L^2 Convergence of Certain Random Walks on Z^d and related Diffusions

One technique for studying the approach to equilibrium of a continuous time Markov process is to consider the restriction to the L^2 space of an invariant distribution. When the process is reversible with respect to this distribution, the generator is a selfadjoint operator. We study the L^2 spectrum of the generator for certain random walks on \mathbb{Z}^d , where the reversible invariant distribution is concentrated near the origin and decays rapidly with distance to the origin. For the related diffusions on \mathbb{R}^d we find that the generators are unitarily equivalent to Schrödinger operators.

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§1 Introduction. One standard approach to continuous time Markov processes is to start with a generator D, construct a transition function $P_t(x, dy)$ which in an appropriate sense satisfies

$$P_t = \exp(tD) \tag{1}$$

and then study the properties of P_t , e.g. invariant measures. For certain physical systems it is more natural to start from a probability measure μ and develop processes which leave μ invariant. Of particular interest are generators which satisfy the detailed balance condition with respect to μ . In terms of μ and P_t this yields the relation

$$\mu(dx)P_t(x,dy) = \mu(dy)P_t(y,dx)$$
(2)

which is the condition of time reversibility for the Markov process with initial distribution μ and transition function P_t .

The assumption of time reversibility introduces additional techniques for the study of the process. The aspect we consider here is convergence in the L^2 sense. When μ and P_t satisfy (2), P_t gives rise to a selfadjoint contraction semigroup in $L^2(\mu)$. The generator D acts as a negative semi-definite selfadjoint operator in $L^2(\mu)$ with eigenvalue zero corresponding to the invariant distribution. If the spectrum of D is otherwise bounded away from zero, then convergence to equilibrium is exponentially fast in $L^2(\mu)$. Such convergence has been shown for a special dynamic spin system having distinct phases and is conjectured for dynamic two-dimensional Ising models in the two phase region (see [4], [5]).

Here we use the spectral approach to study the convergence of some simple random walk models. The original motivation is in the work of Buffet-Pulé-de Smedt on a boson system coupled to a heat bath [1]. Arising in their studies was a Markov process on the positive reals for which an estimate of the rate of convergence was desired. In [6] we gave estimates of convergence for processes of this type and related Markov chains on the positive integers. In the present work we extend the analysis to certain random walks on Z^d and lock briefly at the diffusion limit which yields Schrödinger operators.

§2 Formulation. The L^2 approach is applicable to rather general continuous time Markov processes. We shall formulate here in terms of a countable discrete state space Ω and later specialize to Z^d . To each $x \in \Omega$ we associate a finite subset of Ω denoted ∂x called the neighbours of x. We require that

$$y \in \partial x \iff x \in \partial y.$$

For Z^d we define

$$\partial x = \{ z \pm \mathbf{e}_i : i = 1 \cdots d \}$$
(3)

where $\{e_i\}$ are the standard unit vectors.

We assume that we are given a strictly positive probability distribution π on Ω . We shall construct the generator D from a matrix Q which satisfies the reversibility condition

$$\pi(x)Q(x,y)=\pi(y)Q(y,x)$$

whenever $y \in \partial x$. We define

$$q(x) = \sum_{y \in \partial x} Q(x, y)$$
(4)

and for the real valued function f equal to zero except on a finite subset of Ω

$$(Qf)(x) = \sum_{y \in \partial x} Q(x, y)$$
(5)

$$(Df)(x) = (Qf)(x) - q(x)f(x).$$
 (6)

D is densely defined and dissipative

$$(Dj,f)_{\pi} \leq (j,f)_{\pi}$$

2.

Theorem 1. Let π be a strictly positive probability distribution on Z. If

in
$$\ell^2(\pi)$$
 where

 $(f,g)_{\pi} = \sum f(x)g(x)\pi(x).$

We now introduce some particular generators in terms of Q_i , i = 0, 1, 2, 3. We need only define $Q_i(x, y)$ for $y \in \partial x$ and take q_i , Q_i and D_i as above:

$$Q_0(x, y) = \pi(y) / [\pi(x) + \pi(y)]$$

$$Q_1(x, y) = \min\{1, \pi(y) / \pi(x)\}$$

$$Q_2(x, y) = \sqrt{\pi(y) / \pi(x)}$$

$$Q_3(x, y) = \max\{1, \pi(y) / \pi(x)\}$$

All of these are reversible for π and we have

$$(D_{i+1}f,f)_{\pi} \le (D_if,f)_{\pi}$$
 (7)

for i = 0, 1, 2.

Proposition 1. The closure of D_2 is the generator of a positive contraction semigroup in $\ell^1(\pi)$ provided that the cardinality of ∂x is uniformly bounded for $x \in \Omega$.

Conclusions about the spectral properties of D presume that the closure of D is the generator of a positive contraction semigroup on $\ell^1(\pi)$. When ∂x is uniformly bounded, this obtains for D_0 and D_1 as bounded operators and for D_2 by Proposition 1. Related methods can prove that this property holds for D_3 in the case of π of the form in Theorem 2.

When the closure of D is the generator of a positive contraction semigroup on $\ell^1(\pi)$, the associated P_t is a Feller semigroup which extends to ℓ^p , $1 \le p \le \infty$. The action of the generator in $\ell^2(\pi)$, which we also denote by D, is a negative semidefinite selfadjoint operator. We use the following notation:

$$\lambda_1(D) = \inf_{\lambda \in \mathcal{L}^2} \{\lambda \in \ell^2(\pi) \text{ spectrum of } -D\}$$

 $\lambda_{\infty}(D) = \inf_{\lambda>0} \{ \text{the } [0,\lambda] \text{ spectral projection of } -D \text{ is infinite dimensional} \}$

The value of λ_1 is significant because it determines the rate of exponential convergence to equilibrium in $\ell^2(\pi)$. In [6] we give direct estimates for λ_1 , but for $Z^d, d > 1$, the methods seem more suited for estimating λ_{∞} . We note that if $\lambda_{\infty} > 0$, then $\lambda_1 > 0$. From (7) we hav.

3.

$$\lambda_j(D_i) \le \lambda_j(D_{i+1}) \tag{8}$$

for $j = 1, \infty, i = 0, 1, 2$.

For Z^1 we have the following

$$\limsup_{n \to \infty} \sum_{n}^{\infty} \pi(x)/\pi(n) < \infty$$
$$\limsup_{n \to \infty} \sum_{n}^{\infty} \pi(-x)/\pi(-n) < \infty$$

then we have $\lambda_{\infty}(D_i) > 0$, i = 0, 1, 2, 3. Conversely, if either limit superior is infinite, then $\lambda_{\infty}(D_i) = 0$, i = 0, 1, 2.

In general the condition is not sufficient for $\lambda_{\infty}(D_3) = 0$, but this is the case for π of the type in Theorem 2.

For D > 1, the results are for a specific family of examples. We consider probability distributions on Z^d of the form

$$\pi(x) = K \exp -c|x|^{\alpha}$$

$$c, \alpha > 0 \quad |x| = \sqrt{x_1^2 + \dots + x_d^2}$$

with K the normalizing constant.

Theorem 2. For π as given above we have

$$0 < \alpha < 1 \Longrightarrow \lambda_{\infty}(D_i) = 0, \ i = 0, 1, 2, 3$$

$$\alpha = 1 \Longrightarrow 0 < \lambda_{\infty}(D_i) < \infty, \ i = 0, 1, 2, 3$$
(10)

 $\alpha > 1 \Longrightarrow 0 < \lambda_{\infty}(D_i) < \infty, \ i = 0, 1 \tag{11}$

$$\alpha > 1 \Longrightarrow \lambda_{\infty}(D_i) = \infty, \ i = 2,3 \tag{12}$$

§3 The Diffusion Limit. Before proving the above results we shall take an elementary look at the diffusion limit of operators like those above. The limiting diffusion operators on $L^2(\mathbb{R}^d, \pi dx)$ when symmetrized to $L^2(\mathbb{R}^d)$ take the form

 $\Delta - V$

with Δ denoting the Laplace operator and V a multiplicative operator. Thus, apart from irrelevant constants, the limiting operators are Schrödinger operators (see [3]).

We shall consider limits of operators based on D_2 . The reader may verify that D_1 and D_3 lead to these same limiting operators, while D_0 yields half these limits. Let $\pi : \mathbb{R}^d \longrightarrow \mathbb{R}$ be a strictly positive twice continuously differentiable function such that

$$\sum \pi(x/n) < \infty$$

for each positive integer n, with the sum over $x \in Z^d$. Define

$$e(x) \equiv -\frac{1}{2}\log \pi(x)$$

The generator $_nD$ is defined by the matrix $_nQ$, where

$$\partial x = \{ x \pm \mathbf{e_j}/n : j = 1 \cdots d \}$$

 ${}_nQ(x, y) = n^2 \sqrt{\pi(y)/\pi(x)}$

Proposition 2. Let $f: \mathbb{R}^d \longrightarrow \mathbb{R}$ be twice continuously differentiable. Then

$$\lim_{n \to \infty} {}_{n} D f = \Delta f - 2\nabla e \cdot \nabla f$$
(13)

pointwise. This operator acting on $f \in L^2(\mathbb{R}^d, \pi dx)$ is formally unitarily equivalent to

$$\Delta g - (|\nabla e|^2 - \Delta e) g \tag{14}$$

acting on $g \in L^2(\mathbb{R}^d)$.

Proof. To get (13), expand f to second order in a Taylor series and take limits. The mapping taking $f \in L^2(\mathbb{R}^d, \pi dx)$ to $g \in L^2(\mathbb{R}^d)$ is given by

$$g(x) = f(x) \sqrt{\pi(x)}. \tag{15}$$

Expression (14) follows from a straightforward calculation.

Thus we obtain Schrödinger operators which can be expressed with V of the form

$$V = |\nabla e|^2 - \Delta e.$$

For example, $e(x) = |x|^2$ corresponds to the harmonic oscillator potential. The following shows that quite a broad class of Schrödinger operators can be expressed in this way.

Proposition 3. Let the Schrödinger operator $-\Delta + V$ possess a strictly positive twice continuously differentiable eigenfunction ψ :

$$-\Delta \psi + V\psi = \lambda \psi$$

for the real constant λ . Then V can be expressed in the form

$$V = \lambda + |\nabla e|^2 - \Delta e$$

with $e = -\log \psi$. Proof. Calculation

5.

§4 Remaining proofs. For Proposition 1: If $\sharp \partial x$ is uniformly bounded in $x \in \Omega$, then Q_2 acts as a bounded linear operator in $\ell^2(\pi)$. Multiplication by -q is the generator of a contraction semigroup in $\ell^2(\pi)$. By Theorem 13.2.1 of Hille-Phillips [2], the closure of D_2 generates a contraction semigroup in $\ell^2(\pi)$. Then for $\lambda > 0$ and any $f \in \ell^2(\pi)$ there exists $g \in \ell^2(\pi)$ with

$$(\lambda - D_2)g = f$$

Now $\ell^2(\pi) \subset \ell^1(\pi)$ and is dense. We verify that the above holds in $\ell^1(\pi)$ and the result follows from the Hille-Yosida Theorem.

Proof of Theorem 1. If we have for all $n \ge 0$ and some $\alpha > 0$

$$\sum_{n=1}^{\infty} \frac{\pi(x)}{\pi(n)} \leq \frac{1}{\alpha}, \ \sum_{n=1}^{\infty} \frac{\pi(-x)}{\pi(-n)} \leq \frac{1}{\alpha},$$

an adaptation of the proof of Theorem 1 of [6] shows that

$$\lambda_1(D_3) \ge \alpha^2/4$$

$$\lambda_1(D_2) \ge \sqrt{\alpha/(1-\alpha)}\alpha^2/4$$

$$\lambda_1(D_1) \ge [\alpha/(1-\alpha)]\alpha^2/4$$

$$\lambda_1(D_0) \ge \alpha \cdot \alpha^2/4.$$

As the null space of D is one dimensional

 $\lambda_{\infty} > \lambda_1 > 0$

in each case

For the case where one of the inferior limits is infinite— for definiteness we assume

$$\liminf_{n \to \infty} \pi(n) / \sum_{n}^{\infty} \pi(x) = 0, \qquad (16)$$

consider the functions

$$f_n(x) = 0 \text{ for } x_1 < n, = 1 \text{ for } x_1 \ge n$$
 (17)

As d = 1, $x_1 = x$, but the above definition will be used again below. We have

$$(-D_2 f_n, f_n)_{\pi}/(f_n, f_n)_{\pi} = \sqrt{\pi(n-1)\pi(n)} / \sum_{n=1}^{\infty} \pi(x)$$

It is not difficult to deduce from (16) and the above that

$$\liminf_{n\to\infty}(-D_2f_n,f_n)_{\pi}/(f_n,f_n)_{\pi}=0,$$

so $\lambda_{\infty}(D_2) = 0$ by Lemma 1 below. The result for D_0 and D_1 follows from (8). Lemma 1. If there exists a constant a and a sequence of functions $\{f_n\} \in \ell^2(\pi)$ such that

$$f_n(x) = 0 \text{ for } |x| < n$$

$$\liminf_{n \to \infty} (-Df_n, f_n)_{\pi} / (f_n, f_n)_{\pi} \leq a \qquad (18)$$

then $\lambda_{\infty} \leq a$.

Proof. If $b < \lambda_{\infty}$, then the [0, b] spectral projection of -D is finite dimensional, so the contribution of this part of the spectrum to (18) goes to zero as $n \to \infty$, hence $b \leq a$.

Lemma 2. If there exists a constant a and a positive function o such that with $Q(x,y) = Q(x,y)\sqrt{\pi(x)\rho(y)/(\rho(x)\pi(y))}$

$$f(x,y) = Q(x,y)\sqrt{\pi(x)\rho(y)}/{(\rho(x)\pi(y))}$$

 $s(x) = \sum_{y \in \partial x} Q(x,y)$

we have that

 $\liminf_{|x|\to\infty} q(x) - s(x) \geq a,$

then $\lambda_{\infty} \geq a$.

Proof. Assume that for all $|x| \ge n$

$$q(x)-s(x)\geq b.$$

For f such that f(x) = 0 for |v| < n and $\{x : f(x) \neq 0\}$ is finite, with $g(x) = \sqrt{\pi(x)/\rho(x)}f(x)$ we have

$$(f, f)_{\pi} = (g, g)_{\rho}$$

$$(-Df, f)_{\pi} = ([g - s]f, f)_{\pi} + (sg, g)_{\rho} + (-Qg, g)_{\rho}.$$

By an adaptation of Lemma 1 of [6], the last two terms together are nonnegative so

$$(-Df, f)_{\pi} \geq b(f, f)_{\pi}.$$

This inequality extends to all f in the $\ell^2(\pi)$ domain of D which satisfy f(x) = 0 for |x| < n, which implies $\lambda_{\infty} \ge b$.

Proof of Theorem 2. For $0 < \alpha < 1$, if we apply D_3 to f_n given by (17) for n > 0

$$(-D_3 f_n, f_n)_{\pi}/(f_n, f_n)_{\pi} \leq \pi \{x_1 = n\}/\pi \{x_1 \geq n\}$$

For fixed integer k we hav.

$$\lim_{k \to \infty} \pi \{ x_1 = n \} / \pi \{ x_1 = n + k \} = 1.$$

Then

$$\lim_{n \to \infty} (-D_3 f_n, f_n)_{\pi} / (f_n, f_n)_{\pi} = 0$$

and Lemma 1 together with (8) gives conclusion (9).

For D_2 and $\alpha \ge 1$ we employ Lemma 2 with $\rho(x) \equiv 1$. for this case we have

$$-s(x) + q(x) = -2d + \sum_{i=1}^{3} [\pi(x + \mathbf{e}_i)^{\frac{1}{2}} + \pi(x - \mathbf{e}_i)^{\frac{1}{2}}]/\pi(x)^{\frac{1}{3}}$$
(19)

For $\alpha > 1$ the right hand side of (19) approaches $+\infty$ as $|x| \to \infty$. Hence we have (12). For $\alpha = 1$ the right hand side of (19) can for large |x| be approximated arbitrarily closely by a sum of d terms of the form r + 1/r - 2with at least one value of r satisfying $r \leq \exp[-c/(2d^{\frac{1}{2}})]$. Also for $\alpha = 1$,

 $Q_2 \leq \cosh(c/2) Q_0 ,$

so we have conclusion (10).

Now we consider D_1 for $\alpha > 1$ and take

$$\rho(x) = \exp[-c|x|^{\alpha} + 2\beta|x|]$$

with $\beta > 0$ constant. Then q(x) - s(x) can be represented as the sum of 2d terms of the following two types. With $y = x \pm e_i$ for |y| < |x| the term is of the form $1 - \exp \beta [|y| - |x|]$, while for |y| > |x| the term is of the form

$$\left(\exp c[|x|^{\alpha} - |y|^{\alpha}]\right)\left(1 - \exp \beta[|x| - |y|]\right) \tag{20}$$

It is not difficult to deduce that terms of the form (20) go to zero as $|x| \to \infty$ so that

$$\liminf_{|x|\to\infty} q(x) - s(x) \ge 1 - \exp(-\beta/d^{\frac{1}{2}}).$$

Since $\beta > 0$ is arbitrary, $\lambda_{\infty}(D_1) \ge 1$. Also $2Q_0 \ge Q_1$ and both D_1 and D_0 are bounded so we have (11).

Concluding remarks. The random walks on Z^d we considered showed the following behavior. If the reversible invariant distribution π decays as $|x| \to \infty$ at a rate less than exponential, then 0 is an accumulation point of the spectrum of the generator. If the rate of decay is exponential or greater, then 0 is an isolated point of the spectrum.

We have given a very elementary approach to the diffusion limit. With a bit more effort it is possible to relate the spectral properties of the limit to those of the discrete approximations. For this to be useful we need better estimates on the spectra of the discrete models. Since Schrödinger operators have received such considerable study, it might be more useful to be able to make assertions about the spectra of the discrete models based on the properties of the diffusion limit.

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