Eigenvalue Sums of Theta Laplacians on Finite Graphs

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Abstract

We study a class of laplacian operators on finite directed graphs. We study some
general properties of operators in this class before applying the Harrell-Stubbe Aver-
gaged Variational Principle to develop a bound of sums of eigenvalues of such operators.

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cian, half-band, eigenvalue sums.

1 Background

A graph $G$ can be regarded as a pair of maps $s, t : \mathcal{E} \to \mathcal{V}$ of finite sets. The maps $s, t$ are
called the source and target, respectively. The set $\mathcal{E}$ is called the set of edges and the set $\mathcal{V}$
is called the set of vertices.

Given a graph $G$ let $E, V$ be the free complex vector spaces spanned by $\mathcal{E}, \mathcal{V}$, respec-
tively. Note that since these spaces are generated by finite sets, they are finite dimen-
sional Hilbert spaces in an obvious way with canonical bases and inner products. As a
convention we take all inner products to be conjugate linear in the first argument. $V$
is isomorphic to the space of complex valued functions on $\mathcal{V}$ under the identification
$f : \mathcal{V} \to \mathbb{C} \leftrightarrow \sum_v f(v)v$, analogously for $E$. We will use both notations interchange-
ably.

Note that $s, t$ induce maps $s, t : E \Rightarrow V$ by extending by linearity. Let $D := ss^* + tt^*$. $D$
is called the degree operator. Let $A = st^* + ts^*$. Then $A$ is called the (undirected)
adjacency operator. Additionally, we call $A_s := ts^* - st^*$ the skew adjacency operator as
it is plainly skew-adjoint. Let $d^* = t - s$ and $d = (d^*)^* = t^* - s^*$. Then the standard graph
laplacian is $dd^* = (t - s)(t^* - s^*) = D - A$. In the following section we generalize this
definition to construct a wider class of operators.
2 A Construction of Graph Laplacian Operators

2.1 A general construction

We generalize the construction of the standard graph laplacian as follows. See [4], [10], and [11] for similar approaches to constructing discrete laplacian operators. If $\mathcal{H}$ is a Hilbert space, then $B(\mathcal{H})$ is the space of bounded linear operators on $\mathcal{H}$.

For $f : \mathcal{E} \to \mathbb{C}$ any complex valued function, we may consider the corresponding multiplication operator $f : E \to E$, defined by its action on the basis $\mathcal{E}$, $e \mapsto f(e)e$. Then the adjoint of $f$ is the multiplication operator, again defined by its values on $\mathcal{E}$, $e \mapsto \overline{f(e)}e$. By the above notation we denote it by $\overline{f}$.

Proof. Define $D_{\alpha,\beta} := s_\alpha(s_\alpha)^* + t_\beta(t_\beta)^* = s|\alpha|^2s^* + t|\beta|^2t^*$, $A_{\alpha,\beta} := s_\alpha(t_\beta)^* + t_\beta(s_\alpha)^* = d^*_{\alpha,\beta} = t_\beta - s_\beta$, and $d_{\alpha,\beta} = (d^*_{\alpha,\beta})^* = t_\beta^* - s_\beta^*$. Then let $\Delta_{\alpha,\beta} := d_{\alpha,\beta}d^*_{\alpha,\beta} = D_{\alpha,\beta} - A_{\alpha,\beta}$. Note, by its factorization as a square, $\Delta_{\alpha,\beta}$ is a positive self-adjoint operator.

For $v$ a vertex, let $d_v = \langle v, Dv \rangle$ be the degree of $v$, and define $\alpha, \beta$ by $\alpha(e) := \frac{1}{\sqrt{d_{\alpha,\beta}^2\beta(e)} := \frac{1}{\sqrt{d_{\alpha,\beta}^2}}$. Then $\Delta_{\alpha,\beta}$ is the normalized laplacian.

It’s not difficult to see that $s^*(v) = \sum_{e:te=v}e$ and $t^*(v) = \sum_{e:se=v}e$ so that $d^*_{\alpha,\beta}(v) = (t\beta)^* - (s\alpha)^* = \overline{\beta}^*t^*v - \overline{\alpha}^*s^*v = \sum_{e:te=v}\overline{\beta(e)}e - \sum_{e:se=v}\overline{\alpha(e)}e'$.

Let $Q_{\alpha,\beta} : V \times V \to \mathbb{C} :: (v, w) \mapsto \langle v, \Delta_{\alpha,\beta}w \rangle$ be the sesquilinear form associated with $\Delta_{\alpha,\beta}$. Let $Q_{\alpha,\beta}(v) := Q_{\alpha,\beta}(v, v)$ be the associated quadratic form. We then have the following useful calculation.

Lemma 2.1. $Q_{\alpha,\beta}(f) = \sum_e |\beta(e)f(te) - \alpha(e)f(se)|^2$.

Proof. Define $T$ by $T(f, g) := \sum_e \overline{\beta(e)}f(te) - \overline{\alpha(e)}f(se))\overline{(\beta(e)g(te) - \alpha(e)g(se))}$. $T$ is sesquilinear by inspection. Set $T(f) := T(f, f)$. By the polarization identity $T$ is completely determined by its quadratic form, as is $Q_{\alpha,\beta}$. Moreover, since $T$ is determined by its action on basis vectors, it suffices to show $T(v, w) = Q_{\alpha,\beta}(v, w)$ for any $v, w \in \mathcal{V}$.

However, $T(v, w) = \sum_e \overline{\beta(e)}\delta_{v,te} - \overline{\alpha(e)}\delta_{v,se})(\beta(e)\delta_{w,te} - \overline{\alpha(e)}\delta_{w,se}) = \sum_e \langle v, \beta(e)te - \alpha(e)se \rangle \langle \beta(e)te - \alpha(e)se, w \rangle = \sum_e \langle v, d^*_{\alpha,\beta}e \rangle \langle d^*_{\alpha,\beta}e, w \rangle = \sum_e \langle d_{\alpha,\beta}v, e \rangle \langle e, d_{\alpha,\beta}w \rangle = \langle d_{\alpha,\beta}v, d_{\alpha,\beta}w \rangle = \langle v, \Delta_{\alpha,\beta}w \rangle = Q_{\alpha,\beta}(v, w)$. 

2.2 Theta Laplacians

For the remainder of the paper we shall restrict primarily to the following choices for $\alpha$ and $\beta$. Let $\theta : \mathcal{E} \to (0, 2\pi)$. Then let $\alpha = e^{-i\theta}$ and $\beta = 1$ so that $\alpha(e) = e^{-i\theta(e)}$ and $\beta(e) = 1$ for all $e \in \mathcal{E}$. Then let $A_\theta := A_{\alpha,\beta} = se^{-i\theta}t^* + te^{i\theta}s^*$, $d_\theta := d_{\alpha,\beta}$, and define the (combinatorial) theta laplacian $\Delta_\theta := \Delta_{\alpha,\beta} = d^*_\theta d_\theta = (t - se^{-i\theta})(t^* - e^{i\theta}s^*)$. By the previous lemma, $Q_\theta(f) = \sum_e |f(te) - e^{i\theta(e)}f(se)|^2$. 


By expanding the product \((t - se^{-i\theta})(t^* - s^*e^{i\theta})\) we see \(\Delta_\theta = D - A_\theta\). Note that \(\Delta_0 = D - A_0 = D - A\) is the standard graph laplacian and that \(D_\pi = D + A\).

We note in passing the following connections of the operators \(\Delta_\theta\) to electromagnetism, which would also justify calling the operators \(\Delta_\theta\) magnetic graph laplacians. In \(\mathbb{R}^n\), let \(A\) be a continuous vector field. Suppose \(f : \mathbb{R}^n \to \mathbb{C}\) is continuously differentiable. Let \(x \in \mathbb{R}^n\). Let \(u\) be a unit vector in \(\mathbb{R}^n\). Then for \(h \in \mathbb{R}\), let \(\gamma_{u,h}\) the arc-length parameterized linear path connecting \(x\) and \(x + uh\), \(\gamma_{u,h}(t) = x + ut\) for \(0 \leq t \leq h\). Then define \(\theta_u : \mathbb{R} \to \mathbb{R}\) by \(\theta_u(h) = \int_{\gamma_{u,h}} A(r) \cdot dr = \int_0^h (A(x + tu) \cdot u)dt\). Then \(\lim_{h \to 0^+} \int_{\gamma_{u,h}} f(x + hu) - e^{-i\theta_u(b)} f(x) ) = (\nabla f(x) + iA(x)f(x))u\). On the right hand side one recognizes the gauge covariant derivative.

Another connection to electromagnetism may be seen as follows. Consider the lattice \(\mathbb{Z}^2\). Adopt the Landau gauge \((0, Bx, 0)\) to model a constant electromagnetic field normal to the plane. We may consider \(\mathbb{Z}^2\) as an infinite oriented graph with oriented edges of the form \((m, n) \to (m, n + 1)\) or \((m, n) \to (m + 1, n)\). Then we see that if \(\gamma_1, \gamma_2\) are the arc-length parameterized linear paths along the edges \((m, n) \to (m + 1, n)\) and \((m, n) \to (m, n + 1)\), respectively, then \(\int_{\gamma_1} A(r) \cdot dr = 0\) and \(\int_{\gamma_2} A(r) \cdot dr = B(m + \frac{1}{2})\). We define \(\theta\) by \(\theta((m, n) \to (m, n + 1)) = 0\) and \(\theta((m, n) \to (m + 1, n)) = B(m + \frac{1}{2})\). Let \(\mathcal{B}(l^2(\mathbb{Z}^2))\) be the space of bounded linear operators on \(l^2(\mathbb{Z}^2)\). Then \(\Delta_\theta = D - A_\theta \in \mathcal{B}(l^2(\mathbb{Z}^2))\) is defined by \(A_\theta f(m, n) = e^{-iB(m+\frac{1}{2})} f(m, n + 1) + e^{iB(m+\frac{1}{2})} f(m, n - 1) + f(m + 1, n) + f(m - 1, n)\). Define \(T_1, T_2 \in \mathcal{B}(l^2(\mathbb{Z}^2))\) by \(T_1 f(m, n) = f(m + 1, n)\) and \(T_2 f(m, n) = e^{-iB(m+\frac{1}{2})} f(m, n + 1) + e^{iB(m+\frac{1}{2})} f(m, n - 1)\). Then \(A_\theta = T_1 + T_2 + T_3, T_3 = 0, A_\theta\) is a form of the Harper operator or discrete magnetic laplacian \([2][8]\). Now define \(S_1, S_2 \in \mathcal{B}(l^2(\mathbb{Z}))\) by \(S_1 f(k) = f(k + 1)\) and \(S_2 f(k) = e^{-iB(k+\frac{1}{2})} f(k)\). Then let \(H_\theta = S_1 + S_1^* + S_2 + S_2^*\). So \(H_\theta f(k) = f(k + 1) + f(k - 1) + 2 \cos(B(k + \frac{1}{2}))\), which may be recognized as a form of the almost Mathieu operator. Note \(H_\theta\) may be obtained from \(A_\theta\) by restricting \(A_\theta\) to functions that are constant in the second argument. We have that \(S_1 S_2 = e^{iB} S_2 S_1\) and \(T_1 T_2 = e^{iB} T_2 T_1\). When the algebra is simple, which is known to be the case when \(B\) is irrational, they generate isomorphic noncommutative tori and have the same spectrum \([6]\). Similar discrete magnetic operators have been studied for various infinite and periodic graphs \([8][9][5]\).

For constant \(\theta\), we have that \(A_\theta = \cos(\theta) A + i \sin(\theta) A_s\), as can be checked by expanding both sides using the definitions. Hence for constant theta independent of the edges, we have \(-i \frac{d\theta}{d\theta} A_\theta = i \sin \theta A + \cos \theta A_s = -e^{-i\theta} st^* + e^{i\theta} ts^*\). So \(-i \frac{d\theta}{d\theta} A_\theta|_0 = A_s\). But \(i A_s = A_{\pi/2}\). In particular, \(\frac{d\Delta_\theta}{d\theta}|_0 = -i A_s = -A_{\pi/2}\). Now since the constant vector 1 corresponds to the 0 eigenvalue of \(\Delta_\theta\), if \(\mu_{\theta,0}\) is the lowest eigenvalue of \(\Delta_\theta\), by Feynman-Hellmann we have \(\frac{d\mu_{\theta,0}}{d\theta}|_0 = (1, -A_{\pi/2}) = -\sum_{j,k} (A_{\pi/2})_{j,k} = 0\), since \((A_{\pi/2})_{j,k} = -(A_{\pi/2})_{k,j}\) for all \(j, k\).

It can be seen from either the definition in terms of \(s, t\) or from the quadratic form that both the standard laplacian \(\Delta_0\) and \(\Delta_s\) are independent of orientation, since interchanging the roles of \(se, te\) for any given edge leaves them invariant. Note, however, that in general \(\Delta_\theta\) is highly dependent on the orientation.

Since \(\det(\Delta_\theta) = 0\) if and only if the lowest eigenvalue \(\inf_{\|f\|_2 = 1} Q_\theta f = 0\), and since the
set $|f|_2 = 1$ is compact, as the space $V$ is finite dimensional, we have $\det(\Delta_\theta) = 0$ if and only if there exists an $f \neq 0$ with $Q_\theta(f) = 0$. This occurs, by the form of $Q_\theta$ given above, if and only if $f(te) = e^{i\theta(e)}f(se)$ for all $e$. This suggests the following result.

**Proposition 2.2.** An undirected graph is bipartite if and only if $\det(\Delta_\pi) = 0$. Additionally it is bipartite if and only if $\det(\Delta_{2\pi}) = 0$ for some orientation. An undirected graph is tripartite if and only if $\det(\Delta_{\frac{3\pi}{2}}) = 0$ for some orientation.

**Proof.** Without loss of generality we may assume the graph is connected since we may consider its components separately. Suppose $Q_\pi(f) = \sum_e |f(te) + f(se)|^2 = 0$ for some $f \neq 0$. By rescaling $f$ if necessary, since $f \neq 0$ we may assume $f(v_0) = 1$ for some vertex $v_0$. Then every $f$ must take the value $-1$ on every vertex connected to $v_0$ and the value 1 on every vertex distance 2 from $v_0$, etc. Hence $f$ only takes on values $\pm 1$ and two + vertices and two − vertices cannot be connected by an edge. Hence we may define a bipartition by the + and − vertices. Conversely, suppose $A, B$ is a bipartition for the graph. Define $f := 1_A - 1_B$. Then for any edge $e$ we have $|f(te) + f(se)|^2 = 0$. Hence $Q_\pi(f) = 0$. Since the argument did not depend on choice of orientation, this proves the first assertion.

As for the second claim, we proceed similarly. Suppose for some orientation that $Q_{\pi}(f) = \sum_e |f(te) - if(se)|^2 = 0$ for some $f \neq 0$. Again by rescaling if necessary we may assume that $f(v_0) = 1$ for some $v_0$. Then since the graph is connected we have that $f$ takes on at most the values $1, -1, i, -i$ and +1 vertices cannot be connected to −1 vertices and +i vertices cannot be connected to −i vertices. So define a bipartition by letting $A$ be the set of all +1, −1 vertices and $B$ be the set of all +i, −i vertices. Conversely, suppose $A, B$ is a bipartition of an undirected graph. Then define $f := 1_A + i1_B$. Define an orientation by having $s$ always take values in $A$, $t$ values in $B$. Then for any $e : se \to te$ we have $|f(te) - if(se)|^2 = |i - i(1)|^2 = 0$. Hence $Q_{\pi}(f) = 0$. This proves the second assertion.

As for the last assertion, let $\omega := e^{2i\pi}$ and suppose for some orientation that $Q_{\frac{\pi}{2}}(f) = \sum_e |f(te) - \omega f(se)|^2 = 0$ for some $f \neq 0$. Again by rescaling if necessary we may assume that $f(v_0) = 1$ for some $v_0$. Then since the graph is connected we have that $f$ takes on at most the values $1, \omega, \omega^2$ and any two $\omega^j$ vertices cannot be connected for the same $j$. So define a tripartition with $A_j$, for $j = 0, 1, 2$, the $\omega^j$ vertices. Conversely, suppose $A, B, C$ is a tripartition of an undirected graph. Then define $f := 1_A + \omega 1_B + \omega^2 1_B$. Then define an orientation by the following rules. For any edge $e$ between an $A$ vertex and a $B$ vertex take $se$ to be the $A$ vertex, $te$ the $B$ vertex. For any edge $e$ between a $B$ vertex and an $C$ vertex set $se$ to be the $B$ vertex, $te$ the $C$ vertex. For any edge between a $C$ vertex and an $A$ vertex set $se$ to be the $C$ vertex, $te$ the $A$ vertex. Then, by construction, for any directed $e : se \to te$ we have $|f(se) - \omega f(te)|^2 = 0$. Hence $Q_{\frac{\pi}{2}}(f) = 0$ and the proof is complete.

Following [7], we call a unitary operator $U : V \to V$ a gauge transformation if it is multiplication operator with respect to the basis of vertices. So $Uv = \phi(v)v$ where $\phi : \mathcal{V} \to \mathbb{C}$ with $|\phi| = 1$. 

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Proposition 2.3. $\Delta_\phi$ is unitarily equivalent under a gauge transformation to the standard laplacian $\Delta_0$ if and only if $\det(\Delta_\phi) = 0$.

Proof. We may assume the underlying graph is connected since $\Delta_\phi$ has a decomposition as a direct sum of corresponding $\Delta_\phi$ operators on each connected component.

Since $\det(\Delta_0) = 0$, one direction is clear. For the other, suppose $\det(\Delta_\phi) = 0$. Let $\phi$ be normalized such that $\langle \phi, \Delta_\phi \phi \rangle = 0$. Since $\phi$ is normalized and the graph is connected, the vanishing of $\langle \phi, \Delta_\phi \phi \rangle$ ensures that $|\phi| = 1$. Define $U : V \to V$ by $U(v) := \phi(v)v$ and extending linearly. Since $|\phi| = 1$, $U$ is a gauge transformation.

Define sesquilinear forms $Q, T$ by $Q(f, g) := \langle f, \Delta_\phi U g \rangle, T(f, g) := \langle f, U \Delta_\phi g \rangle$. Let $v, w \in \mathcal{V}$. We have $Q(v, w) = \langle v, \Delta_\phi U w \rangle = \langle v, \Delta_\phi \phi(w)w \rangle = \phi(w)\langle v, \Delta_\phi w \rangle = \phi(w)(\langle v, Dw \rangle - \langle v, A_\phi w \rangle) = \phi(w)(\delta_{e, w} \deg(v) - \langle v, (e^{-i\theta(e)}s^*t + e^{i\theta(e)}t^*s)w \rangle)$. Then if $v = w$ the result is $\phi(v)\deg(v)$ and if $v \neq w$ and $v, w$ non-adjacent then the result is 0. If $e : v \to w$ is an edge then since $\phi$ is an eigenvector of 0, $\phi(w) = e^{i\theta(v \to w)}\phi(v)$. So $e$ contributes $e^{i\theta(v \to w)}(-e^{-i\theta(v \to w)}) = -1$ to the result. Similarly and edge of the form $w \to v$ contributes $1$. But also $T(v, w) = \langle v, U \Delta_0 w \rangle = \langle U^*v, \Delta_0 w \rangle = \langle \phi(v)v, \Delta_0 w \rangle = \phi(v)\langle v, \Delta_0 w \rangle$, which is $\phi(v)\deg(v)$ if $v = w$, 0 if $v \neq w$ and non-adjacent, and any edge between $v$ and $w$ contributes $-1$. Hence $Q = T$. Therefore $\Delta_\phi U = U \Delta_0$, which implies $\Delta_\phi$ is unitarily equivalent to $\Delta_0$ under a gauge transformation.

If $e$ is an oriented edge, say $uv$, let $\bar{e} = vu$ be the reverse edge. Then extend $\theta$ by $\theta(\bar{e}) = -\theta(e)$. Then if $v = v_0, ..., v_m = v$ is a closed (unoriented) walk, the flux is defined by $\sum_{j=0}^{m-1} \theta(v_jv_{j+1}) \mod 2\pi$. Hence if $v_jv_{j+1}$ is an oriented edge then it contributes $\theta(v_jv_{j+1})$ to the flux, and if $v_{j+1}v_j$ is an edge then $\theta(v_jv_{j+1}) = \theta(v_jv_{j+1})$, $\theta(v_{j+1}v_j) = -\theta(v_{j+1}v_j)$ to the flux.

One direction of the following proposition, in the case of $A_\theta$, may be found in [7]. In order to derive the other from the one presented there, note that gauge transformations are diagonal in the standard basis for $V$ and thus commute with $D$.

Proposition 2.4. Two theta Laplacians $\Delta_{\theta_1}, \Delta_{\theta_2}$ are unitarily equivalent under a gauge transformation if and only if $\theta_1$ and $\theta_2$ induce the same fluxes through closed walks.

Proof. As in the previous proposition, we may assume $G$ is connected. Moreover, for notational convenience we adopt the following convention. If $vw$ is an oriented edge, we extend the definition of $\theta$ to the reverse edge $uw$ by $\theta(uw) = -\theta(vw)$.

Suppose $\Delta_{\theta_1}$ and $\Delta_{\theta_2}$ are unitarily equivalent under a gauge transformation $U$ with $U^*\Delta_{\theta_1}U = \Delta_{\theta_2}$, and for $v \in \mathcal{V}, Uv = \phi(v)$ with $\phi(v) = e^{i\phi_v}$. If $vw$ is an edge or reverse edge then $\langle v, \Delta_\phi w \rangle = \langle v, U^*\Delta_\phi U w \rangle = e^{-i\theta_1(vw) + \phi_v - \phi_w}$. So if $v = v_0, ..., v_m = v$ is a closed walk, then $\sum_{j=0}^{m-1} \theta_1(v_jv_{j+1}) \mod 2\pi = \sum_{j=0}^{m-1} \theta_1(v_jv_{j+1}) + \sum_{j=0}^{m-1} (\phi_{v_j} - \phi_{v_{j+1}}) \mod 2\pi = \sum_{j=0}^{m-1} \theta_1(v_jv_{j+1}) \mod 2\pi$ since $v_0 = v_m = v$.

Conversely, suppose $\theta_1, \theta_2$ induce the same fluxes through closed walks. Let $v_0 \in \mathcal{V}$. Then for $v \in \mathcal{V}$, since $G$ is connected, let $v_0, v_1, ..., v_m = v$ be a closed walk connecting $v_0$ and $v$. Set $\phi_v = \sum_{j=0}^{m-1} \theta_2(v_jv_{j+1}) - \theta_1(v_jv_{j+1}) \mod 2\pi$. Then since $\theta_1, \theta_2$ induce
the same fluxes through closed walks, \( \phi_v \) is well defined. Define \( U \) by \( Uv = e^{i\theta_v} \) for \( v \in \mathcal{V} \) and extending by linearity. Now let \( v, w \in \mathcal{V} \) with \( vw \) an edge or reverse edge. Then let \( v_0, \ldots, v_m = v \) a walk connecting \( v_0 \) and \( v \) and \( v_{l+m} = v_0, v_{l+m-1}, \ldots, v_{m+1} = w \) a walk connecting \( v_0 \) and \( w \). Since \( vw = v_mv_{m+1} \) is an edge in the underlying unoriented graph then \( v_0, \ldots, v_m, v_{m+1}, \ldots, v_{l+m} \) is a closed walk. Hence \( e^{i\theta_1(wv)}\langle w|U^*\Delta_{\theta_2}Uv \rangle = e^{i(\sum_{j=m}^{m+l} \theta_2(v_jv_{j+1}) - \theta_1(v_jv_{j+1}))}e^{i\theta_1(wv)}\langle w|\Delta_{\theta_1}v \rangle = e^{i(\sum_{j=m}^{m+l} \theta_2(v_jv_{j+1}) - \theta_1(v_jv_{j+1}))} = 1 \), by the equal flux condition since \( v_0 = v_{m+l} \). But \( e^{-i\theta_1(wv)} = \langle w|\Delta_{\theta_1}v \rangle \). Hence \( \Delta_{\theta_1} \) and \( \Delta_{\theta_2} \) are unitarily equivalent under a gauge transformation.

\( \square \)

### 3 Averaged Variational Principle

In this section we develop a tool (see [3]) for its origin) that will allow estimates on sums of eigenvalues of finite laplacian operators.

If \( M \) is a self-adjoint \( n \times n \) matrix, we denote its eigenvalues by \( \mu_0 \leq \mu_1 \leq \ldots \leq \mu_{n-1} \) and a corresponding orthonormal basis of eigenvectors by \( \langle u_j \rangle_{j=0}^{n-1} \). If \( V \) is any \( k \) dimensional subspace of \( \mathbb{C}^n \) and \( \langle v_j \rangle_{j=0}^{k-1} \) an orthonormal basis for \( V \), then we define \( \text{Tr}(M|V) := \sum_{i=0}^{k-1} \langle v_i, Mv_i \rangle \). \( \text{Tr}(M|V) \) is independent of the basis chosen. Indeed, let \( P_V \) be the projection onto \( V \). Then \( P_V = \sum_{i=0}^{k-1} v_i v_i^* \). So \( \sum_{j=0}^{n-1} \mu_j \|P_Vu_j\|^2 = \sum_{j=0}^{k-1} \sum_{i=0}^{n-1} \mu_j \langle v_i, u_j \rangle \|^2 = \sum_{i=0}^{k-1} v_i^* Mv_i \), using the spectral decomposition of \( M \). Since the left hand side of the above string of equalities is independent of basis, the result holds.

We begin with the following classical result. The proof is an adaptation of the proof found in [1].

**Proposition 3.1.** With notation as above, for \( 1 \leq k \leq n \), we have

\[
\sum_{j=0}^{k-1} \mu_j = \inf_{\dim(V)=k} \text{Tr}(M|V).
\]

In particular if \( \langle v_j \rangle_{j=0}^{k-1} \subset \mathbb{C}^n \) is any collection of orthonormal vectors, we have

\[
\sum_{j=0}^{k-1} \mu_j \leq \sum_{j=0}^{k-1} \langle v_j, Mv_j \rangle.
\]

**Proof.** If \( V \) is 1-dimensional, say spanned by unit vector \( v_0 \), using the spectral decomposition \( A = \sum_{i=0}^{n-1} \mu_i u_i u_i^* \), we have \( \langle v_0, Mv_0 \rangle = \sum_{i=0}^{n-1} \mu_i |\langle u_0, v_i \rangle|^2 \geq \mu_0 \sum_{i=0}^{n-1} |\langle u_0, v_i \rangle|^2 = \mu_0 \|u_0\|^2 = \mu_0 \). Moreover, take \( v_0 = u_0 \) for the other inequality. Now suppose the statement holds for any \( n \) and any subspace of dimension at most \( k-1 \). Then suppose \( V \) is a subspace of dimension \( k \). Let \( \langle v_j \rangle_{j=0}^{k-1} \) be an orthonormal basis for \( V \). If \( V \subset u_0^\perp \), then \( V' := v_0^\perp \) is a \( k-1 \) dimensional subspace of \( V \) contained in \( u_0^\perp \). Else let \( V' \) be the projection of \( V \) onto \( u_0^\perp \).
In any case there is a $k - 1$ dimensional subspace $V'$ of $V$ contained in $u_0^\perp$. Note $M$ leaves $u_0^\perp$ invariant. So let $M'$ be the restriction of $M$ to $u_0^\perp$. Then $M'$ is self adjoint with eigenvalues $\mu_1 \leq \cdots \leq \mu_{n-1}$. Then by the induction hypothesis, since $V = V' \bigoplus C u_0$, we have 
\[
\Tr(M|V) = \Tr(M|V') + \Tr(M|C u_0) = \Tr(M'|V') + \Tr(M|C u_0) \geq (\sum_{j=1}^{k-1} \mu_j) + \mu_0 = \sum_{j=0}^{k-1} \mu_j.
\]
The other inequality follows by taking $V$ to be the space spanned by the $u_j$ for $j \leq k - 1$.  

The following is an immediate application to the first eigenvalue of $\Delta_\theta$.

**Proposition 3.2.** If $\mu_0$ is the first eigenvalue of $\Delta_\theta$ then $\mu_0 \leq \frac{1}{|\mathcal{E}|} \sum_{v \in \mathcal{E}} (2 - 2 \cos(\theta(e)))$.

In particular, for $\theta$ constant, $\mu_0 \leq \frac{|\mathcal{E}|}{|\mathcal{E}|} (2 - 2 \cos \theta)$.

**Proof.** Apply Proposition 2.1 with $v_0 = \frac{1}{\sqrt{|\mathcal{E}|}} \sum_{v \in \mathcal{E}} v$ the constant vector and use the formula from Lemma 1.2. \qed

The following variational principle from [3] is a generalization of Proposition 3.1.

**Theorem 3.3.** Let $M$ a self adjoint $n \times n$ matrix with eigenvalues $\mu_0 \leq \mu_1 \leq \cdots \leq \mu_{n-1}$ and corresponding normalized eigenvectors $(u_i)_{i=0}^{n-1}$. Suppose $(Z, \mathcal{M}, \mu)$ is (a positive) measure space and $\phi : Z \to \mathbb{C}^n$ is measurable with $\int_Z \|\phi(z)\|^2 \, d\mu(z) < \infty$. Then if $Z_0 \in \mathcal{M}$, then for any $0 \leq k \leq n - 1$, we have

$$
\mu_k \left( \int_{Z_0} \|\phi\|^2 \, d\mu - \sum_{j=0}^{k-1} \int_Z |\langle \phi, u_j \rangle|^2 \, d\mu \right) \leq \int_{Z_0} \langle \phi, M\phi \rangle \, d\mu - \sum_{j=0}^{k-1} \int_Z \mu_j |\langle \phi, u_j \rangle|^2 \, d\mu.
$$

We recall the proof, following [3].

**Proof.** Let $x \in \mathbb{C}^n$. Since the eigenvalues are non-decreasing, $\mu_k \sum_{i=k}^{n-1} |\langle u_i, x \rangle|^2 \leq \sum_{i=k}^{n-1} \mu_i |\langle u_i, x \rangle|^2$. But $\mu_k \sum_{i=k}^{n-1} |\langle u_i, x \rangle|^2 = \mu_k (\|x\|^2 - \sum_{j=0}^{k-1} |\langle x, u_j \rangle|^2)$ and $\sum_{i=k}^{n-1} \mu_i |\langle u_i, x \rangle|^2 = |\langle x, Mx \rangle - \sum_{j=0}^{k-1} \mu_j |\langle x, u_j \rangle|^2|$. Hence $\mu_k (\|\phi\|^2 - \sum_{j=0}^{k-1} |\langle \phi, u_j \rangle|^2) \leq |\langle \phi, M\phi \rangle - \sum_{j=0}^{k-1} \mu_j |\langle \phi, u_j \rangle|^2|$ holds for all $z$. Hence integrating over $Z_0$ we get

$$
\mu_k \left( \int_{Z_0} \|\phi\|^2 \, d\mu - \sum_{j=0}^{k-1} \int_{Z_0} |\langle \phi, u_j \rangle|^2 \, d\mu \right) \leq \int_{Z_0} \langle \phi, M\phi \rangle \, d\mu - \sum_{j=0}^{k-1} \int_{Z_0} \mu_j |\langle \phi, u_j \rangle|^2 \, d\mu. \quad (1)
$$

Now integrating $\sum_{j=0}^{n-1} \mu_j |\langle u_j, \phi \rangle|^2 \leq \mu_k \sum_{j=0}^{k-1} |\langle u_j, \phi \rangle|^2$ over $Z_0^c$ yields

$$
- \mu_k \sum_{j=0}^{k-1} \int_{Z_0^c} |\langle u_j, \phi \rangle|^2 \, d\mu \leq - \sum_{j=0}^{n-1} \int_{Z_0^c} \mu_j |\langle u_j, \phi \rangle|^2 \, d\mu. \quad (2)
$$

Then adding (1) and (2) we obtain the result. \qed
Note that provided that \( \mu_k \sum_{j=0}^{k-1} \int_Z |\langle \phi, u_j \rangle|^2 d\mu \leq \mu_k \int_{Z_0} \| \phi \|^2 d\mu \), we have that

\[
\sum_{j=0}^{k-1} \int_Z \mu_j |\langle \phi, u_j \rangle|^2 d\mu \leq \int_{Z_0} \langle \phi, M\phi \rangle d\mu. \tag{3}
\]

We now show that Proposition 3.1 follows from the theorem 3.3, in particular from (3). Let \( v_1, ..., v_{k-1} \) be a collection of orthonormal vectors in \( \mathbb{C}^n \). Take \( Z := \{0, 1, ..., n-1\} \) and \( Z_0 := \{0, 1, ..., k-1\} \) with the counting measure. Extend the \( v_j \) to an orthonormal basis for all of \( \mathbb{C}^n \). Then let \( \phi(l) := v_l \). Then \( \sum_{j=0}^{k-1} \int_Z |\langle \phi, u_j \rangle|^2 d\mu = k = \int_{Z_0} \| \phi \|^2 d\mu \). Hence (3) then states \( \sum_{j=0}^{k-1} \mu_j \sum_{t=0}^{n-1} |\langle v_t, u_j \rangle|^2 = \sum_{j=0}^{k-1} \mu_j \leq \sum_{j=0}^{k-1} \langle v_j, Mv_j \rangle \), and we recover Proposition 3.1.

### 4 Inequalities for Sums of Eigenvalues of Theta Laplacians

We now apply the averaged variational principle, Theorem 3.3, to \( \Delta_\theta \). For the remainder of this section we take all graphs to be loopless directed graphs without multiple edges. We assume \( G \) is connected on \( n \) vertices. Let \( \lambda_0 \leq \lambda_1 \leq ... \leq \lambda_{n-1} \) be the eigenvalues of \( \Delta_\theta \).

Orient \( K_n \) with some orientation such that its restriction to \( G \) is the orientation on \( G \). Suppose \( H \) is a \( d \)-regular directed subgraph of \( K_n \) with \( G \) a directed subgraph of \( H \). Note this is always possible by taking \( H = K_n \) and with \( d = n-1 \). However, for example, for \( G = C_6 \), \( d \) may be taken to be 2, 3, 4, or 5. Let \( H^c \) be the graph complement of \( H \) in \( K_n \) with the induced orientation. We shall denote pairs \( (u, v) \) in \( Z \) by \( uv \). If \( e = uv \) is an oriented edge in \( K_n \) we shall denote \( \bar{e} := vu \). We shall also denote directed edges \( e : u \to v \) by \( u \to v \), omitting the \( e \), when convenient. We call two vertices \( u, v \) adjacent and write \( u \sim v \) if there is some oriented edge between them, either \( u \to v \) or \( v \to u \). If the graph \( G \) is not clear from the context, we write \( \sim_G \) if we wish to restrict the relation to \( G \). Then let \( Z := \mathcal{V} \times \mathcal{V} \) and \( \mathcal{M} := \mathcal{P}(Z) \). Let \( a, b \geq 0 \). Define \( \mu \) on \( \mathcal{M} \) by \( \mu(e) = \mu(\bar{e}) = 1 \) for \( e \) an edge in \( H \), \( \mu(e) = \mu(\bar{e}) = a \) for \( e \) an edge in \( H^c \), and \( \mu(u, u) = b \) for all \( u \). Let \( \alpha : \mathcal{E} \to [0, 2\pi) \). Then extend \( \alpha \) and \( \theta \) to all of \( K_n \) by setting them equal to 0 outside of edges of \( G \).

Define \( \phi_{\alpha,H} : Z \to V \cong \mathbb{C}^n \) by \( \phi_{\alpha,H}(uv) := b_{uv} \), where

\[
b_{uv} := \begin{cases} v - e^{i\alpha(uv)}u, & uv \in \mathcal{E}_{K_n} \\ v + e^{-i\alpha(vu)}u, & vu \in \mathcal{E}_{K_n} \\ u, & u = v. \end{cases}
\]

Hence for any \( f \),

\[
|\langle f, b_{uv} \rangle|^2 = \begin{cases} |f(u)|^2 + |f(v)|^2 - 2\text{Re}(e^{i\alpha(uv)}f(u)f(v)) & uv \in \mathcal{E}_{K_n} \\ |f(u)|^2 + |f(v)|^2 + 2\text{Re}(e^{-i\alpha(vu)}f(u)f(v)) & vu \in \mathcal{E}_{K_n} \\ |f(u)|^2 & u = v. \end{cases}
\]
We wish to calculate $\sum_{uv \in \mathcal{Z}} \mu(\langle f, b_{uv} \rangle)$. Note that for $uv$ an edge in $K_n$, we have $|\langle f, b_{uv} \rangle|^2 + |\langle f, b_{vu} \rangle|^2 = 2|f(u)|^2 + 2|f(v)|^2$. For $u$ fixed, for any vertex $v$, exactly one of the following possibilities occurs: $v = u$, $v$ is adjacent to $u$ in $H$, or $v$ is adjacent to $u$ in $H^c$. Hence, since edges and their opposites occur in pairs in both $H$ and $H^c$, and since $H$ is $d$-regular and $H^c$ is $n-1-d$-regular, we have

$$\sum_{uv \in \mathcal{Z}} \mu(\langle f, b_{uv} \rangle) =\sum_{uv \in \mathcal{Z}} \mu(\langle f, b_{vu} \rangle) = \sum_{uv \in \mathcal{Z}} (|f(u)|^2 + |f(v)|^2) + a(\sum_{uv \in \mathcal{Z}} (|f(u)|^2 + |f(v)|^2)) + b(\sum_{uv \in \mathcal{Z}} |f(u)|^2) = (d+a(n-1-d)+b)|f|^2 + (n-1-d-a)|f|^2 = 2(d+a(n-1-d)+b)|f|^2.$$ Let $C(a,b,d) := d + a(n-1-d) + b$. Then $\sum_{uv \in \mathcal{Z}} \mu(\langle f, b_{uv} \rangle)^2 = 2C(a,b,d)|f|^2$.

Let $Z_0 \subset Z$. Now we calculate $\sum_{uv \in Z_0} \langle b_{uv}, \Delta \theta b_{uv} \rangle$. There are four cases. If $uv$ is an oriented edge in $G$ then $\langle b_{uv}, \Delta \theta b_{uv} \rangle = |1 + e^{i\theta(\langle f, b_{uv} \rangle)}|^2 + d_u - 1 + d_v - 1 = d_u + d_v + 2\cos(\theta(\langle f, b_{uv} \rangle))$. If $vu$ is an oriented edge in $G$ then $\langle b_{uv}, \Delta \theta b_{uv} \rangle = |1 - e^{-i\theta(\langle f, b_{uv} \rangle)}|^2 + d_u - 1 + d_v - 1 = d_u + d_v - 2\cos(\theta(\langle f, b_{uv} \rangle))$. If $u \neq v$ and neither $uv$ nor $vu$ is an oriented edge in $G$ then $\langle b_{uv}, \Delta \theta b_{uv} \rangle = d_u + d_v$. Lastly, for any $v$, $\langle b_{uv}, \Delta \theta b_{uv} \rangle = d_u$.

Hence $\sum_{uv \in Z_0} \langle b_{uv}, \Delta \theta b_{uv} \rangle = \sum_{uv \in Z_0} \langle b_{uv}, \Delta b_{uv} \rangle = \sum_{uv \in Z_0} \mu(\langle f, b_{uv} \rangle) = \sum_{uv \in Z_0} \mu(\langle f, b_{vu} \rangle) = \sum_{uv \in Z_0} \mu(\langle f, b_{uv} \rangle) + \sum_{uv \in Z_0} \mu(\langle f, b_{vu} \rangle) = \sum_{uv \in Z_0} \mu(\langle f, b_{uv} \rangle) + \sum_{uv \in Z_0} \mu(\langle f, b_{vu} \rangle)$.

For $A$ a finite set let $|A|$ denote the cardinality of $A$. Then we have $\sum_{uv \in Z_0} \mu(\langle f, b_{uv} \rangle) = 2|\{uv \in Z_0 \mid uv \in \mathcal{E}_G \}| + 2a|\{uv \in Z_0 \mid uv \in \mathcal{E}_H \}| + b|\{uv \in Z_0 \}| := N(a,b,H,Z_0)$.

It follows by the remark following Theorem 3.3, that if $k$ is such that $2kC(a,b,d) \leq N(a,b,H,Z_0)$ then $\sum_{j=0}^{k} \lambda_j \leq \frac{M(a,b,Z_0,H,\alpha,\theta)}{2C(a,b,d)}$.

We may achieve great simplifications of the above inequality if we take $Z_0$ to contain only edges or reverse edges of $\mathcal{E}$ or also, if needed, elements of the form $uu$. Before continuing, we note the following. Let $Z_G := \sum_{\alpha \in \mathcal{E}_G} a_{\alpha} \alpha$ be the first Zagreb index of $G$, where $d_v$ is the degree of $v$ in $G$. Then $\sum_{\alpha \in \mathcal{E}_G} (d_u + d_v) = Z_G$. Indeed, for each $v$, $d_v$ appears once in exactly $d_v$ terms in the sum.

We provide several examples. First let $Z_0 = \mathcal{E}$. Then $\sum_{uv \in Z_0} \langle b_{uv}, \Delta \theta b_{uv} \rangle = Z_G + 2\sum_{\alpha \in \mathcal{E}_G} \cos(\alpha(e) + \theta(e))$. Since we will be wishing to minimize this quantity, we define $\alpha$ such that $\alpha(e) + \theta(e) \equiv \pi$ (mod $2\pi$). Then $\sum_{uv \in Z_0} \langle b_{uv}, \Delta \theta b_{uv} \rangle = Z_G - 2|\mathcal{E}|$.

Applying theorem 3.3, we have that if $2kC(a,b,d) \leq 2|\mathcal{E}|$ then $2C(a,b,d) \sum_{j=0}^{k} \lambda_j \leq Z_G - 2|\mathcal{E}|$. However, since $C(a,b,d)$ can take on any number greater than or equal to $d$, if $k \leq \frac{|\mathcal{E}|}{d}$ then the optimal choice is $C(a,b,d) = \frac{|\mathcal{E}|}{k}$. Hence we have proven the following theorem.

**Theorem 4.1.** Let $G$ be a connected, directed, loopless, graph on $n$ vertices without repeated edges. Let $d_0$ be the degree of a regular subgraph $H$ of $K_n$ containing $G$ as a subgraph. Then if $k$ is an integer with $k \leq \frac{|\mathcal{E}|}{d_0}$, we have

$$\sum_{j=0}^{k-1} \lambda_j \leq \frac{k}{2|\mathcal{E}|} (Z_G - 2|\mathcal{E}|).$$
Note that if $D$ is the degree matrix, $|\mathcal{E}| = \frac{1}{2} \text{Tr}(D)$ and $Z_G = \text{Tr}(D^2)$. Hence we may rewrite the above inequality as follows. For $G$ as in the previous theorem, we have

$$\frac{1}{k} \sum_{j=0}^{k-1} \lambda_j \leq \frac{\text{Tr}(D^2)}{\text{Tr}(D)} - 1, \text{ for } k \text{ a positive integer with } k \leq \frac{1}{2d_0} \text{Tr}(D).$$

We may increase the bound on $k$ by admitting a combination of reverse edges of $G$ and loops $uu$ to $Z_0$. Then the cosine terms cancel in pairs for reverse edges and loops add terms proportional to the degree.

In [7] the half-filled band, corresponding to the case that $k = \frac{n}{2}$, is studied. As a corollary we provide an inequality for the half-filled band in the case of a $d-$regular graph. Let $H = G$. Then $d_0 = d$. Note in this case $Z_G = nd^2$ and $2|\mathcal{E}| = nd$. Note further that any $\Delta_\theta$ is a sum of theta laplacians corresponding to individual edges, each being a positive operator. It follows that eigenvalue sums for a subgraph are bounded above by corresponding sums for the graph. Hence we have the following result for the half-band.

**Corollary 4.2.** Let $G$ be a connected, directed, loopless, subgraph of a $d-$regular graph on $n$ vertices without repeated edges. Then for $k \leq \frac{n}{2}$ we have

$$\sum_{j=0}^{k-1} \lambda_j \leq k(d - 1).$$

We give two simple examples. Let $G = K_3$ with some orientation. The condition is $k \leq \frac{3}{2}$, so the only non-trivial choice for $k$ is 1. The above inequality reduces to $\lambda_0 \leq 1$. This is sharp since taking $\theta$ constant equal to $\pi$ on any orientation yields a spectrum of $1, 1, 4$.

Consider the cycle $C_4$. Then the spectrum of the standard Laplacian is $0, 2, 2, 4$. Hence the inequality is sharp at $k = 2$ for this example, as the sum of the first half of the spectrum is $2 = \frac{n}{2}(d - 1)$, where $n = 4, d = 2$.

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