BOUNDS ON THE L^2 SPECTRUM FOR MARKOV CHAINS AND MARKOV PROCESSES: A GENERALIZATION OF CHEEGER'S INEQUALITY

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ABSTRACT. We prove a general version of Cheeger's inequality for discrete-time Markov chains and continuous-time Markovian jump processes, both reversible and nonreversible, with general state space. We also prove a version of Cheeger's inequality for Markov chains and processes with killing. As an application, we prove L^2 exponential convergence to equilibrium for random walk with inward drift on a class of countable rooted graphs.

1. Introduction. Twenty years ago, Cheeger [1] proved a beautiful lower bound on the next-to-smallest eigenvalue (smallest strictly positive eigenvalue) λ_1 of the Laplacian on a compact Riemannian manifold M, in terms of an isoperimetric constant for M. This result inspired many further lower and upper bounds on λ_1 in terms of global geometric invariants of M (see, e.g., [2-4] for reviews). Very recently, Alon [5] proved an analogous bound for the Laplacian on a finite graph. From a probabilistic point of view, these bounds concern the rate of exponential convergence of a positive-recurrent reversible Markov process (the Brownian motion on M) to its unique invariant distribution (normalized Lebesgue measure on M).

In the same paper, Cheeger also proved a lower bound on the smallest eigenvalue λ_0 (necessarily strictly positive) of the Laplacian on a compact Riemannian manifold M with Dirichlet boundary ∂M . More recently, Dodziuk [6] proved an analogous bound for the Laplacian on a finite graph with Dirichlet boundary. From a probabilistic point of view, these bounds concern the exponential decay rate of a reversible Markov process with killing (the Brownian motion on M killed at ∂M).

In this note we prove a general version of Cheeger's inequality for positive-recurrent discrete-time Markov chains and continuous-time Markovian jump processes, both reversible and nonreversible, with general state space. In addition, we prove a general version of Cheeger's inequality for Markov chains and Markov processes with killing. As an application, we prove bounds on the L^2 spectrum for a random walk with inward drift on a certain class of countable rooted graphs, generalizing an earlier result of Sokal and Thomas [7].

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We emphasize that our methods in this paper are not new: our proofs are, by and large, close analogues of Cheeger's original argument. However, we think it is worthwhile to generalize and unify a number of results which have been scattered in the literature of fields as diverse as differential geometry, graph theory, linear algebra, probability theory and mathematical physics. We have tried hard to make our exposition comprehensible to specialists in all these fields. In §2 we present our main result in the positive-recurrent case. In §3 we present our main result for Markov chains and processes with killing, and derive an alternate version of the positive-recurrent result as a corollary. In §4 we prove some lemmas which are useful in applying our bounds. In §5 we study the random walk with inward drift on a countable rooted graph. Finally, in §6 we discuss previous work which is related to ours.

2. Cheeger's inequality for positive-recurrent Markov chains and processes. Consider a positive-recurrent discrete-time Markov chain with measurable state space (S, \mathcal{S}) , transition probability kernel P(x, dy) and invariant probability measure π . Then P induces a positivity-preserving linear contraction on $L^2(\pi)$ [and in fact on all the spaces $L^p(\pi)$] by

$$(2.1) (Pf)(x) = \int P(x, dy) f(y).$$

The constant function 1 is an eigenvector of P (and of its adjoint P^*) with eigenvalue 1. The goal of this section is to prove bounds on the spectrum of $P \upharpoonright 1^{\perp}$.

The analogue of Cheeger's isoperimetric constant is the rate of probability flow, in the stationary Markov chain, from a set A to its complement A^c , normalized by the invariant probabilities of A and A^c :

(2.2)
$$k \equiv \inf_{\substack{A \in \mathcal{N}' \\ 0 < \pi(A) < 1}} k(A)$$

with

(2.3)
$$k(A) \equiv \frac{\int \pi(dx)\chi_A(x)P(x,A^c)}{\pi(A)\pi(A^c)} = \frac{(\chi_A, P\chi_{A^c})_{L^2(\pi)}}{\pi(A)\pi(A^c)}.$$

If, for some set A, the flow from A to A^c is very small compared to the invariant probabilities of A and A^c , then intuitively the Markov chain must have very slow convergence to equilibrium (the sets A and A^c are "metastable"). Another way of expressing this intuition is to note that if there exists a set A with $0 < \pi(A) < 1$ for which $\int \pi(dx)\chi_A(x)P(x,A^c) = 0$, then the Markov chain is reducible, and

(2.4a)
$$f \equiv \pi(A^c)\chi_A - \pi(A)\chi_{A^c}$$

$$(2.4b) = \chi_A - \pi(A)\mathbf{1}$$

is an eigenvector of $P \upharpoonright 1^{\perp}$ with eigenvalue 1. Thus, a small value of k indicates that the Markov chain is "almost reducible", and hence ought to have spectrum very near 1. For reversible Markov chains a trivial variational argument makes this intuition rigorous (Theorem 2.1, upper bound).

Much deeper is the reverse inequality, due in the differential-geometric setting to Cheeger [1]: it states that if there does not exist a set A for which the flow from A to A^c is unduly small, then the Markov chain must have rapid convergence to

equilibrium—or more precisely, that $P \upharpoonright 1^{\perp}$ must not have spectrum near 1.¹ We prove here results of this kind first for reversible Markov chains (Theorem 2.1, lower bound) and then for nonreversible Markov chains (Theorem 2.3b). We discuss the intuitions in more detail following the proofs. For convenience we introduce the operator $\tilde{P} \equiv I - P$ and discuss the spectrum of $\tilde{P} \upharpoonright 1^{\perp}$ near 0. We recall that a Markov chain is called *reversible* (with respect to π) if

$$(2.5) \pi(dx)P(x,dy) = \pi(dy)P(y,dx).$$

Equivalently, the chain is reversible if the operator P on $L^2(\pi)$ is selfadjoint. In this case we define

(2.6)
$$\lambda_1(\tilde{P}) = \lambda_0(\tilde{P} \upharpoonright \mathbf{1}^{\perp}) \equiv \inf \operatorname{spec}(\tilde{P} \upharpoonright \mathbf{1}^{\perp}).$$

Now consider a positive-recurrent continuous-time Markovian jump process with measurable state space (S, \mathcal{S}) , transition rate kernel J(x, dy) and invariant probability measure π . We consider only processes in which the transition rates are essentially bounded, i.e.,

(2.7)
$$\pi - \operatorname{ess \ sup}_{x} J(x, \{x\}^{c}) \le M < \infty.$$

Then the infinitesimal generator \tilde{J} of this jump process,

$$(\tilde{J}f)(x) = \int J(x, dy)[f(x) - f(y)],$$

defines a bounded linear operator (of norm $\leq 2M$) on $L^2(\pi)$ [and in fact on all the spaces $L^p(\pi)$]. The constant function $\mathbf{1}$ is an eigenvector of \tilde{J} (and of its adjoint \tilde{J}^*) with eigenvalue 0. The goal of this section is to prove bounds on the spectrum of $\tilde{J} \upharpoonright \mathbf{1}^{\perp}$.

The analogue of Cheeger's isoperimetric constant is now

(2.9)
$$k \equiv \inf_{\substack{A \in \mathscr{S} \\ 0 < \pi(A) < 1}} k(A)$$

with

(2.10a)
$$k(A) \equiv \frac{\int \pi(dx) \chi_A(x) J(x, A^c)}{\pi(A) \pi(A^c)}$$

(2.10b)
$$= \frac{-(\chi_A, \tilde{J}\chi_{A^c})_{L^2(\pi)}}{\pi(A)\pi(A^c)} = \frac{(\chi_A, \tilde{J}\chi_A)_{L^2(\pi)}}{\pi(A)\pi(A^c)}.$$

A jump process is called reversible if

$$(2.11) \pi(dx)J(x,dy) = \pi(dy)J(y,dx),$$

or equivalently if the operator \tilde{J} on $L^2(\pi)$ is selfadjoint. In this case we define

(2.12)
$$\lambda_1(\tilde{J}) = \lambda_0(\tilde{J} \upharpoonright \mathbf{1}^{\perp}) \equiv \inf \operatorname{spec}(\tilde{J} \upharpoonright \mathbf{1}^{\perp}).$$

 $^{^{1}}P \upharpoonright 1^{\perp}$ could have spectrum near other points of the unit circle (e.g., -1 for reversible Markov chains). Spectrum of this kind is associated with the Markov chain being "almost periodic". This phenomenon occurs only for discrete-time Markov chains, not for continuous-time Markov processes.

Note that the transition probability P of a discrete-time Markov chain can also serve as the transition rate kernel of a continuous-time jump process (the process which waits an exponentially distributed time of mean 1 and then jumps according to P). Thus, we need only state our results for the generators \tilde{J} of continuous-time jump processes; the analogous results for the operators \tilde{P} associated to discrete-time Markov chains follow immediately as a special case (just put M=1).

Finally, we note that the sesquilinear form associated with the operator \tilde{J} can be written as

(2.13)
$$(f, \tilde{J}g)_{L^{2}(\pi)} = \int \mu(dx, dy) \overline{f(x)} [g(x) - g(y)],$$

where

(2.14)
$$\mu(dx, dy) \equiv \pi(dx)J(x, dy)\chi(x \neq y)$$

is a positive measure on $S \times S$ whose marginals are equal and are $\leq M\pi(dx)$. The measure μ is symmetric if and only if \tilde{J} is selfadjoint, and in this case the sesquilinear form can equivalently be written as

$$(2.15) (f, \tilde{J}g)_{L^2(\pi)} = \frac{1}{2} \int \mu(dx, dy) \overline{[f(x) - f(y)]} [g(x) - g(y)],$$

which is manifestly positive-semidefinite.

Before stating Theorem 2.1, we define a positive constant κ by

(2.16)
$$\kappa \equiv \inf_{\mathcal{L}} \sup_{c} \frac{(E|(X+c)^2 - (Y+c)^2|)^2}{E[(X+c)^2]},$$

where the infimum is taken over all distributions of i.i.d. real-valued random variables (X,Y) with variance 1. A priori it is not obvious that $\kappa \neq 0$; but in Proposition 2.2 we will show that $\kappa \geq 1$. (We suspect, however, that this bound is not sharp.)

THEOREM 2.1. Let \tilde{J} be a bounded selfadjoint operator on $L^2(\pi)$ whose associated sesquilinear form is given by (2.15), where μ is a symmetric positive measure whose marginals are $\leq M\pi$. Then

(2.17)
$$\kappa k^2 / 8M \le \lambda_1(\tilde{J}) \le k,$$

where k is defined by (2.9), (2.10b).

PROOF OF UPPER BOUND ON $\lambda_1(\tilde{J})$. Let $A \in \mathcal{S}$ with $0 < \pi(A) < 1$, and consider the trial function f defined in (2.4). Clearly $\int f d\pi = 0$, i.e., $f \perp 1$. A simple computation yields the Rayleigh quotient

(2.18)
$$\frac{(f, \tilde{J}f)_{L^2(\pi)}}{(f, f)_{L^2(\pi)}} = \frac{(\chi_A, \tilde{J}\chi_A)_{L^2(\pi)}}{\pi(A)\pi(A^c)} = k(A).$$

It then follows from the Rayleigh-Ritz principle that $\tilde{J} \upharpoonright \mathbf{1}^{\perp}$ must have spectrum in the interval [0, k]. \square

PROOF OF LOWER BOUND ON $\lambda_1(\tilde{J})$. Since \tilde{J} is real and selfadjoint, it suffices to consider real trial functions. For real $f \in L^2(\pi)$, we have

$$(2.19) (f, \tilde{J}f)_{L^2(\pi)} = \frac{1}{2} \int \mu(dx, dy) [f(x) - f(y)]^2.$$

Let c be a real constant (to be determined later) and define g = f + c. Then

$$(f, \tilde{J}f)_{L^{2}(\pi)} = \frac{1}{2} \int \mu(dx, dy) [g(x) - g(y)]^{2}$$

$$\geq \frac{1}{2} \frac{(\int \mu(dx, dy) [g(x)^{2} - g(y)^{2}])^{2}}{\int \mu(dx, dy) [g(x) + g(y)]^{2}} \quad \text{[by Schwarz]}$$

$$\geq \frac{1}{2} \frac{(\int \mu(dx, dy) [g(x)^{2} - g(y)^{2}])^{2}}{\int \mu(dx, dy) [2g(x)^{2} + 2g(y)^{2}]}$$

$$\geq \frac{1}{8M} \frac{(\int \mu(dx, dy) [g(x)^{2} - g(y)^{2}])^{2}}{\int \pi(dx) g(x)^{2}}.$$

Now

$$(2.21)$$

$$\int \mu(dx, dy)|g(x)^2 - g(y)^2|$$

$$= 2 \int \mu(dx, dy)\chi(g(x)^2 > g(y)^2)(g(x)^2 - g(y)^2) \quad \text{[by symmetry of } \mu\text{]}$$

$$= 2 \int_0^\infty d\alpha \int \mu(dx, dy)\chi(g(x)^2 > \alpha \ge g(y)^2)$$

$$= 2 \int_0^\infty d\alpha - (\chi_{A_\alpha}, \tilde{J}\chi_{(A_\alpha)^c})_{L^2(\pi)}$$

where $A_{\alpha} \equiv \{x \colon g(x)^2 > \alpha\}$. By hypothesis this is

(2.22)
$$\geq 2 \int_0^\infty d\alpha k \pi(A_\alpha) \pi((A_\alpha)^c)$$

$$= 2k \int_0^\infty d\alpha \int \pi(dx) \pi(dy) \chi(g(x)^2 > \alpha \geq g(y)^2)$$

$$= 2k \int \pi(dx) \pi(dy) \chi(g(x)^2 > g(y)^2) (g(x)^2 - g(y)^2)$$

$$= k \int \pi(dx) \pi(dy) |g(x)^2 - g(y)^2|.$$

Combining (2.20)–(2.22), we have

$$(2.23) (f, \tilde{J}f)_{L^2(\pi)} \ge \frac{k^2}{8M} \frac{(\int \pi(dx)\pi(dy)|g(x)^2 - g(y)^2|)^2}{\int \pi(dx)g(x)^2},$$

where $g \equiv f + c$. We now optimize the choice of c; by definition of κ (and an obvious scaling) we have

$$(2.24) \qquad \qquad (f,\tilde{J}f)_{L^2(\pi)} \geq \frac{\kappa k^2}{8M} \left[\int f^2 d\pi - \left(\int f d\pi \right)^2 \right].$$

In particular, if $f \perp 1$, then

$$(2.25) (f, \tilde{J}f)_{L^2(\pi)} \ge \frac{\kappa k^2}{8M} \|f\|_{L^2(\pi)}^2.$$

This proves that $\lambda_1(\tilde{J}) \geq \kappa k^2/8M$. \square

The following proposition, which proves that $\kappa \geq 1$, is perhaps of some interest in its own right.

PROPOSITION 2.2. Let X and Y be i.i.d. real-valued random variables with finite variance σ^2 . Then

(2.26)
$$\sup_{c} \frac{(E|(X+c)^2 - (Y+c)^2|)^2}{E[(X+c)^2]} \ge \sigma^2.$$

PROOF. Without loss of generality we may assume that EX = 0 and $\sigma^2 = E[X^2] = 1$. An easy estimate gives

(2.27)
$$\lim_{c \to \pm \infty} \frac{(E|(X+c)^2 - (Y+c)^2|)^2}{E[(X+c)^2]} = 4(E|X-Y|)^2.$$

By Jensen's inequality, $E|X-Y| \ge E|X-EY| = E|X|$. If $E|X| \ge \frac{1}{2}$ we are done; otherwise we set c=0 and use the estimate

$$(2.28) E|X^2 - Y^2| \ge 2(1 - E|X|).$$

To prove (2.28), note that

(2.29)

$$|E|X^2 - Y^2| \ge 2E[(X^2 - Y^2)\chi(X^2 \ge 1, Y^2 < 1)]$$

$$= 2[E(X^2\chi(X^2 \ge 1))P[X^2 < 1] - E[X^2\chi(X^2 < 1)]P[X^2 \ge 1]].$$

(But
$$E[X^2\chi(X^2 \ge 1)] + E[X^2\chi(X^2 < 1)] = 1$$
.) Hence

$$(2.30) = 2[P[X^2 < 1] - E[X^2 \chi(X^2 < 1)]].$$

On the other hand,

(2.31)
$$E[X^{2}\chi(X^{2} < 1)] \le E[|X|\chi(X^{2} < 1)]$$
$$= E|X| - P[|X| \ge 1]E[|X| | |X| \ge 1]$$
$$< E|X| - P[|X| > 1],$$

which gives the result. \square

REMARK. We suspect that in fact κ is strictly greater than 1, but a proof of this will almost certainly have to consider values of c other than just 0 and $\pm \infty$.

Now we turn to the nonselfadjoint case. For any bounded linear operator T on a *complex* Hilbert space, the *numerical range* W(T) is defined to be the set of all numbers (f, TF) as f ranges over unit vectors. Recall the following facts [8, 9]:

- (i) W(T) is convex (but not necessarily closed).
- (ii) spec $(T) \subset \overline{W(T)}$.
- (iii) If T is normal, then $\overline{W(T)}$ is the convex hull of $\operatorname{spec}(T)$. But if T is non-normal, then $\overline{W(T)}$ can be much larger than the convex hull of $\operatorname{spec}(T)$. [Example: nilpotent operators.]

THEOREM 2.3. Let \tilde{J} be a bounded linear operator on $L^2(\pi)$ whose associated sesquilinear form is given by (2.13), where μ is a positive measure whose marginals are equal and are $\leq M\pi$. Then

- (a) The closure of the numerical range of \tilde{J} contains the number k.
- (b) The closure of the numerical range of \tilde{J} , and hence also the spectrum, is contained in the set

(2.32)
$$\{\lambda \colon |\lambda| \le 2M \text{ and } \operatorname{Re} \lambda \ge \kappa k^2 / 8M\}.$$

PROOF. The computation (2.18) is valid whether or not \tilde{J} is selfadjoint (since $\tilde{J}\mathbf{1} = \tilde{J}^*\mathbf{1} = 0$); this proves (a).

(b) follows from Theorem 2.1 applied to the operator $\frac{1}{2}(\tilde{J} + \tilde{J}^*)$; the point is that

(2.33)
$$\operatorname{Re}(f, \tilde{J}f)_{L^{2}(\pi)} = (f, \frac{1}{2}(\tilde{J} + \tilde{J}^{*})f)_{L^{2}(\pi)}$$

for arbitrary (complex) $f \in L^2(\pi)$; and (2.10b) ensures that \tilde{J} and $\frac{1}{2}(\tilde{J} + \tilde{J}^*)$ have the same constant k. \square

Theorem 2.3(a) is unfortunately not very useful if \tilde{J} is nonnormal, since spec(\tilde{J}) could be much smaller than $W(\tilde{J})$. Indeed, it appears to be an open question whether there exists an inclusion theorem for the spectrum of \tilde{J} in terms of k alone. On the other hand, Theorem 2.3(b) is very strong. It even implies results about the numerical range (and hence the spectrum) of operators $F(\tilde{J})$ for certain analytic functions F [10]; one case of interest is $F(\tilde{J}) = \tilde{J}^{-1}$, which arises in the central limit theorem (see, e.g., [11, 12]).

Here are some examples (for simplicity in discrete time) which illuminate Theorems 2.1 and 2.3:

1. Two-state Markov chain. Let the transition probability matrix be

$$(2.34) P = \begin{pmatrix} 1-a & a \\ b & 1-b \end{pmatrix}.$$

Then the invariant probability distribution is

$$\pi = \left(\frac{b}{a+b}, \frac{a}{a+b}\right),\,$$

the "Cheeger" constant is k = a + b, and the next-to-smallest eigenvalue of \tilde{P} is $\lambda_1(\tilde{P}) = a + b$. So in this example the upper bound in Theorem 2.1 is sharp.

2. Symmetric random walk on $\{1, 2, ..., n\}$ with elastic barriers. The nonzero elements of $P = \{p_{ij}\}_{i,j=1}^n$ are

$$p_{i,i+1} = \frac{1}{2} \qquad (1 \le i \le n-1),$$

$$p_{i,i-1} = \frac{1}{2} \qquad (2 \le i \le n),$$

$$p_{11} = p_{nn} = \frac{1}{2}.$$

Then $\pi = (1/n, ..., 1/n),$

$$k = \left\{ egin{array}{ll} 2/n & (n \ {
m even}), \ 2n/(n^2-1) & (n \ {
m odd}), \end{array}
ight.$$

and $\lambda_1(\tilde{P}) = 1 - \cos(\pi/n) \approx \pi^2/2n^2$. So the order of magnitude in the lower bound in Theorem 2.1 is sharp (but the constant is not sharp).

3. Random walk on the cyclic group \mathbf{Z}_n . The nonzero elements of $P = \{p_{ij}\}_{i,j=1}^n$ are

$$p_{i,i+1} = a, \qquad p_{i,i-1} = 1 - a.$$

Then $\pi = (1/n, \dots, 1/n)$; P is selfadjoint if and only if $a = \frac{1}{2}$. The "Cheeger" constant is

$$k = \begin{cases} 4/n & (n \text{ even}), \\ 4n/(n^2 - 1) & (n \text{ odd}), \end{cases}$$

and the eigenvalues of $\tilde{P} \upharpoonright \mathbf{1}^{\perp}$ with smallest real part are $\lambda = 1 - \cos(2\pi/n) \pm i(2a-1)\sin(2\pi/n)$. So the order of magnitude in Theorem 2.3(b) is sharp for all a, including the extreme cases of reversibility $(a=\frac{1}{2})$ and determinism (a=0,1).

It can be seen from these examples that there are two distinct physical situations which can lead to slow convergence to equilibrium (more precisely, to spectrum of $P \upharpoonright \mathbf{1}^{\perp}$ near 1).² The first situation is small flow from some set A to its complement A^c ; as seen in the two-state Markov chain, this leads to a spectral gap $\lambda_1(\tilde{P})$ of order k. The second situation is the necessity to traverse a long "tunnel", of length n; random walk through this "tunnel" takes a time of order n^2 , so the spectral gap $\lambda_1(\tilde{P})$ is of order n^{-2} . What is quite remarkable is that the second of this physical effects can be bounded in terms of the first: the maximum possible length of a "tunnel" turns out to be $n \sim k^{-1}$, so the spectral gap is always at least const $\times k^2$.

3. Cheeger's inequality for Markov chains and processes with killing. Consider a continuous-time Markovian jump process with killing, with measurable state space (S, \mathcal{S}) , transition rate kernel J(x, dy) and killing rate $K(x) \geq 0$. We assume that the corresponding process without killing is positive-recurrent with finite invariant measure π . We consider only processes in which the transition and killing rates are essentially bounded, i.e.,

(3.1)
$$\pi$$
-ess $\sup_{x} [J(x, \{x\}^c) + \frac{1}{2}K(x)] \le M < \infty.$

Then the infinitesimal generator $L = \tilde{J} + K$ of this jump process,

(3.2)
$$(Lf)(x) = \int J(x, dy)[f(x) - f(y)] + K(x)f(x),$$

defines a bounded linear operator (of norm $\leq 2M$) on $L^2(\pi)$ [and in fact on all the spaces $L^p(\pi)$]. The goal of this section is to prove bounds on the spectrum of L.

The analogue of Cheeger's isoperimetric constant is now

(3.3)
$$h \equiv \inf_{\substack{A \in \mathcal{S} \\ \pi(A) > 0}} h(A)$$

with

(3.4a)
$$h(A) \equiv \frac{\int \pi(dx) \chi_A(x) [J(x, A^c) + K(x)]}{\pi(A)}$$

$$=\frac{(\chi_A, L\chi_A)_{L^2(\pi)}}{\pi(A)}.$$

Thus, the numerator is the total rate of probability flow out of the set A, including both the flow to A^c and the killing. Note that the denominator is $\pi(A)$, not $\pi(A)\pi(A^c)$. As usual, the process is called *reversible* (with respect to π) if the transition rates satisfy (2.11), or equivalently if the operator L on $L^2(\pi)$ is selfadjoint. In this case we define

(3.5)
$$\lambda_0(L) \equiv \inf \operatorname{spec}(L).$$

²Slow convergence to equilibrium can also be associated with spectrum of $P \upharpoonright \mathbf{1}^{\perp}$ near other points of the unit circle. Different physical phenomena are involved in these cases. These phenomena occur only for discrete-time Markov chains, not for continuous-time Markov processes.

The sesquilinear form associated with the operator L can be written as

$$(3.6) \qquad (f, Lg)_{L^2(\pi)} = \int \mu(dx, dy) \overline{f(x)} [g(x) - g(y)] + \int \pi(dx) K(x) \overline{f(x)} g(x),$$

where μ is defined by (2.14). In the selfadjoint case this can be written as (3.7)

$$(f,Lg)_{L^2(\pi)}=rac{1}{2}\int \mu(dx,dy)\overline{[f(x)-f(y)]}[g(x)-g(y)]+\int \pi(dx)K(x)\overline{f(x)}g(x),$$

which is manifestly positive-semidefinite. This sesquilinear form can be written in a form more closely resembling (2.13)–(2.15) by introducing an enlarged state space $S^* = S \cup \{\infty\}$ (where $\infty \notin S$). We then define, for any function f on S, the extended function f^* on S^* by

(3.8)
$$f^*(x) = \begin{cases} f(x) & \text{if } x \in S, \\ 0 & \text{if } x = \infty. \end{cases}$$

We further define a positive measure μ^* on $S^* \times S^*$ by

(3.9a)
$$\mu^*(C) \equiv \mu(C) = \int \pi(dx) J(x, dy) \chi(x \neq y) \chi_C(x, y)$$
 if $C \subset S \times S$,

(3.9b)
$$\mu^*(A \times \{\infty\}) = \mu^*(\{\infty\} \times A) \equiv \int \pi(dx) K(x) \chi_A(x) \quad \text{if } A \subset S,$$

(In probabilistic terms, we are implicitly defining a modified process in which the particle returns from the "cemetery" state ∞ with rates $J^*(\infty, A) \equiv \mu^*(\{\infty\} \times A)/\pi^*(\{\infty\})$, where $\pi^*(\{\infty\})$ is an arbitrary strictly positive number. However, neither $J^*(\infty, A)$ nor $\pi^*(\{\infty\})$ plays any role in our analysis; only the naturally defined measure μ^* enters.) With these definitions, we can write

(3.10)
$$(f, Lg)_{L^2(\pi)} = \int \mu^*(dx, dy) \overline{f^*(x)} [g^*(x) - g^*(y)]$$

in general, and

$$(3.11) (f, Lg)_{L^2(\pi)} = \frac{1}{2} \int \mu^*(dx, dy) \overline{[f^*(x) - f^*(y)]} [g^*(x) - g^*(y)]$$

in the selfadjoint case.

THEOREM 3.1. Let L be a selfadjoint operator on $L^2(\pi)$ whose associated sesquilinear form is given by (3.7), where μ is a symmetric positive measure whose marginals are $\leq [M - \frac{1}{2}K(x)]\pi(dx)$. Then

$$(3.12) h^2/2M \le \lambda_0(L) \le h,$$

where h is defined by (3.3), (3.4b).

PROOF OF UPPER BOUND ON $\lambda_0(L)$. Let $A \in \mathcal{S}$ with $\pi(A) > 0$, and consider the trial function χ_A . Obviously

(3.13)
$$\frac{(\chi_A, L\chi_A)_{L^2(\pi)}}{(\chi_A, \chi_A)_{L^2(\pi)}} = \frac{(\chi_A, L\chi_A)_{L^2(\pi)}}{\pi(A)} = h(A). \quad \Box$$

PROOF OF LOWER BOUND ON $\lambda_0(L)$. Since L is real and selfadjoint, it suffices to consider real trial functions. For real $f \in L^2(\pi)$, we have

$$(f, Lf)_{L^{2}(\pi)} = \frac{1}{2} \int_{S \times S} \mu(dx, dy) [f(x) - f(y)]^{2} + \int_{S} \pi(dx) K(x) f(x)^{2}$$

$$= \frac{1}{2} \int_{S^{*} \times S^{*}} \mu^{*}(dx, dy) [f^{*}(x) - f^{*}(y)]^{2}$$

$$\geq \frac{1}{2} \frac{\left(\int_{S^{*} \times S^{*}} \mu^{*}(dx, dy) [f^{*}(x)^{2} - f^{*}(y)^{2}]\right)^{2}}{\int_{S^{*} \times S^{*}} \mu^{*}(dx, dy) [f^{*}(x) + f^{*}(y)]^{2}} \quad \text{[by Schwarz]}.$$

Now the denominator is

$$= \int_{S \times S} \mu(dx, dy) [f(x) + f(y)]^2 + 2 \int_S \pi(dx) K(x) f(x)^2$$

$$\leq \int_{S \times S} \mu(dx, dy) [2f(x)^2 + 2f(y)^2] + 2 \int_S \pi(dx) K(x) f(x)^2$$

$$\leq 4M \int_S \pi(dx) f(x)^2.$$

On the other hand,

$$\int_{S^{*}\times S^{*}} \mu^{*}(dx, dy)|f^{*}(x)^{2} - f^{*}(y)^{2}|$$

$$= 2 \int_{S^{*}\times S^{*}} \mu^{*}(dx, dy)\chi(f^{*}(x)^{2} > f^{*}(y)^{2})(f^{*}(x)^{2} - f^{*}(y)^{2})$$
[by symmetry of μ]
$$= 2 \int_{0}^{\infty} d\alpha \int_{S^{*}\times S^{*}} \mu^{*}(dx, dy)\chi(f^{*}(x)^{2} > \alpha \geq f^{*}(y)^{2})$$

$$= 2 \int_{0}^{\infty} d\alpha \int_{S^{*}\times S^{*}} \mu^{*}(dx, dy)\chi_{A_{\alpha}}(x)[\chi_{A_{\alpha}}(x) - \chi_{A_{\alpha}}(y)]$$

$$= 2 \int_{0}^{\infty} d\alpha(\chi_{A_{\alpha}}, L\chi_{A_{\alpha}})_{L^{2}(\pi)}$$

where $A_{\alpha} \equiv \{x \in S : f(x)^2 > \alpha\}$. By hypothesis this is

Combining (3.14)–(3.17), we have

$$(3.18) (f, Lf)_{L^2(\pi)} \ge \frac{h^2}{2M} ||f||_{L^2(\pi)}^2.$$

This proves that $\lambda_0(L) \geq h^2/2M$. \square

A version of Theorem 3.1 for nonreversible Markov chains with killing can be proven by an argument similar to that used in Theorem 2.3; we leave the details to the reader.

One common way of obtaining a Markov process with killing is to take a positiverecurrent Markov process on a state space S and kill it whenever it leaves some specified subset $B \subset S$. More precisely, consider a positive-recurrent reversible continuous-time Markovian jump process with measurable state space (S, \mathcal{S}) , transition rate kernel J(x, dy) [satisfying (2.7)] and finite invariant measure π , and assume now that the process is killed when it leaves the subset B ($B \in \mathcal{S}$). This latter process is, therefore, a reversible Markovian jump process on B with transition rate kernel $J^B(x,dy) \equiv J(x,dy)\chi_B(y)$ and killing rate $K^B(x) \equiv J(x,S\backslash B)$ $[x \in B]$. Its infinitesimal generator $L^B = \widetilde{J}^B + K^B$.

(3.19)
$$(L^B f)(x) = \int_B J^B(x, dy)[f(x) - f(y)] + K^B(x)f(x) [x \in B],$$

defines a bounded linear operator (of norm $\leq 2M$) on the space $L^2(B,\pi)$ [and in fact on all the spaces $L^p(B,\pi)$]. (Note that the assumed reversibility (2.11) for the pair (π, J) implies the same relation for the pair $(\pi \upharpoonright B, J^B)$; in particular, $\pi \upharpoonright B$ is an invariant measure for J^B .) The sesquilinear form associated with the operator L^B can be written as

(3.20a)

$$(f, L^B g)_{L^2(B,\pi)} = \int_{B \times B} \mu^B(dx, dy) \overline{f(x)} [g(x) - g(y)] + \int_B \pi(dx) K^B(x) \overline{f(x)} g(x)$$

$$(3.20b) \qquad = \int_{S \times S} \mu(dx, dy) \overline{f(x)} [g(x) - g(y)]$$

where μ is defined by (2.14), μ^B is its restriction to $B \times B$, and f and g are defined to vanish outside B. In other words, the sesquilinear form associated with L^B is just the restriction to the subspace $L^2(B,\pi) \subset L^2(\pi)$ of the sesquilinear form associated with \tilde{J} .

It follows that if we define

(3.21)
$$h_B \equiv \inf_{\substack{A \subset B \\ \pi(A) > 0}} h(A)$$

with

(3.22a)

$$h(A) \equiv \frac{\int \pi(dx)\chi_A(x)J(x,S\backslash A)}{\pi(A)} = \frac{\int \pi(dx)\chi_A(x)[J^B(x,B\backslash A) + K^B(x)]}{\pi(A)}$$

$$h(A) \equiv \frac{\int \pi(dx)\chi_A(x)J(x,S\backslash A)}{\pi(A)} = \frac{\int \pi(dx)\chi_A(x)[J^B(x,B\backslash A) + K^B(x)]}{\pi(A)}$$

(3.22b)
$$= \frac{(\chi_A, \tilde{J}\chi_A)_{L^2(\pi)}}{\pi(A)} = \frac{(\chi_A, L^B\chi_A)_{L^2(B,\pi)}}{\pi(A)},$$

then we obtain immediately from Theorem 3.1 the following corollary:

COROLLARY 3.2. Let L^B be a bounded selfadjoint operator on $L^2(B,\pi)$ whose associated sesquilinear form is the restriction to $L^2(B,\pi)$ of the sesquilinear form (2.15) on $L^2(S,\pi)$, where $B \subset S$ and μ is a symmetric positive measure on $S \times S$ whose marginals are $\leq M\pi$. Then

$$(3.23) h_B^2/2M < \lambda_0(L^B) < h_B,$$

where h_B is defined by (3.21), (3.22b).

Now return to the set-up of §2, in which \tilde{J} is the generator of a positive-recurrent Markovian jump process on S. We can use Corollary 3.2 to give an alternate proof of (a slight variant of) Theorem 2.1. First we demonstrate a very interesting relation between λ_1 for a positive-recurrent process and λ_0 for the associated killed processes on subsets $B \subset S$.

For any bounded selfadjoint operator H on $L^2(\pi)$ and any $B \in \mathcal{S}$, we define $H_B \equiv I_B H I_B \upharpoonright L^2(B,\pi)$, where I_B is the operator of multiplication by χ_B . [Equivalently, H_B is the operator on $L^2(B,\pi)$ whose associated sesquilinear form is the restriction to $L^2(B,\pi)$ of the sesquilinear form associated with H.] For example, $(\tilde{J})_B = L^B$.

PROPOSITION 3.3. Let H be a bounded selfadjoint operator on $L^2(\pi)$ whose associated quadratic form is given by

$$(3.24) (f, Hf)_{L^2(\pi)} = \frac{1}{2} \int \mu(dx, dy) |f(x) - f(y)|^2,$$

where μ is a finite symmetric positive measure. Then

(3.25)
$$\lambda_1(H) \ge \inf_{R} \max[\lambda_0(H_B), \lambda_0(H_{B^c})].$$

We first prove this proposition in a special case:

LEMMA 3.4. Proposition 3.3 holds if $\lambda_1(H)$ is an eigenvalue of H.

PROOF. To shorten the notation, write λ in place of $\lambda_1(H)$. Let $f \in L^2(\pi)$ be real-valued, $\not\equiv 0$ and satisfy $Hf = \lambda f$. Define $V^+ = \{x \colon f(x) > 0\}$ and $f_+(x) = \max[f(x), 0]$. Note that $\|f_+\|_{L^2(\pi)} \neq 0$ since $f \perp 1$. Then

(3.26)
$$\lambda = \frac{\int \chi_{V} + \lambda f^2 d\pi}{\int \chi_{V} + f^2 d\pi} = \frac{(f_+, Hf)_{L^2(\pi)}}{(f_+, f_+)_{L^2(\pi)}}.$$

Now

$$(f_{+}, Hf)_{L^{2}(\pi)} = \int \mu(dx, dy) f_{+}(x) [f(x) - f(y)]$$

$$\geq \int \mu(dx, dy) f_{+}(x) [f_{+}(x) - f_{+}(y)]$$

$$= (f_{+}, Hf_{+})_{L^{2}(\pi)}.$$

Hence

(3.28)
$$\lambda \ge \frac{(f_+, Hf_+)_{L^2(\pi)}}{(f_+, f_+)_{L^2(\pi)}} \ge \lambda_0(H_{V^+}).$$

An analogous argument with $V^-=(V^+)^c=\{x\colon f(x)\leq 0\},\ f_-(x)=\max[-f(x),0]$ shows that $\lambda\geq \lambda_0(H_{V^-}).$

PROOF OF PROPOSITION 3.3 IN GENERAL CASE. Let \mathscr{S}' be a finitely generated subfield of \mathscr{S} , and let E be the conditional expectation $E^{\pi}(\cdot|\mathscr{S}')$. [Analytically, E is the orthogonal projection in $L^2(\pi)$ onto the subspace $L^2(\mathscr{S}',\pi)$ of \mathscr{S}' -measurable functions.] Now define $H' = EHE \upharpoonright L^2(\mathscr{S}',\pi)$. Obviously

$$(3.29) (f, H'f)_{L^2(\pi)} = (f, Hf)_{L^2(\pi)} = \frac{1}{2} \int \mu(dx, dy) |f(x) - f(y)|^2$$

for $f \in L^2(\mathcal{S}', \pi)$. Since $L^2(\mathcal{S}', \pi)$ is a finite-dimensional space, Lemma 3.4 applies to H', so

(3.30)
$$\lambda_1(H') \ge \inf_{B \in \mathscr{D}'} \max[\lambda_0((H')_B), \lambda_0((H')_{B^c})].$$

Now

$$(3.31a) \lambda_0((H')_B) \ge \lambda_0(H_B),$$

(3.31b)
$$\lambda_0((H')_{B^c}) \ge \lambda_0(H_{B^c})$$

by the Rayleigh-Ritz principle (since the LHS is the infimum of (f, Hf)/(f, f) over a smaller class of functions). Now let $\{S'_{\alpha}\}$ be the net of all finitely generated subfields of S, directed by inclusion, and let $\{E'_{\alpha}\}$ be the corresponding conditional expectations. Clearly $\lim_{\alpha} E'_{\alpha} f = f$ for all $f \in L^2(\pi)$. Moreover, if $f \perp 1$, then $E'_{\alpha} f \perp 1$ for all α . Thus, for all $f \perp 1$,

(3.32)
$$(f, Hf) = \lim_{\alpha} (E'_{\alpha}f, HE'_{\alpha}f)$$
 [by boundedness of H]

and for each α ,

$$(E'_{\alpha}f, HE'_{\alpha}f) \geq \lambda_{1}(H'_{\alpha})\|E'_{\alpha}f\|^{2}$$

$$\geq \left(\inf_{B \in \mathscr{S}'_{\alpha}} \max[\lambda_{0}((H'_{\alpha})_{B}), \lambda_{0}((H'_{\alpha})_{B^{c}})]\right) \|E'_{\alpha}f\|^{2}$$

$$\geq \left(\inf_{B} \max[\lambda_{0}(H_{B}), \lambda_{0}(H_{B^{c}})]\right) \|E'_{\alpha}f\|^{2}$$

$$\rightarrow \left(\inf_{B} \max[\lambda_{0}(H_{B}), \lambda_{0}(H_{B^{c}})]\right) \|f\|^{2}.$$

This proves the proposition. \square

REMARK. One consequence of Proposition 3.3 is that

(3.34)
$$\lambda_1(H) \ge \sup_x \lambda_0(H_{\{x\}^c})$$

(since for every B, either $\{x\}^c \supset B$ or $\{x\}^c \supset B^c$). This result can also be proven by the min-max theorem, and has interesting applications [13, 7]. Proposition 3.3 gives additional insight into why (3.34) is true (and why it is not optimal).

We can now prove a slight variant of Theorem 2.1. Define the modified Cheeger constant

$$h^* \equiv \inf_{\substack{A \in \mathcal{S} \\ 0 < \pi(A) < 1}} h^*(A)$$

with

$$(3.36a) h^*(A) \equiv \max[h(A), h(A^c)]$$

(3.36b)
$$= \frac{(\chi_A, \tilde{J}\chi_A)_{L^2(\pi)}}{\min[\pi(A), \pi(A^c)]}.$$

Note that $h^*(A) \leq k(A) \leq 2h^*(A)$ and hence that $h^* \leq k \leq 2h^*$. We have

THEOREM 3.5. Let \tilde{J} be a bounded selfadjoint operator on $L^2(\pi)$ whose associated sesquilinear form is given by (2.15), where μ is a symmetric positive measure whose marginals are $\leq M\pi$. Then

where h^* is defined by (3.35), (3.36).

PROOF. By Proposition 3.3 and Corollary 3.2,

(3.38)
$$\lambda_{1}(\tilde{J}) \geq \inf_{B} \max[\lambda_{0}((\tilde{J})_{B}), \lambda_{0}((\tilde{J})_{B^{c}})]$$

$$\geq \inf_{B: \pi(B) \leq 1/2} \lambda_{0}((\tilde{J})_{B}) \geq \inf_{B: \pi(B) \leq 1/2} \inf_{\substack{A \subseteq B \\ \pi(A) > 0}} \frac{h(A)^{2}}{2M}$$

$$= \inf_{A: 0 < \pi(A) \leq 1/2} \frac{h(A)^{2}}{2M} = \frac{h^{*2}}{2M}. \quad \Box$$

REMARKS. 1. Since $h^* \geq k/2$, Theorem 3.5 implies that $\lambda_1(\tilde{J}) \geq k^2/8M$. Thus, if $\kappa = 1$, then Theorem 3.5 is stronger than Theorem 2.1; but if $\kappa > 1$, then the two theorems are incomparable.

2. It is useful to note that

$$(3.39) h^* \ge \sup_x h_{\{x\}^c}$$

[since the $A \leftrightarrow A^c$ symmetry in (3.36) means that the infimum in (3.35) can be restricted without loss to $A \not\ni x$, and then $h^*(A) \ge h(A)$]. This relation is analogous to (3.34).

4. Some lemmas for evaluating k, h and h^* . The theorems of the preceding sections are, as they stand, rather difficult to apply, since k is defined as the infimum of k(A) over all measurable sets A (and likewise for h and h^*). In this section we prove some useful lemmas which show that the infimum can be restricted to much smaller classes of sets A.

A family $\mathcal{S}_0 \subset \mathcal{S}$ is said to be *dense* if for all $A \in \mathcal{S}$ and all $\varepsilon > 0$ there exists $B \in \mathcal{S}_0$ such that $\pi(A \triangle B) \leq \varepsilon$.

LEMMA 4.1. Let \mathcal{S}_0 be a dense subfamily of \mathcal{S} . Then

(4.1)
$$k \equiv \inf_{\substack{A \in \mathcal{S} \\ 0 < \pi(A) < 1}} k(A) = \inf_{\substack{A \in \mathcal{S}_0 \\ 0 < \pi(A) < 1}} k(A)$$

and likewise for h and h^* .

PROOF. Immediate. \square

For example, if S is a metric space, \mathcal{S}_0 can be taken to be the family of closed (or open) sets; if S is a topological space and π is a Radon measure, \mathcal{S}_0 can be taken to be the family of compact sets; or if S is an n-dimensional smooth manifold, \mathcal{S}_0 can be taken to be the family of n-dimensional smooth submanifolds of S with smooth boundary.

We say that sets A and B are separated (for the operator L) if $\pi(A \cap B) = (\chi_A, L\chi_B)_{L^2(\pi)} = (\chi_B, L\chi_A)_{L^2(\pi)} = 0$.

LEMMA 4.2. Let $\{A_i\}_{i\in I}$ be a countable family of pairwise separated sets of nonzero π -measure, and define $A=\bigcup_i A_i$. Then either $h(A_i)=h(A)$ for all i, or else there exists an index i_0 such that $h(A_{i_0})< h(A)$.

PROOF. We have

(4.2)
$$h(A) = \frac{(\chi_A, L\chi_A)_{L^2(\pi)}}{\pi(A)} = \frac{\sum_i (\chi_{A_i}, L\chi_{A_i})_{L^2(\pi)}}{\sum_i \pi(A_i)}$$

since A_i and A_j are separated for $i \neq j$. The claim easily follows. \square

LEMMA 4.3. Let $\{A_i\}_{i\in I}$ be a countable family of pairwise separated sets of nonzero π -measure, such that $B \equiv A^c \equiv (\bigcup_i A_i)^c$ also has nonzero π -measure. Then

- (a) Either $h^*(A_i) = h^*(A)$ for all i, or else there exists an index i_0 such that $h^*(A_{i_0}) < h^*(A)$.
 - (b) Provided that $|I| \geq 2$, there exists an index i_0 such that $k(A_{i_0}) < k(A)$.

PROOF. (a) We have

(4.3)
$$h^*(A) = \frac{(\chi_A, \tilde{J}\chi_A)_{L^2(\pi)}}{\min[\pi(A), \pi(A^c)]} \ge \frac{\sum_i (\chi_{A_i}, \tilde{J}\chi_{A_i})_{L^2(\pi)}}{\sum_i \min[\pi(A_i), \pi((A_i)^c)]}.$$

The claim easily follows.

(b) We have

(4.4)
$$k(A) = \frac{(\chi_A, \tilde{J}\chi_A)_{L^2(\pi)}}{\pi(A)\pi(B)} = \frac{\sum_i (\chi_{A_i}, \tilde{J}\chi_{A_i})_{L^2(\pi)}}{[\sum_i \pi(A_i)]\pi(B)}$$

and

(4.5)
$$k(A_i) = \frac{(\chi_{A_i}, \tilde{J}\chi_{A_i})_{L^2(\pi)}}{\pi(A_i)[\pi(B) + \sum_{j \neq i} \pi(A_j)]} < \frac{(\chi_{A_i}, \tilde{J}\chi_{A_i})_{L^2(\pi)}}{\pi(A_i)\pi(B)}.$$

The claim follows as before. \Box

If the state space S is countable, we define the (undirected) graph associated to the transition rate J by declaring that x is adjacent to y $(x, y \in S)$ if $x \neq y$ and either J(x, y) > 0 or J(y, x) > 0 (or both). A set $A \subset S$ is said to be connected if for every pair $x, y \in A$ $(x \neq y)$ there is a path from x to y lying entirely in A. Lemmas 4.2 and 4.3 then have the following consequence:

COROLLARY 4.4. If the state space S is countable, then

(4.6)
$$h \equiv \inf_{A} h(A) = \inf_{A \text{ connected}} h(A)$$

and likewise for h* and k. If, in addition, S is connected, then

$$h^* = \inf_{A : A \text{ so both connected}} h^*(A)$$

and likewise for k.

PROOF. Take any set A with $\pi(A) > 0$, and decompose it into its connected components $\{A_i\}$. Then $h(A) = h(\bigcup_{i: \pi(A_i) > 0} A_i)$, and Lemma 4.2 implies that $h(A_{i_0}) \leq h(A)$ for at least one index i_0 with $\pi(A_{i_0}) > 0$. This proves (4.6). Analogous arguments work for h^* and k.

Now assume that S is connected, and consider any connected set A with 0 < $\pi(A) < 1$. Decompose A^c into its connected components $\{B_i\}$. Then $h^*(A) =$ $h^*(A^c) = h^*(\bigcup_{j: \pi(B_j) > 0} B_j)$, and Lemma 4.3 implies that $h^*(B_{j_0}) \leq h^*(A)$ for at least one index j_0 with $\pi(B_{j_0}) > 0$. But by Lemma 4.5 below, $(B_{j_0})^c$ is connected. This proves (4.7). Analogous arguments work for k.

LEMMA 4.5. Let G be a connected graph, let A be a connected subset of G, and let B be a connected component of A^c . Then B^c is connected.

PROOF. Write $C \equiv A^c \backslash B$, so that $B^c = A \cup C$. To show that B^c is connected, it suffices to show that every $y \in C$ can be connected to some point in A by a path in B^c . Now we know that there exists a path in G from y to A (because G is connected); but this path cannot pass through B before entering A, since B is a connected component of A^c and $y \notin B$. \square

REMARK. The strict inequality in Lemma 4.3(b) implies also that if k(A) = k, then A must be connected (and its complement must be connected if S is connected) except possibly for components of π -measure zero.

5. Random walk with inward drift on a countable rooted graph. In this section we use Theorem 2.1, Corollary 3.2 and Theorem 3.5 to study the L^2 spectrum of a random walk with inward drift on a countable rooted graph. This Markov chain is an abstraction of a Monte Carlo algorithm for the self-avoiding walk proposed by Berretti and Sokal [14]. Our results, together with those of Sokal and Thomas [7], go part way toward analyzing a conjecture made by Berretti and Sokal concerning the autocorrelation time of their Markov chain.

Let $G = (V, E, \mathbf{0})$ be a countable connected rooted graph with vertex set V, edge set E, and a distinguished vertex $\mathbf{0}$, called the root. The level of a vertex x, denoted |x|, is the number of edges in the shortest path which connects x to the root. We write c_N for the number of vertices of level N (N = 0, 1, 2, ...). If x is adjacent to y, then |y| must be either |x|-1, |x| or |x|+1; we call y a parent, sibling or child of x, respectively, and write p(x), s(x) and c(x) for the number of parents, siblings and children of x. Each vertex other than the root must have at least one parent. We remark that G is a tree if and only if each vertex other than the root has precisely one parent and no siblings. Finally, we say that y is a descendant of x (and that x is an ancestor of y), denoted $x \leq y$, if there exists a path of length |y| from y to the root which contains x. Equivalently, y is a descendant of x iff it is either x itself, or a child of x, or a child of a child of x, etc. We denote by V_x the set of all descendants of x, and by $G_x = (V_x, E_x, x)$ the associated rooted graph with x as the root.

We restrict attention to graphs satisfying

$$\sup_{x \to \infty} p(x) \le M_p < \infty,$$

(5.1)
$$\sup_{x} p(x) \leq M_{p} < \infty,$$
(5.2)
$$\sup_{x} c(x) \leq M_{c} < \infty.$$

It follows that

(5.3)
$$\mu \equiv \limsup_{N \to \infty} c_N^{1/N} \le M_c < \infty.$$

We call μ the growth factor of the rooted graph G. We define for $\beta \geq 0$ the generating function

(5.4)
$$Z(\beta) \equiv \sum_{x \in V} \beta^{|x|} = \sum_{N=0}^{x} c_N \beta^N.$$

 $Z(\beta)$ is finite for $0 \le \beta < \mu^{-1}$ and infinite for $\beta > \mu^{-1}$.

We now fix $\beta \geq 0$, and define a continuous-time jump process on V with transition rates

(5.5)
$$J(x,y) = \begin{cases} 1 & \text{if } y \text{ is a parent of } x, \\ \beta & \text{if } y \text{ is a child of } x, \\ 0 & \text{otherwise.} \end{cases}$$

This process is a reversible Markov process with invariant measure

(5.6)
$$\pi(x) = \operatorname{const} \times \beta^{|x|}.$$

 π is finite iff $Z(\beta) < \infty$ (as we assume from now on); in this case we normalize it to be a probability measure

(5.7)
$$\pi(x) = Z(\beta)^{-1} \beta^{|x|}.$$

Finally, we define

(5.8)
$$Z_x(\beta) \equiv \sum_{y \in V_x} \beta^{|y|-|x|} = \beta^{-|x|} Z(\beta) \pi(V_x)$$

[this is the generating function of the rooted graph $G_x = (V_x, E_x, x)$] and

(5.9)
$$R_1 = R_1(\beta) \equiv \sup_{x \neq \mathbf{0}} Z_x(\beta),$$

(5.10)
$$R_2 = R_2(\beta) \equiv \sup_{x \neq 0} \min \left[1, \frac{1 - \pi(V_x)}{\pi(V_x)} \right] Z_x(\beta),$$

(5.11)
$$R_3 = R_3(\beta) \equiv \sup_{x \neq \mathbf{0}} [1 - \pi(V_x)] Z_x(\beta),$$

(5.12)
$$R_4 = R_4(\beta) \equiv \limsup_{|x| \to \infty} Z_x(\beta).$$

Clearly $R_1 \ge R_2 \ge R_3 \ge R_4$ and $R_3 \ge 2R_2$. We can now state our main technical result:

PROPOSITION 5.1. Let $\beta \geq 0$ be such that $Z(\beta) < \infty$. Then, for the process defined by (5.5):

(a) If each vertex other than the root has precisely one parent (e.g., if G is a tree), then $h_{\{0\}^c} = R_1^{-1}$, $h^* = R_2^{-1}$ and $k = R_3^{-1}$.

(b) In general,
$$k \ge h^* \ge h_{\{0\}^c} \ge R_1^{-1}$$
.

PROOF. (a) By deleting all edges between siblings (they play no role anyway), we can assume that G is a tree. First consider $h_{\{0\}^c}$. By Corollary 4.3 (applied to the operator $L^{\{0\}^c}$), we can restrict the infimum to sets $A \subset \{0\}^c$ which are connected. It is not hard to convince oneself that all such sets are of the form $A = V_{x^*} \setminus (\bigcup_i V_{x_i})$ where $x^* \neq 0$, $x^* \leq x_i$ for all i, and the $\{V_{x_i}\}$ are disjoint. Now

(5.13)
$$h(A) = \frac{\sum_{y \in A, z \in A^c} \pi(y) J(y, z)}{\pi(A)},$$

from which it easily follows that

$$(5.14) h(A) \ge h(V_{x^*}) = \pi(V_{x^*})^{-1} Z^{-1} \beta^{|x^*|} = Z_{x^*}^{-1}.$$

Thus $h_{\{0\}^c} = R_1^{-1}$, as claimed.

For h^* and k, we can restrict the infimum to sets A with $0 < \pi(A) < 1$ such that both A and A^c are connected; again, it is easy to see that the only such sets are either V_x or $(V_x)^c$ for some vertex $x \neq 0$. The equalities $h^* = R_2^{-1}$ and $k = R_3^{-1}$ easily follow.

(b) It is a general fact that $2h^* \ge k \ge h^* \ge h_{\{x\}^c}$ for all x [cf. (3.39)]. So we need only show that $h_{\{0\}^c} \ge R_1^{-1}$.

Let $\hat{G} = (V, \hat{E}, \mathbf{0})$ be the rooted spanning tree in G formed by deleting all edges between siblings and deleting all but one (arbitrarily chosen) of the edges from each vertex $x \neq \mathbf{0}$ to its parents. The level numbering of vertices in \hat{G} is easily seen to be the same as that in G. We have (in an obvious notation) $\hat{Z} = Z$, $\hat{\pi} = \pi$, $\hat{V}_x \subset V_x$, $\hat{R}_1 \leq R_1$ and $\hat{h}_{\{\mathbf{0}\}^c} \leq h_{\{\mathbf{0}\}^c}$. Now, by part (a), we know that $\hat{h}_{\{\mathbf{0}\}^c} \geq \hat{R}_1^{-1}$. It therefore follows immediately that $h_{\{\mathbf{0}\}^c} \geq R_1^{-1}$. \square

Proposition 5.1 together with Theorems 2.1 and 3.5 immediately yields a bound on the spectral gap for the operator \tilde{J} :

THEOREM 5.2. Let $\beta \geq 0$ be such that $Z(\beta) < \infty$, and define

$$M \equiv \sup_{x} [p(x) + \beta c(x)].$$

Then, for the process defined by (5.5),

- (a) $\lambda_1(\tilde{J}) \ge \lambda_0((\tilde{J})_{\{0\}^c}) \ge R_1^{-2}/2M$.
- (b) $\lambda_1(\tilde{J}) \ge \max[R_2^{-2}/2M, \kappa R_3^{-2}/8M].$
- (c) If each vertex other than the root has precisely one parent (e.g., if G is a tree), then $\lambda_1(\tilde{J}) \leq R_3^{-1}$.

In particular, if G is a tree, then $\lambda_1(\tilde{J}) > 0$ if and only if $R_3 < \infty$.

It is thus necessary to obtain bounds on R_1, R_2 and R_3 . One case is easy:

PROPOSITION 5.3. If
$$0 \le \beta < M_c^{-1}$$
, then $R_1(\beta) \le (1 - \beta M_c)^{-1} < \infty$.

PROOF. For any $x \in V$,

(5.15)
$$Z_x(\beta) \equiv \sum_{y \in V_x} \beta^{|y| - |x|} \le \sum_{k=0}^x (M_c \beta)^k = (1 - \beta M_c)^{-1} < \infty. \quad \Box$$

It follows that for $\beta < M_c^{-1}$, the process (5.5) has a nonzero L^2 spectral gap and is geometrically ergodic. These facts can alternatively be proven by a Lyapunov-function argument [7]. On the other hand, Proposition 5.3 is, in a very strong sense, the best one can do without further assumptions on the structure of the graph G:

PROPOSITION 5.4. Let $c_0 \equiv 1, c_1, c_2, \ldots$ be any sequence of positive integers satisfying $\lim_{N\to x} c_N = +\infty$ and $\sup_{N\geq 0} (c_{N+1}/c_N) < \infty$, and let M_c be any integer $\geq \sup_{N\geq 0} (c_{N+1}/c_N)$. Then there exists a countable rooted tree $T=(V,E,\mathbf{0})$ such that:

- (a) $\#(\{x\colon |x|=N\})=c_N,$
- (b) $\sup_x c(x) \leq M_c$,

(c)
$$R_1(\beta) = R_4(\beta) = \begin{cases} (1 - \beta M_c)^{-1} & \text{if } 0 \le \beta < M_c^{-1}, \\ +\infty & \text{if } \beta \ge M_c^{-1}. \end{cases}$$

PROOF. We construct a "maximally unbalanced" tree having the given $\{c_N\}$: the root has c_1 children, which are labelled "eldest", "second-eldest", etc.; these children procreate, beginning with the eldest, each one having the maximum allowable number of children (M_c) until c_2 children have been generated; and so on. [In other words, of the c_N vertices at level N, the $\lfloor c_{N+1}/M_c \rfloor$ eldest of these have M_c children each, the one next-eldest has $c_{N+1} - M_c \lfloor c_{N+1}/M_c \rfloor$ children, and the rest have no children. Moreover, if |x| = |y| and x is "elder" to y, then all the children of x are elder to all the children of x.] Now let x_N^* be the eldest vertex of level x, then the tree of descendants of x_N^* contains a complete x-ary rooted tree of x-ary rooted tree of x-ary support x-ary rooted tree of x-ary rooted

(5.16)
$$Z_{x_N^*}(\beta) \ge \sum_{k=0}^{K_N} (M_c \beta)^k.$$

Now $K_N \ge \inf_{k\ge 0} \log c_{N+k}/\log M_c \to +\infty$ as $N\to\infty$. It follows that

(5.17)
$$R_4(\beta) \ge \begin{cases} (1 - \beta M_c)^{-1} & \text{if } 0 \le \beta < M_c^{-1}, \\ +\infty & \text{if } \beta \ge M_c^{-1}. \end{cases}$$

The rest follows from Proposition 5.3. \square

Thus, for $\beta \geq M_c^{-1}$ it is impossible to prove the existence of an L^2 spectral gap (much less lower bounds on it) given only the $\{c_N\}_{N=0}^{\infty}$ and M_c ; it is necessary to have more detailed information about the structure of the graph G. One tractable case is that of a *sub-Cayley* rooted graph:

Rooted graphs $G = (V, E, \mathbf{0})$ and $G' = (V', E', \mathbf{0}')$ are said to be *isomorphic* if there is an isomorphism of (V, E) onto (V', E') which takes $\mathbf{0}$ onto $\mathbf{0}'$. A rooted subgraph of $G = (V, E, \mathbf{0})$ is a rooted graph $G_1 = (V_1, E_1, \mathbf{0})$ where (V_1, E_1) is a subgraph of (V, E) containing $\mathbf{0}$. A connected rooted graph $G = (V, E, \mathbf{0})$ is said to be Cayley (resp. sub-Cayley) if, for each $x \in V$, the rooted graph $G_x = (V_x, E_x, x)$ is isomorphic to G (resp. to a rooted subgraph of G). Some important examples of sub-Cayley rooted graphs (both trees and nontrees) will be given below.

For a sub-Cayley rooted graph we obviously have $Z_x(\beta) \leq Z(\beta)$ for all x, and hence $R_1(\beta) \leq Z(\beta) < \infty$ for all $\beta < \mu^{-1}$. We have thus proven

COROLLARY 5.5. Let G be a sub-Cayley rooted graph, let $\beta \geq 0$ be such that $Z(\beta) < \infty$, and define $M \equiv \sup_x [p(x) + \beta c(x)]$. Then, for the process defined by (5.5), $\lambda_1(\tilde{J}) \geq \lambda_0((\tilde{J})_{\{0\}^c}) \geq Z^{-2}/2M$.

EXAMPLES. 1. Consider the countable rooted tree in which the root has q children, each of these has q children, and so on indefinitely. We call this graph the Cayley rooted tree of order q. For this graph, explicit computation shows that the lower bound in Theorem 5.2 and Corollary 5.5 is sharp in order of magnitude (but not in constants) as $\beta \uparrow q^{-1}$.

- 2. Let V be the set of all nearest-neighbor self-avoiding walks on \mathbf{Z}^d (of arbitrary length) starting at the origin and ending anywhere. We give V the structure of a rooted tree by declaring the zero-step walk to be the root, and declaring ω' to be a child of ω if it is a one-step extension of ω . This is a sub-Cayley rooted tree: every descendant $\tilde{\omega}$ of ω can be written uniquely as $\tilde{\omega} = \omega \circ \omega'$ where $\omega, \omega' \in V$, since every segment of a self-avoiding walk must itself be self-avoiding. However, this is not a Cayley rooted tree, since not every walk of the form $\omega \circ \omega'$ with $\omega, \omega' \in V$ is self-avoiding. The discrete-time analogue of (5.5) [see (5.18) below], with $M = 1 + 2d\beta$, is the transition matrix of a Monte Carlo algorithm for self-avoiding walks first proposed by Berretti and Sokal [14].
- 3. More generally, let $\mathscr A$ be a finite "alphabet" (of cardinality q), and let V^* be the set of all finite words (including the empty word) formed from the "letters" in $\mathscr A$. We give V^* the structure of a rooted tree by declaring the empty word \varnothing to be the root, and declaring ω' to be a child of ω if it is a one-letter extension of ω . Clearly, V^* is the Cayley rooted tree of order q. Now let $F \subset V^* \setminus \{\varnothing\}$ be a set (finite or infinite) of "forbidden phrases", and let V be the set of all words $\omega \in V^*$ which do not contain any element of F as a sub-word. Then V is a rooted subtree of V^* , and it is easily seen that V is sub-Cayley. (This example includes the preceding one as a special case: the alphabet $\mathscr A$ is the set of neighbors of the origin in $\mathscr L$, and the forbidden phrases F are (for example) the walks which return to the origin.)
- 4. Let $G = (V, E, \mathbf{0})$ be an arbitrary connected rooted graph, and define $G^* = (V^*, E^*, \mathbf{0}^*)$ to be the (connected) rooted graph with $V^* = V \times \mathbf{Z}_+$, $E^* = \{\{(x, k), (y, k)\} \colon (x, y) \in E\} \cup \{\{(\mathbf{0}, k), (\mathbf{0}, k+1)\} \colon k \in \mathbf{Z}_+\}$ and $\mathbf{0}^* = (\mathbf{0}, 0)$. Then G^* is sub-Cayley (resp. a tree) whenever G is. An easy computation shows that $Z^*(\beta) = (1 \beta)^{-1}Z(\beta)$. Thus, if $\mu > 1$, then $\mu^* = \mu$ and Z^* has the same singularity at $\beta = \mu^{-1}$ that Z has. Moreover, $Z_x^*(\beta) = Z^*(\beta)$ for all $x = (\mathbf{0}, k)$; hence $R_4^*(\beta) = Z^*(\beta)$. In other words, for any type of singularity which is achievable in a sub-Cayley rooted graph, there exists a sub-Cayley rooted graph with this singularity and with $R_4(\beta) = Z(\beta)$. So the bound $R_1(\beta) \leq Z(\beta)$ for sub-Cayley rooted graphs cannot in general be improved.

We note, however, that Sokal and Thomas [7] have proven a lower bound on $\lambda_0((\tilde{J})_{\{0\}^c})$ and $\lambda_1(\tilde{J})$ for random walk on a sub-Cayley tree, which should in many cases be strictly stronger than that given by Corollary 5.5. (Their proof is based on a detailed analysis of the hitting time to the root.) Assume, for example, that $c_N \sim \mu^N N^{\gamma-1}$ as $N \to \infty$ for some exponent γ . Then the sub-Cayley property implies that the $\{c_N\}$ are submultiplicative and hence that $\gamma \geq 1$. In this case, the lower bound of Sokal and Thomas yields $\lambda_1(\tilde{J}) \geq \lambda_0((\tilde{J})_{\{0\}^c}) \gtrsim (1-\beta\mu)^{1+\gamma}$, while Corollary 5.5 yields only the weaker bound $\lambda_1(\tilde{J}) \geq \lambda_0((\tilde{J})_{\{0\}^c}) \gtrsim (1-\beta\mu)^{2\gamma}$. Thus, if G is a sub-Cayley rooted tree with $\mu > 1$ and $\gamma > 1$, then for the graph G^* the lower bound in Theorem 2.1 does *not* give the optimal order of magnitude. We note that for self-avoiding walks (Example 2) in dimensions d = 2 and 3, it is believed that $c_N \sim \mu^N N^{\gamma-1}$ with $\gamma > 1$ (and it is trivial to see that $\mu \geq d$). However, the authors do not know any examples of sub-Cayley rooted trees for which such a behavior is rigorously proven.

³The symbol \circ denotes concatenation. That is, if $\omega=(\omega_0,\ldots,\omega_M)$ and $\omega'=(\omega_0',\ldots,\omega_N')$ with $\omega_0=\omega_0'=0$, then $\omega\circ\omega'=(\omega_0,\ldots,\omega_M,\omega_M+\omega_1',\ldots,\omega_M+\omega_N')$.

Finally, we remark that our analysis of the continuous-time jump process (5.5) applies almost without change to the discrete-time Markov chain given by

(5.18)
$$P(x,y) = \begin{cases} 1/M & \text{if } y \text{ is a parent of } x, \\ \beta/M & \text{if } y \text{ is a child of } x, \\ (M = [p(x) + \beta c(x)])/M & \text{if } y = x, \\ 0 & \text{otherwise,} \end{cases}$$

where M is any number $\geq \sup_x [p(x) + \beta c(x)]$. This includes, as a special case, the Monte Carlo algorithm of Berretti and Sokal [14].

6. Discussion. In this section we discuss the meaning of our theorems and their relation with results obtained previously by other authors.

Consider first Theorem 3.1. According to the Rayleigh-Ritz principle, $\lambda_0(L)$ is the infimum of the Rayleigh quotient (f, Lf)/(f, f) over all $f \in L^2(\pi)$. On the other hand, h is the infimum of this same Rayleigh quotient over the particular class of functions $f = \chi_A$ (which are a total set in $L^2(\pi)$ but not, of course, a linear subspace). The upper bound in Theorem 3.1 is therefore trivial; the lower bound is the striking statement that the Rayleigh quotient for arbitrary f can be controlled in terms of that for $f = \chi_A$ —the price being that the lower bound involves h squared.

Theorem 2.1 has a similar interpretation: By the Rayleigh-Ritz principle, $\lambda_1(\tilde{J})$ is the infimum of the Rayleigh quotient $(f, \tilde{J}f)/(f, f)$ over all $f \in \mathbf{1}^{\perp}$. On the other hand, k is the infimum of this same Rayleigh quotient over the particular class of functions $f = \chi_A - \pi(A)\mathbf{1}$ (which are a total set in $\mathbf{1}^{\perp}$ but not a linear subspace). The upper bound in Theorem 2.1 is therefore trivial; the lower bound says that the Rayleigh quotient for arbitrary f can be controlled in terms of that for $f = \chi_A - \pi(A)\mathbf{1}$ —the price, again, being that the lower bound involves k squared.

Our argument in §3 follows very closely the original proof of Cheeger [1], adapted to the class of operators we are considering. Our proof of Theorem 3.1 is very close to that of Dodziuk [6, Theorem 2.3]. An alternate proof of a weakened version of Theorem 3.1—namely, $\lambda_0 \geq h^2/(4M+2h)$ —can be given along the lines of Alon [5, Lemma 2.4], using the max-flow-min-cut theorem (we omit the details).⁴ Proposition 3.3 is implicit in both Cheeger [1] and Alon [5]; our proof of the special case (Lemma 3.4) is a direct adaptation of Alon's. Finally, it is known [2] that the constant in Cheeger's original inequality is sharp in both the Dirichlet-boundary and no-boundary cases, so we wonder if the constants in Theorems 3.1 and 3.5 may be sharp as well. It would be interesting to prove this by constructing explicit examples of finite graphs which saturate (or asymptotically saturate) the inequality.

Our argument in §2 is somewhat different from Cheeger's (all integrations are extended over the entire space S), but is clearly inspired by it. (In fact, our proof of Theorem 2.1 was inspired by our initial mis-reading of Cheeger's paper, in which we failed to notice that the integrations were restricted to the subset where f > 0, and we therefore failed to understand why f was taken to be an eigenvector of \tilde{J} rather than an arbitrary vector in $\mathbf{1}^{\perp}$!) It would be interesting to find the optimal

⁴We remark that Alon's bound $\lambda_0 \geq c^2/(4+2c^2)$ is significantly weaker than this one, since his constant c involves the number of vertices in A^c that are adjacent to A, whereas h involves the number of edges that connect A^c to A, which could be much larger.

constant in Proposition 2.2, but we suspect that this will not give the optimal constant in Theorem 2.1.

Our methods do not apply directly to Markovian diffusions, but might be employed indirectly. One strategy would be to apply Theorem 2.1 (or 3.5) to the time-t evolution operator $P_t = e^{-tH}$ and then invoke the spectral mapping theorem to deduce bounds on the spectrum of H. For sets A with smooth boundary, it should be possible to compute $k_t(A)$ for $t \to 0$ in terms of the behavior at the boundary ∂A . For example, for $H = -\Delta$ on a compact Riemannian manifold, we expect that

(6.1)
$$k_t(A) = \frac{\pi^{-1/2}\operatorname{area}(\partial A)}{\pi(A)\pi(A^c)}t^{1/2} + O(t).$$

However, in order to get an analogous formula for k_t it is necessary to control the interchange of $t \to 0$ with the infimum over A, and this seems to be a difficult technical problem. Moreover, this approach, even if it can be carried through, will give suboptimal constants in the final bounds. Probably a better approach is to work directly with the generator H and imitate Cheeger's original argument.

Davies [15–19], in a series of papers on metastability in reversible Markov processes, has proven results which appear to be closely related to the lower bound in Theorem 2.1. His results are stated in the contrapositive form: if (among other hypotheses) the spectral gap λ_1 is small, then there must exist a set A which is "metastable" (in several senses which Davies defines, one of which implies the smallness of k(A)). However, his hypotheses are considerably stronger than just the smallness of λ_1 : he assumes that the remainder of the spectrum of \tilde{J} is far separated from λ_1 . Thus, his results do not appear to contain Theorem 2.1, but rather prove stronger results under stronger hypotheses.

On the other side, a result closely related to the upper bound in Theorem 2.1 (and which in fact strengthens it for a certain class of operators) was proven recently by Alon and Milman [20, Lemma 2.1]. Some related results can be found in [21–23].

Further results on the spectrum of the Laplacian on a finite graph can be found in [24–29, 13]. In particular, Thomas and Zhong Yin [13] use (3.34) to prove a lower bound on λ_1 which is in some cases significantly better (and in other cases significantly worse) than that of Theorems 2.1 and 3.5.

Two papers by Fiedler [30, 31] are also worth mentioning. He considers finite stochastic matrices P, and introduces a quantity which is identical to the numerator of k or h^* . He then obtains a lower bound on λ_1 which closely resembles that of Theorems 2.1 and 3.5, but is a factor $\sim n^2$ worse, where n is the order of the matrix. A subsequent paper by Fiedler and Pták [32] proves, by similar means, bounds on the eigenvalues of P near -1, in terms of an additional quantity which measures how near the matrix is to being periodic of even period. It would be interesting to extend this result to general discrete-time Markov chains, and to spectrum near other points of the unit circle.

Finally, we mention the papers of Pignataro and Sullivan [33] and Dodziuk et al. [34], which prove bounds on the spectrum of the Laplacian for certain hyperbolic surfaces, both compact and noncompact. The hyperbolicity allows them to prove lower bounds which are roughly of the form k rather than k^2 (hence of the same order as the upper bound). We remark that from a probabilistic point of view, the results for noncompact manifolds concern a transient Markov process: a nonzero lower bound on λ_0 shows that the process is " L^2 geometrically transient".

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