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Heat diffusion on graphs

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City University of New York, 1994

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Heat Diffusion on Graphs

by

Debe Bednarchak

A dissertation submitted to the Graduate Faculty in Mathematics in partial fulfillment of the requirements for the degree of Doctor of Philosophy, The City University of New York.

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THE CITY UNIVERSITY OF NEW YORK

Abstract

Heat Diffusion on Graphs

by

Debe Bednarchak

Advisor: Professor Edgar Feldman

We derive the heat kernel for integer lattices and for regular trees, and use it to investigate the evolution of heat distribution on sets of various geometries, with particular attention to the movement over time of the locus of maximum temperature.

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Contents

Chapter 1

Background

1.1 The Heat Kernel for Riemannian Manifolds

We briefly review the heat kernel for Riemannian manifolds [3]. Let M be a connected Riemannian manifold with Laplace-Beltrami operator Δ. M is viewed as a homogeneous isotropic medium. We begin, at time $t = 0$, with a temperature distribution concentrated at a point y in M, with total temperature 1, and ask for the temperature at x in M at time t. The equation that describes the conduction of heat through M is the heat equation $\Delta = \frac{\partial}{\partial t}$. That is, the temperature at x at time t will be given by a continuous function $p(x, y, t)$ that is C^2 in the space variable x, C^1 in the time variable t, and satisfies

$$\begin{aligned} \Delta_x p(x,y,t) &= \frac{\partial}{\partial t} p(x,y,t) \\ \lim_{t \to 0} p(x,y,t) &= \delta_y(x) \end{aligned}$$

where δ_y is the Dirac delta function. The function $p(x, y, t)$ is called the *heat kernel* of M. If the initial temperature distribution is given by $\phi(y)$ then the solution of the heat equation

$$\Delta u(x,t) = \frac{\partial}{\partial t} u(x,t)$$

will be given by

$$u(x,t) = \int_M p(x,y,t)\phi(y)\, dV(y)$$

satisfying

$$\phi(x) = \lim_{t \to 0} \int_M p(x,y,t)\phi(y) dV(y).$$

To derive the heat equation, we observe that given a regular domain Ω in M, and assuming that for $t > 0$ heat is neither supplied to nor withdrawn from Ω, the instantaneous change in total temperature in Ω, with respect to time, must equal the flow of heat across the boundary of Ω. That is,

$$\iint_\Omega \frac{\partial u}{\partial t}(x,t)\, dV(x) = \int_{\partial\Omega} \frac{\partial u}{\partial \nu}(w,t)\, dA(w)$$

where ν is the outward unit normal vector field on $\partial\Omega$. Applying Green's formula, we have

$$\iint_\Omega \frac{\partial u}{\partial t} u(x,t)\, dV(x) = \iint_\Omega \Delta u(x,t)\, dV(x)$$

or

$$\iint_\Omega (\Delta - \frac{\partial}{\partial t}) u(x,t) dV(x) = 0$$

for all such domains Ω.

For compact manifolds, the existence of the heat kernel follows from a construction of Minakshisundaram and Pleijel, and the uniqueness from an application of Green's formulas ([3], Chapter VI). For noncompact manifolds, we want the minimal positive solution to the heat equation. It is constructed as follows ([7], [3], Chapter VIII): Choose a sequence $\Omega_1, \Omega_2, \ldots$ of regular domains in M, with smooth boundaries, such that

$$\begin{aligned} \overline{\Omega}_j &\subseteq \Omega_{j+1} \\ \bigcup_{j=1}^{\infty} \Omega_j &= M. \end{aligned}$$

For each j, let q_j be the heat kernel on Ω_j with *Dirichlet* boundary condition, i.e.:

$$\begin{aligned} q_j : \overline{\Omega}_j \times \overline{\Omega}_j &\times [0,\infty) \to R \\ \Delta q_j(x,y,t) &= \frac{\partial}{\partial t} q_j(x,y,t) \\ q_j(x,y,t) &= 0 \text{ if } x \text{ or } y \in \partial\Omega_j. \end{aligned}$$

We can regard $q_j(x,y,t)$ as a function on $M \times M \times [0,\infty)$ by defining it to be zero if either x or y is outside Ω_j. By the maximum principle, $\{q_j\}$ is an increasing sequence, and we define

$$p(x,y,t) = \lim_{j\to\infty} q_j(x,y,t).$$

It can be shown that $p(x,y,t)$ is a fundamental solution of the heat equation on M and is minimal in the sense that $p(x,y,t) \leq q(x,y,t)$ for any other positive fundamental solution q.

In both cases, the heat kernel is positive, finite, and symmetric in the space variables. For compact manifolds, and for M noncompact but complete with Ricci curvature bounded below, the heat kernel satisfies the conservation of heat property

$$\int_M p(x,y,t)dV(y) = 1.$$

For arbitrary noncompact M we have

$$\int_M p(x,y,t)dV(y) \leq 1.$$

On R^n, a fundamental solution of the heat equation is

$$p(x,y,t) = (4\pi t)^{-n/2} e^{\frac{-|x-y|^2}{4t}}.$$

Note that the heat kernel is a function only of t and the *distance* between x and y. Furthermore, p decreases as the distance between x and y increases. For hyperbolic spaces the heat kernel also depends only on t and the distance between x and y, and for each $t > 0$, decreases as the distance increases ([3], Chapters VI,X,XI).

1.2 Hot Spots in Riemannian Manifolds

The starting point for our work is the paper "Movement of Hot Spots in Riemannian Manifolds" by Isaac Chavel and Leon Karp [5]. In this section, we present those theorems and proofs that we will refer to in later sections.

As in Section 1.1, for a Riemannian manifold M, let $p(x,y,t)$ be the minimal positive heat kernel. Then, for any smooth, non-negative function

ϕ with compact support in M,

$$P_t\phi(x) = \int_M p(x,y,t)\phi(y)dV(y)$$

is the minimal positive solution to the heat equation satisfying

$$\lim_{t\to 0} P_t\phi = \phi.$$

The "hot spots" are the points in the set

$$H(t;\phi) = \{x : P_t\phi(x) = \max_y P_t\phi(y)\}.$$

We are interested in the behavior of $H(t;\phi)$ as $t \to \infty$.

For $M = R^n$,

$$P_t\phi(x) = \int_{R^n} (4\pi t)^{-n/2} e^{\frac{-|x-y|^2}{4t}} \phi(y)d(y).$$

Let S_ϕ denote the support of ϕ, and C_ϕ the closed convex hull of S_ϕ. We recall that the center of mass of ϕ is the point m_ϕ such that

$$\int_{R^n} (m_\phi - y)\phi(y)dy = 0.$$

Theorem 1 *(Chavel, Karp) For each $t > 0$, the function $P_t\phi$ has a maximum value, and it can only be attained at points of C_ϕ, i.e.,*

$$H(t;\phi) \subseteq C_\phi. \tag{1.1}$$

Furthermore,

$$H(t;\phi) \to \{m_\phi\} \quad \text{as} \quad t \to \infty. \tag{1.2}$$

Proof: For each $x \in R^n \setminus C_\phi$, there is a unique point $p_x \in \partial C_\phi$ for which $d(x, C_\phi) = |x - p_x|$. For any y in the interior of S_ϕ, the function

$$\xi \mapsto |\xi - y|$$

decreases as ξ moves from x to p_x along the line segment $\overline{xp_x}$. Since the heat kernel increases as the distance between x and y decreases, $P_t\phi$ increases as ξ moves from x to p_x along $\overline{xp_x}$. This implies (1.1).

For (1.2), note that we have

$$(\nabla P_t\phi)(x) = -(4\pi t)^{-n/2} \int \frac{(x-y)}{2t} e^{\frac{-|x-y|^2}{4t}} \phi(y)dy.$$

This implies that for every maximum point h_t of $P_t\phi$,

$$\int (h_t - y) e^{\frac{-|h_t-y|^2}{4t}} \phi(y)dy = 0.$$

Let (t_k) be a sequence converging to $+\infty$ as $k \to \infty$. Since all the points h_{t_k} are in the compact set C_ϕ, (h_{t_k}) possesses a subsequence (h_{t_l}) which converges to some point $h_\infty \in C_\phi$. Consequently

$$\int (h_\infty - y)\phi(y)dy = 0,$$

i.e., $h_\infty = m_\phi$. Therefore, the sequence (h_{t_k}) converges to m_ϕ. Since the sequence (h_{t_k}) is arbitrary, we have (1.2). ▮

From another point of view, one might ask to what extent does the asymptotic behavior of $P_t\phi$ determine the initial data ϕ. In particular, if for two domains Ω_1, Ω_2, $P_t 1_{\Omega_1}$ agrees with $P_t 1_{\Omega_2}$ on an open set up to order $t^{-\frac{n}{2}+1}$ as $t \to \infty$, must $\Omega_1 = \Omega_2$? We will discuss this question in Section 2.2. Chavel and Karp prove the following "Hot Potato Kugel Theorem":

Theorem 2 *(Chavel, Karp) Given a relatively compact open set (resp., a solid) Ω and an n-disk B in R^n, suppose that the limit*

$$L(x) = \lim_{t\to\infty} t^{\frac{n}{2}+1} P_t(1_\Omega - 1_B)(x)$$

exists and is identically equal to 0 for x in some open set U contained in the interior of $R^n \setminus (B \cup \Omega)$. Then $\Omega = B$ up to a set of measure 0 (resp. $\Omega = \overline{B}$).

Proof:

$$\begin{aligned}
&(4\pi)^{\frac{n}{2}} t^{\frac{n}{2}+1} P_t(1_\Omega - 1_B)(x) \\
&= t\int_{R^n} e^{\frac{-|x-y|^2}{4t}} (1_\Omega - 1_B)(y)dy \\
&= t\sum_{k=0}^{\infty} \frac{(-4t)^{-k}}{k!} \int_{R^n} |x-y|^{2k}(1_\Omega - 1_B)(y)dy \\
&= t\int_{R^n} (1_\Omega - 1_B)(y)dy - \frac{1}{4}\int_{R^n} |x-y|^2(1_\Omega - 1_B)(y)dy + O(t^{-2}).
\end{aligned}$$

The existence of the limit implies $Vol(\Omega) = Vol(B)$ and therefore

$$\int \{|x|^2 - 2\langle x, y\rangle + |y|^2\}(1_\Omega - 1_B)(y)dy = 0$$

on U. Differentiating with respect to x we have

$$\int y(1_\Omega - 1_B)(y)dy = 0$$

so Ω and B have the same center of mass. This implies

$$\int |y|^2(1_\Omega - 1_B)(y)dy = 0$$

which implies $\Omega = B$ up to a set of measure zero. ∎

The terminology is derived from the Potato Kugel Theorem of [1], a result about the uniqueness of gravitational potentials. Consider the question: Given two solids Ω_1, Ω_2 in R^3 whose gravitational potentials

$$Pot_\Omega(x) = \int_\Omega \frac{1}{|x-y|}dy$$

agree on some open subset of the unbounded component of $R^3 \setminus (\Omega_1 \cup \Omega_2)$, must $\Omega_1 = \Omega_2$? It is shown in [1] (see also [13]) that the answer is yes if one of the solids is a 3–disk in R^3, but no for arbitrary solids.

Chavel and Karp also investigate the movement of hot spots in H^n, the n-dimensional hyperbolic space. The solution to the heat equation with initial data ϕ is

$$P_t\phi(x) = \int_{H^n} p(x,y,t)\phi(y)dV(y),$$

where $p(x,y,t)$ is the heat kernel of H^n. $p(x,y,t)$ depends only on t and the distance between x and y so we have

$$p(x,y,t) = P(d(x,y),t).$$

It is known that for each $t > 0$, $P(d(x,y),t)$ decreases as d increases.

Theorem 3 *(Chavel, Karp) In H^n, for any $\phi \geq 0$, $H(t;\phi) \subseteq C_\phi$ for all $t > 0$.*

Proof: For any $x \in H^n \backslash C_\phi$, there is a unique $p_x \in \partial C_\phi$ for which $d(x, C_\phi) = d(x, p_x)$. Let γ_x be the geodesic connecting x to p_x. Using the first variation of arc length formula it can be shown that for any $y \in C_\phi, d(\xi, y)$ decreases as ξ moves along γ_x from x to p_x. Consequently, $P_t\phi(\xi)$ increases. ∎

Chavel and Karp also prove that in H^n hot spots do not necessarily tend to one fixed point in C_ϕ. If S_ϕ is sufficiently small then there is a single point h_∞ such that $H(t,\phi) \to \{h_\infty\}$, but if S_ϕ is large enough then there may be more than one hot spot.

1.3 The Combinatorial Laplacian

The analogue for graphs of the Laplace-Beltrami operator on manifolds is the combinatorial Laplacian. Combinatorial Laplacians have been studied by many authors (see [6], [8], [9], [11], [10], [4]). Many properties of the Laplace-Beltrami operator on manifolds have analogues in the discrete case including the maximum principle, the Harnack inequality, and Cheeger's theorem bounding the lowest eigenvalue. In this section we present definitions and collect those properties that we will need.

A *graph* G consists of a set V of *vertices* and a set E of unordered pairs of elements of V. For $x, y \in V$ we say there is an *edge* joining x and y if $(x,y) \in E$. G is an *infinite* graph if V is an infinite set. A *path* from x to y is a sequence $x_0, x_1, \ldots, x_n$ of elements of V with $x_0 = x, x_n = y$ and $(x_i, x_{i+1}) \in E$ for $i = 0, \ldots, n-1$. The *length* of this path is n. G

is *connected* if for all $x, y \in V$ there is a path from x to y. G is *simple* if E contains no elements of the form (x, x) and if there is at most one edge joining any pair of distinct vertices. The *degree* $m(x)$ of a vertex x is the number of edges with x as an endpoint. A graph is *q-regular* if $m(x) = q$ for all $x \in V$.

If $(x, y) \in E$ we say x and y are *neighbors*. For a fixed $x \in V$, $\sum_{y \sim x}$ will mean the sum over those vertices y that are neighbors of x. We will sometimes want to consider *directed* edges. $[x, y]$ will denote the directed edge from x to y. E^* will denote the set of all directed edges, so if $(x, y) \in E$ then both $[x, y]$ and $[y, x]$ are in E^*.

Let G be a simple, infinite, connected graph. We define the following Hilbert spaces as in [11]:

$$L_0^2 = \{f : V \to R \mid \sum_{x \in V} m(x) f^2(x) < \infty\}$$

and

$$L_1^2 = \{\phi : E^* \to R \quad \mid \quad \phi([x, y]) = -\phi([y, x]) \quad \forall\, [x, y] \in E^*, \\ \sum_{(x,y) \in E} \phi^2([x, y]) < \infty\}$$

The sum in the definition of L_1^2 is independent of the choice of direction for each edge. The inner product in L_0^2 is defined by

$$(f, g) = \sum_{x \in V} m(x) f(x) g(x)$$

and the inner product in L_1^2 by

$$(\phi, \psi) = \frac{1}{2} \sum_{[x,y] \in E^*} \phi([x,y])\psi([x,y]).$$

Consider next the linear operator $d : L_0^2 \to L_1^2$ defined by

$$df([x,y]) = f(y) - f(x).$$

We note that d is bounded since

$$\begin{aligned}
(df, df) &= \sum_{(x,y) \in E} (f(y) - f(x))^2 \\
&\leq 2 \sum_{(x,y) \in E} (f^2(y) + f^2(x)) \\
&= 2(f, f).
\end{aligned}$$

The adjoint of d is the linear operator $\delta : L_1^2 \to L_0^2$ defined by

$$(f, \delta\phi) = (df, \phi)$$

for all $f \in L_0^2$ and $\phi \in L_1^2$, where the inner product on the left side is in L_0^2 and on the right side in L_1^2.

We can calculate $\delta\phi$ as follows:

$$\begin{aligned}
(df, \phi) &= \frac{1}{2} \sum_{[x,y] \in E^*} df([x,y])\phi([x,y]) \\
&= \frac{1}{2} \sum_{[x,y] \in E^*} (f(y) - f(x))\phi([x,y]) \\
&= \sum_{x \in V} \sum_{y \sim x} f(x)\phi([y,x])
\end{aligned}$$

$$\begin{aligned} &= \sum_{x\in V} m(x)f(x)\cdot \frac{1}{m(x)}\sum_{y\sim x}\phi([y,x]) \\ &= (f,\delta\phi). \end{aligned}$$

So

$$\delta\phi(x) = \frac{1}{m(x)}\sum_{y\sim x}\phi([y,x]).$$

The Laplace operator $\Delta : L_0^2 \to L_0^2$ is defined by

$$\Delta = -\delta d.$$

That is,

$$\begin{aligned} \Delta f(x) &= -\delta(df)(x) \\ &= -\frac{1}{m(x)}\sum_{y\sim x} df([y,x]) \\ &= \frac{1}{m(x)}\sum_{y\sim x}(f(y)-f(x)) \\ &= \frac{1}{m(x)}\sum_{y\sim x} f(y) - f(x). \end{aligned}$$

A *domain* D in G is a subset of V along with whatever edges were present in G. The boundary of D is the set of edges with one endpoint in D and one endpoint not in D, i.e. the edges joining D to its complement in G. We have the following Green's formulas:

Lemma 1 *For* $f,g \in L_0^2$, $(g,\Delta f) = -(dg, df)$.

Proof:

$$\begin{aligned}
-(dg,df) &= -\frac{1}{2}\sum_{[x,y]\in E^*}(g(y)-g(x))(f(y)-f(x)) \\
&= \frac{1}{2}\sum_{[x,y]\in E^*}(g(y)f(x)+g(x)f(y)-g(y)f(y)-g(x)f(x)) \\
&= \sum_{x\in V} g(x)\sum_{y\sim x} f(y) \;-\sum_{x\in V} m(x)g(x)f(x) \\
&= \sum_{x\in V} m(x)g(x)\cdot\left(\frac{1}{m(x)}\sum_{y\sim x} f(y)-f(x)\right) \\
&= (g,\Delta f). \quad \blacksquare
\end{aligned}$$

Corollary 1 *For* $f\in L_0^2$, $\quad \sum_{x\in V} m(x)\Delta f(x)=0$

Proof: Apply Lemma 1 with $g=1_V$. $\blacksquare$

Lemma 2 *If* $f,g\in L_0^2$ *and* g *has finite support* D *then*

$$(g,\Delta f)+(dg,df)_D=\sum_{x\in D} g(x)\left(\sum_{\substack{y\sim x\\ y\notin D}}(f(y)-f(x))\right)$$

where $(dg,df)_D$ *means we sum over those edges with both endpoints in* D.

Note that the sum on the right side is an 'integral' over the boundary.

Proof: We split (dg,df) into a sum over edges entirely in D plus sums over edges with at least one endpoint not in D.

$$\begin{aligned}
(dg,df)=(dg,df)_D \;&+\; \sum_{x\in D}\sum_{\substack{y\sim x\\ y\notin D}}(g(y)-g(x))(f(y)-f(x)) \\
&+\; \sum_{x\notin D}\sum_{\substack{y\sim x\\ y\notin D}}(g(y)-g(x))(f(y)-f(x))
\end{aligned}$$

Since support $g = D$, we have

$$\begin{aligned}(dg, df) &= (dg, df)_D \\ &+ \sum_{x \in D} \sum_{\substack{y \sim x \\ y \notin D}} (-g(x))(f(y) - f(x))\end{aligned}$$

or

$$(g, \Delta f) + (dg, df)_D = \sum_{x \in D} \sum_{\substack{y \sim x \\ y \notin D}} g(x)(f(y) - f(x)). \quad \blacksquare$$

1.4 The Heat Kernel for Graphs

Let G be a simple, infinite, connected graph with Laplace operator Δ. To derive the heat equation, we view G as a uniform conductor of heat and observe, as in the Riemannian manifold setting, that the total change in temperature, with respect to time, in a domain $D \subset G$ must be equal to the flow of heat across the boundary (assuming, for $t > 0$, that heat is neither supplied to nor withdrawn from D). Letting $u(x, t)$ be the temperature at vertex x at time t, we have

$$\sum_{x \in D} m(x) \frac{\partial}{\partial t} u(x, t) = \sum_{x \in D} \sum_{\substack{y \sim x \\ y \notin D}} (u(y, t) - u(x, t)).$$

Applying Lemma 2 to the right side, with $f = u(\, , t)$ and g the characteristic function of D, we have

$$\begin{aligned}\sum_{x \in D} m(x) \frac{\partial}{\partial t} u(x, t) &= \sum_{x \in D} \sum_{\substack{y \sim x \\ y \notin D}} (u(y, t) - u(x, t)) \\ &= \sum_{x \in D} g(x) \sum_{\substack{y \sim x \\ y \notin D}} (u(y, t) - u(x, t))\end{aligned}$$

$$
\begin{aligned}
&= (g, \Delta u(\ ,t)) + (dg, du)_D \\
&= (g, \Delta u(\ ,t)) \\
&= \sum_{x \in D} m(x) \Delta u(x,t)
\end{aligned}
$$

i.e., $\Delta u(x,t) = \frac{\partial}{\partial t} u(x,t)$.

The heat kernel, $p(x,y,t)$, is the solution to the heat equation with initial condition one unit of heat concentrated at $y \in G$:

$$
\begin{aligned}
p : G \times G \times [0,\infty) &\rightarrow R \\
\Delta_x p(x,y,t) &= \frac{\partial}{\partial t} p(x,y,t) \\
\lim_{t \to 0} \sum_{x \in G} m(x) p(x,y,t) f(x) &= f(y) \quad \forall f \ \in L_0^2.
\end{aligned}
$$

For an initial temperature distribution $\phi(y)$, the solution to the heat equation is

$$
u(x,t) = \sum_{y \in G} m(y) p(x,y,t) \phi(y).
$$

Theorem 4 *For a simple, infinite, connected graph G,*

$$
\begin{aligned}
&i) \quad \sum_{x \in G} m(x) p(x,y,t) = 1 \qquad \forall t \\
&ii) \quad \sum_{x \in G} m(x) u(x,t) = \sum_{x \in G} m(x) \phi(x).
\end{aligned}
$$

Proof: i)

$$
\begin{aligned}
\sum_{x \in G} m(x) p(x,y,0) &= \sum_{x \in G} m(x) p(x,y,0) \delta_y(x) \\
&= \delta_y(y) = 1
\end{aligned}
$$

and

$$\begin{aligned}\frac{\partial}{\partial t}\sum_{x\in G} m(x)p(x,y,t) &= \sum_{x\in G} m(x)\frac{\partial}{\partial t}p(x,y,t)\\ &= \sum_{x\in G} m(x)\Delta_x p(x,y,t)\\ &= 0 \quad \text{by Corollary 1.}\end{aligned}$$

So $\sum_{x\in G} m(x)p(x,y,t) = \text{constant} = 1$.

ii)

$$\begin{aligned}\frac{\partial}{\partial t}\sum_{x\in G} m(x)u(x,t) &= \sum_{x\in G} m(x)\frac{\partial}{\partial t}u(x,t)\\ &= \sum_{x\in G} m(x)\Delta u(x,t)\\ &= 0.\end{aligned}$$

Therefore,

$$\begin{aligned}\sum_{x\in G} m(x)u(x,t) &= \sum_{x\in G} m(x)u(x,0)\\ &= \sum_{x\in G}\left(m(x)\left(\sum_{y\in G} m(y)p(x,y,0)\phi(y)\right)\right)\\ &= \sum_{x\in G} m(x)\phi(x). \quad \blacksquare\end{aligned}$$

Chapter 2

$\mathbf{Z^n}$

2.1 The Heat Kernel for $\mathbf{Z^n}$

In this section, we extend the results of "Movements of Hot Spots in Riemannian Manifolds" to Z^n.

Let G be the graph whose vertices are the points in the integer lattice Z^n, and whose edges join a vertex $(x_1, x_2, \ldots, x_n)$ to its $2n$ neighbors

$$\{(x_1, x_2, \ldots, x_i + 1, \ldots, x_n), (x_1, x_2, \ldots, x_i - 1, \ldots, x_n)\}, i = 1, \ldots, n.$$

G is obviously simple, infinite, and connected. Let ϕ be a positive real valued function defined on a finite subset of Z^n. We will solve the heat equation $\Delta u(x,t) = \frac{\partial}{\partial t} u(x,t)$, with initial data ϕ, by taking the Fourier transform of each side with respect to the space variable, solving the resulting differential equation, and then applying the inverse transform.

Our goal is to find $u : Z^n \times [0,\infty) \to R$ such that

$$\begin{aligned} \Delta u(x,t) &= \frac{\partial}{\partial t}u(x,t) \\ \lim_{t\to 0} u(x,t) &= \phi(x). \end{aligned} \tag{2.1}$$

The Fourier transform of u is

$$\hat{u}(\zeta,t) = \sum_{x\in Z^n} u(x,t)e^{i(x\cdot\zeta)} \qquad \zeta \in R^n.$$

The Fourier transform of Δu is

$$\begin{aligned}
&\widehat{\Delta u}(\zeta,t) \\
&= \sum_{x\in Z^n} \Delta u(x,t)\, e^{i(x\cdot\zeta)} \\
&= \sum_{x\in Z^n} \left\{ \frac{1}{2n}\sum_{i=1}^{n}(u(x_1,\ldots,x_i+1,\ldots,x_n,t) + u(x_1,\ldots,x_i-1,\ldots,x_n,t))e^{i(x\cdot\zeta)} \right. \\
&\qquad \left. - u(x_1,\ldots,x_n,t)\, e^{i(x\cdot\zeta)} \right\} \\
&= \sum_{x\in Z^n} u(x,t) \left\{ \frac{1}{2n}\left(e^{i(x_1+1)\zeta_1} + e^{i(x_1-1)\zeta_1} + \cdots + e^{i(x_n-1)\zeta_n} + e^{i(x_n-1)\zeta_n}\right) - e^{i(x\cdot\zeta)} \right\} \\
&= \sum_{x\in Z^n} u(x,t)e^{i(x\cdot\zeta)} \left\{ \frac{1}{2n}\left(e^{i\zeta_1} + e^{-i\zeta_1} + \cdots + e^{i\zeta_n} + e^{-i\zeta_n}\right) - 1 \right\} \\
&= \sum_{x\in Z^n} u(x,t)e^{i(x\cdot\zeta)} \left\{ \frac{1}{n}(\cos\zeta_1 + \cdots + \cos\zeta_n) - 1 \right\} \\
&= \hat{u}(\zeta,t) \left\{ \frac{1}{n}(\cos\zeta_1 + \cdots + \cos\zeta_n) - 1 \right\}.
\end{aligned}$$

So (2.1) becomes

$$\left\{ \frac{1}{n}(\cos\zeta_1 + \cdots + \cos\zeta_n) - 1 \right\} \hat{u}(\zeta,t) = \frac{\partial}{\partial t}\hat{u}(\zeta,t).$$

A solution is

$$\hat{u}(\zeta,t) = e^{t(\frac{1}{n}(\cos\zeta_1+\cdots+\cos\zeta_n)-1)}\hat{u}(\zeta,0)$$

or since $\hat{u}(\zeta,0) = \hat{\phi}(\zeta)$,

$$\hat{u}(\zeta,t) = e^{t(\frac{1}{n}(\cos\zeta_1+\cdots+\cos\zeta_n)-1)}\ \hat{\phi}(\zeta)$$

which we will write as

$$\hat{u}(\zeta,t) = e^{-t}e^{\frac{t}{n}C(\zeta)}\hat{\phi}(\zeta).$$

To recover u, we apply the inverse transform

$$\begin{aligned} u(x,t) &= (2\pi)^{-n}\int_{R^n} e^{-t}e^{\frac{t}{n}C(\zeta)}\hat{\phi}(\zeta)\, e^{-i(x\cdot\zeta)}d\zeta \\ &= e^{-t}(2\pi)^{-n}\int_{R^n} e^{\frac{t}{n}C(\zeta)}\sum_{y\in Z^n}\phi(y)e^{i(y\cdot\zeta)}e^{-i(x\cdot\zeta)}d\zeta \\ &= e^{-t}(2\pi)^{-n}\sum_{y\in Z^n}\phi(y)\int_{R^n} e^{\frac{t}{n}C(\zeta)}e^{i(y\cdot\zeta)}e^{-i(x\cdot\zeta)}d\zeta. \end{aligned}$$

For a point source at y,

$$\begin{aligned} u(x,t) &= e^{-t}(2\pi)^{-n}\int_{R^n} e^{\frac{t}{n}C(\zeta)}e^{i(y\cdot\zeta)}e^{-i(x\cdot\zeta)}d\zeta \\ &= e^{-t}(2\pi)^{-n}\int_{R^n} e^{t\cdot\frac{1}{n}\cos\zeta_1}e^{-i(x_1-y_1)\zeta_1}\ldots e^{t\cdot\frac{1}{n}\cos\zeta_n}e^{-i(x_n-y_n)\zeta_n}d\zeta. \end{aligned}$$

Making the substitution $\zeta_j = \theta_j + \frac{\pi}{2}$ we have

$$\begin{aligned} &\frac{1}{2\pi}\int_R e^{\frac{t}{n}\cos\zeta_j}e^{-i(x_j-y_j)\zeta_j}d\zeta_j \\ &= \frac{1}{2\pi}\int_R e^{-i(x_j-y_j)\frac{\pi}{2}}e^{\frac{-t}{n}\sin\theta_j}e^{-i(x_j-y_j)\theta_j}d\theta_j \end{aligned}$$

$$= e^{-i(x_j-y_j)\frac{\pi}{2}} J_{(x_j-y_j)}(it/n)$$

where J_r is the Bessel function of order r. So we have

$$u(x,t) = e^{-t}(e^{-i(x_1-y_1)\frac{\pi}{2}} \dots e^{-i(x_n-y_n)\frac{\pi}{2}}) J_{(x_1-y_1)}(it/n) \dots J_{(x_n-y_n)}(it/n).$$

Since $e^{-ir\frac{\pi}{2}} J_r(it/n) = I_r(t/n)$, the modified Bessel function, we have, writing $p(x,y,t)$ instead of $u(x,t)$ to emphasize the point source,

$$p(x,y,t) = e^{-t} I_{(x_1-y_1)}(t/n) \cdots I_{(x_n-y_n)}(t/n).$$

Theorem 5 *$p(x,y,t)$ is a solution of the heat equation on Z^n.*

Proof: We may assume the point source is at the origin. Then

$$\begin{aligned}
&\Delta_x p(x,0,t) \\
&= \Delta_x \{e^{-t} I_{x_1}(t/n) \cdots I_{x_n}(t/n)\} \\
&= e^{-t} \frac{1}{2n} \sum_{z \sim x} I_{z_1}(t/n) \cdots I_{z_n}(t/n) - e^{-t} I_{x_1}(t/n) \cdots I_{x_n}(t/n) \\
&= e^{-t} \frac{1}{2n} \sum_{i=1}^{n} \{I_{x_1}(t/n) \cdots I_{x_i+1}(t/n) \cdots I_{x_n}(t/n) \\
&\qquad + I_{x_1}(t/n) \cdots I_{x_i-1}(t/n) \cdots I_{x_n}(t/n)\} \\
&\quad - e^{-t} I_{x_1}(t/n) \cdots I_{x_n}(t/n)
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial}{\partial t} p(x,0,t) &= \frac{\partial}{\partial t} \{e^{-t} I_{x_1}(t/n) \cdots I_{x_n}(t/n)\} \\
&= e^{-t} \sum_{i=1}^{n} \left\{ I_{x_1}(t/n) \cdots \left(\frac{I_{x_i+1}(t/n) + I_{x_i-1}(t/n)}{2n} \right) \cdots I_{x_n}(t/n) \right\}
\end{aligned}$$

$$
\begin{aligned}
&-e^{-t}I_{x_1}(t/n)\cdots I_{x_n}(t/n)\\
=\;&\Delta_x p(x,0,t). \quad \blacksquare
\end{aligned}
$$

A path from x to y in Z^n is a sequence of points $x = x_0, x_1, \ldots, x_r = y$, where x_i and x_{i+1} are neighbors. The length of this path is r. The distance between x and y, $d(x,y)$, is the smallest integer r for which there exists a path of length r from x to y. For $x = (x_1, x_2, \ldots, x_n)$ and $y = (y_1, y_2, \ldots, y_n)$, we have

$$d(x,y) = \sum_{j=1}^{n} |y_j - x_j|.$$

A path from x to y is *minimal* if its length is $d(x,y)$.

Theorem 6 *i) $p(x,y,t)$ is symmetric in the space variables.*

ii) $p(x,y,t)$ decreases as the distance between x and y increases.

iii) $p(x,y,t)$ satisfies the conservation of heat property:

$$\sum_x p(x,y,t) = 1 \quad \text{for all t.}$$

Proof: All three assertions follow from well-established facts about modified Bessel functions.

i) is equivalent to $I_k(s) = I_{-k}(s)$ if k is an integer.

For (ii), let γ be a minimal path from y to x. Let z and q be neighbors on γ with $d(z,y) > d(q,y)$. Since z and q are neighbors, they differ in only one coordinate, say the j^{th}. We have

$$
\begin{aligned}
p(z,y,t) &= e^{-t}I_{|y_1-z_1|}(t/n)\cdots I_{|y_j-z_j|}(t/n)\cdots I_{|y_n-z_n|}(t/n)\\
&= e^{-t}I_{|y_1-q_1|}(t/n)\cdots I_{|y_j-q_j|+1}(t/n).\cdots I_{|y_n-q_n|}(t/n)
\end{aligned}
$$

$$
\begin{aligned}
&< e^{-t} I_{|y_1-q_1|}(t/n)\cdots I_{|y_j-q_j|}(t/n).\cdots I_{|y_n-q_n|}(t/n) \\
&= p(q,y,t)
\end{aligned}
$$

since $I_k(s)$ is decreasing as a function of k.

For (iii), we may assume the point source is at the origin. Then

$$
\begin{aligned}
\sum_x p(x,0,t) &= e^{-t}\sum_x I_{x_1}(t/n)\cdots I_{x_n}(t/n) \\
&= e^{-t}\sum_{j=-\infty}^{\infty} I_j(t/n)\cdots\sum_{j=-\infty}^{\infty} I_j(t/n) \\
&= e^{-t}\cdot e^{t/n}\cdots e^{t/n} \\
&= 1
\end{aligned}
$$

since $\sum_{j=-\infty}^{\infty} I_j(s) = e^s$. ∎

For initial data ϕ the solution to the heat equation is

$$
\begin{aligned}
u(x,t) &= e^{-t}\sum_{y\in Z^n}\phi(y)p(x,y,t) \\
&= e^{-t}\sum_{y\in Z^n}\phi(y)I_{|y_1-x_1|}(t/n)\cdots I_{|y_n-x_n|}(t/n).
\end{aligned}
$$

We will often write $P_t\phi(x)$ instead of $u(x,t)$.

2.2 Hot Spots in Z^n

In this section we investigate the movement of hot spots in Z^n. We begin with a description of convex sets.

We recall from the previous section that a path from x to y in Z^n is a sequence of points $x = x_0, x_1, \ldots, x_r = y$, where x_i and x_{i+1} are neighbors.

The length of this path is r. The distance between x and y, $d(x,y)$, is the smallest integer r for which there exists a path of length r from x to y. For $x = (x_1, \ldots, x_n)$ and $y = (y_1, \ldots, y_n)$, we have

$$d(x,y) = \sum_{j=1}^{n} |y_j - x_j|.$$

A path from x to y is *minimal* if its length is $d(x,y)$. Minimal paths are not necessarily unique. We will use the following definition of convexity:

Definition: A set $C \subset Z^n$ is convex if for all $x, y \in C$, C contains all minimal paths in Z^n from x to y.
This is analogous to strong convexity for domains in Riemannian manifolds.

By an interval in Z^1 we mean a subset of the form $\{x \in Z^1 : a \leq x \leq b\}$, which we will denote $[a,b]$. A rectangular solid in Z^n is the Cartesian product of intervals

$$[a_1, b_1] \times \cdots \times [a_n, b_n].$$

It is possible that one or more of these intervals consists of only one point.

Proposition 1 *i) A convex set C in Z^1 is an interval.*
ii) A convex set C in Z^n in a rectangular solid.

Proof: i) If $x, y \in C$ then all points z, $x < z < y$, must be also.

ii) Suppose $x = (x_1, \ldots, x_n)$ and $y = (y_1, \ldots, y_n)$ are in C. Then C must contain all paths from x to y of length $d(x,y)$. Therefore, C must contain all points of the form $(z, x_2, \cdots, x_n)$ where z increases (or decreases) one unit at a time from x_1 to y_1. Similarly for the other coordinates. So C must contain all points in $[x_1, y_1] \times \cdots \times [x_n, y_n]$. ∎

Definition: The convex hull C_B of a set $B \subset Z^n$ is the smallest convex set containing B; that is, if C is any convex set containing B then $C_B \subset C$.

Definition: The distance, $d(x, C)$, between a set $C \subset Z^n$ and a point $x \notin C$ is the smallest integer r for which there exists a path of length r from x to some y in C.

Proposition 2 *If C is a convex set in Z^n and $x \in Z^n \setminus C$, then there is a unique point $\overline{y} \in C$ such that $d(x, C) = d(x, \overline{y})$.*

Proof: In Z^1, convex sets are intervals and $\overline{y}$ is the endpoint of C closer to x.

In $Z^n, n \geq 2$, suppose there were two distinct points $y, z \in C$ with $d(x, C) = d(x, y) = d(x, z)$. For convenience suppose $x = (0, \ldots, 0)$. Since $y \neq z$, some $y_i \neq z_i$; say $|y_i| < |z_i|$. Consider the following path from z to y: start at $(z_1, \ldots, z_n)$, decrease (or increase) the i^{th} coordinate until we reach $(z_1, \ldots, y_i, \ldots, z_n)$, then take any minimal path to $(y_1, \ldots, y_n)$. The length of this path is

$$|z_i - y_i| + \sum_{j=1, j \neq i}^{n} |z_j - y_j| = d(y, z)$$

so $(z_1, \ldots, y_i, \ldots, z_n)$ is in C. But the distance from x to this point is

$$|y_i| + \sum_{j \neq i} |z_j| \quad < \quad \sum_{j=1}^{n} |z_j| = d(x, C)$$

which is a contradiction. ∎

Proposition 3 *Given C, x, and $\overline{y}$ as in Proposition 2, for any $y \in C$,*

$$d(x, y) = d(x, \overline{y}) + d(\overline{y}, y).$$

Proof: Assume x is the origin. C is a product of intervals $[a_1, b_1] \times \cdots \times [a_n, b_n]$. Suppose first that no interval contains 0. Then, by taking reflections if necessary, we may assume all $a_i,\ b_i > 0$. In this case, $\overline{y} = (a_1, \ldots, a_n)$ and

$$d(0, \overline{y}) + d(\overline{y}, y) = \sum_i a_i + \sum_i (y_i - a_i) = \sum_i y_i = d(0, y).$$

Now suppose one interval, say the j^{th}, contains 0. Again by taking reflections if necessary we may assume $a_i, b_i > 0, i \neq j$. In this case $\overline{y} = (a_1, \ldots, 0, \ldots, a_n)$ with the 0 in the j^{th} place. Then

$$\begin{aligned} d(0, \overline{y}) + d(\overline{y}, y) &= \sum_{i \neq j} a_i + \sum_{i \neq j} (y_i - a_i) + |y_j| \\ &= \sum_{i \neq j} y_i + |y_j| \\ &= d(0, y). \end{aligned}$$

The proof can easily be modified if more than one interval contains 0. ∎

Next we discuss the center of mass of a function. We recall for ϕ defined on a domain $B \subset R^n$, $\phi \geq 0$, the center of mass m of ϕ is the point in R^n for which

$$\int_{R^n} (m - y)\phi(y) dy = 0.$$

For Z^1, we make the following definition:

Definition: For a function ϕ defined on a domain $B \subset Z^1, \phi \geq 0$, the center of mass m of ϕ is

$$\left\langle \frac{\sum_{k \in B} k\phi(k)}{\sum_{k \in B} \phi(k)} \right\rangle,$$

where $\langle r \rangle$ means the integer nearest to r; if $\frac{\sum_{k\in B} k\phi(k)}{\sum_{k\in B}\phi(k)}$ is exactly halfway between two integers then m is the set

$$\left\{ \frac{\sum_{k\in B} k\phi(k)}{\sum_{k\in B}\phi(k)} - \frac{1}{2}, \frac{\sum_{k\in B} k\phi(k)}{\sum_{k\in B}\phi(k)} + \frac{1}{2} \right\}.$$

For convenience, let $\langle r \rangle^*$, for $r \in R$, denote the integer nearest to r, if this is well defined, or $\{r - \frac{1}{2}, r + \frac{1}{2}\}$ otherwise.

In comparison with the R^n definition we note that m minimizes

$$\left| \sum_{k\in B} (n-k)\phi(k) \right|$$

for n in Z. To see this, write $|\sum_{k\in B}(n-k)\phi(k)|$ as

$$\left| n \sum_{k\in B} \phi(k) - \sum_{k\in B} k\phi(k) \right|.$$

If n were real, i.e., not necessarily in Z, then the minimum would occur at $n = \frac{\sum_{k\in B} k\phi(k)}{\sum_{k\in B}\phi(k)}$; if we require n in Z, the minimum occurs at $\left\langle \frac{\sum_{k\in B} k\phi(k)}{\sum_{k\in B}\phi(k)} \right\rangle^*$.

Proposition 4 *Let ϕ be a function with finite support $S \subset Z^1$ and let C_S be the convex hull of S. Then the center of mass m of ϕ is in C_S.*

Proof: For $k \in C_S \setminus S$, define $\phi(k) = 0$. C_S is an interval $[a, b]$. If m is one point then

$$m = \left\langle \frac{\sum_{k\in C} k\phi(k)}{\sum_{k\in C}\phi(k)} \right\rangle \leq \left\langle \frac{\sum_{k\in C} b\phi(k)}{\sum_{k\in C}\phi(k)} \right\rangle = b.$$

Similarly, $m \geq a$.

If

$$m = \left\{ \frac{\sum_{k\in C} k\phi(k)}{\sum_{k\in C} \phi(k)} - \frac{1}{2}, \frac{\sum_{k\in C} k\phi(k)}{\sum_{k\in C} \phi(k)} + \frac{1}{2} \right\},$$

then $\frac{\sum_{k\in C} k\phi(k)}{\sum_{k\in C} \phi(k)} + \frac{1}{2}$ must be $\leq b$. Suppose not, i.e., suppose

$$\frac{\sum_{k\in C} k\phi(k)}{\sum_{k\in C} \phi(k)} + \frac{1}{2} \geq b + 1.$$

Then

$$\sum_{k\in C} k\phi(k) \geq \sum_{k\in C} (b + \frac{1}{2})\phi(k),$$

but $k \leq b$ for all k in C.

Similarly, $\frac{\sum_{k\in C} k\phi(k)}{\sum_{k\in C} \phi(k)} - \frac{1}{2} \geq a$. ∎

In Z^n we define the center of mass coordinate by coordinate:

Definition: For a function ϕ defined on a domain $B \subset Z^n$, let

$$m_i = \left\langle \frac{\sum_{x\in B} x_i\phi(x_1, \ldots, x_n)}{\sum_{x\in B} \phi(x_1, \ldots, x_n)} \right\rangle^* .$$

The center of mass m of ϕ is $m_1 \times \cdots \times m_n$.

Note that each m_i is either one integer or a set containing two integers; therefore, the center of mass of ϕ is either one point or a set containing at most 2^n points.

Example: Let $B = [0,3] \times [0,2] \subset Z^2$ and $\phi = 1_B$. Then

$$\begin{aligned} m_1 &= \left\langle \frac{\sum_{x\in B} x_1\phi(x_1,x_2)}{\sum_{x\in B}\phi(x_1,x_2)} \right\rangle^* = \left\langle \frac{18}{12} \right\rangle^* = \{1,2\} \\ m_2 &= \left\langle \frac{\sum_{x\in B} x_2\phi(x_1,x_2)}{\sum_{x\in B}\phi(x_1,x_2)} \right\rangle^* = \left\langle \frac{12}{12} \right\rangle^* = 1, \end{aligned}$$

and the center of mass of ϕ is the set $\{1,2\} \times \{1\}$ or $\{(1,1), (2,1)\}$.

Proposition 5 *Let ϕ be a function defined on a finite set $S \subset Z^n$ and let C_S be the convex hull of S. Then the center of mass m of ϕ is in C_S.*

Proof: For $x \in C_S \setminus S$, define $\phi(x) = 0$.

C_S is a product of intervals $[a_1, b_1] \times \cdots \times [a_n, b_n]$. By Proposition 4, m_i is in $[a_i, b_i]$ for each i, therefore m is in C. ∎

For a function $\phi \geq 0$ with finite support $S \subset Z^n$, the solution to the heat equation with initial data ϕ is

$$P_t\phi(x) = e^{-t} \sum_{y\in Z^n} \phi(y) I_{|y_1-x_1|}(t/n) \cdots I_{|y_n-x_n|}(t/n).$$

Let $H(t;\phi) = \{x \in Z^n : P_t\phi(x) = \max_{z\in Z^n} P_t\phi(z)\}$.

Theorem 7 *$H(t;\phi) \subseteq C_S$ for all t.*

Proof: By Proposition 2, for any $x \in Z^n \setminus C_S$, there is a unique $\overline{y} \in C_S$ such that $d(x,\overline{y}) = d(x, C_S)$.

Let γ be a minimal path from x to $\overline{y}$. For any $z \in \gamma$, $d(z,C) = d(z,\overline{y})$ and by Proposition 3 for any $y \in C$, $d(z,y) = d(z,\overline{y}) + d(\overline{y},y)$. Therefore, $d(z,y)$ decreases as z moves along γ from x to $\overline{y}$. Therefore, by Theorem 6, $p(z,y,t)$ increases as z moves along γ from x to $\overline{y}$. ∎

Theorem 8 *For large $t, H(t;\phi) = m$, the center of mass of ϕ.*

Proof: Suppose first that m is one point.

We may assume that m is the origin.

We then want to show $P_t\phi(0) > P_t\phi(x)$ for large t, for all x.

For large t,

$$I_r(t) \sim (2\pi t)^{-1/2}e^t\left\{1 - \frac{4r^2-1}{8t} + O(t^{-2})\right\}.$$

Therefore,

$$\begin{aligned} P_t\phi(0) &= e^{-t}\sum_y \phi(y)I_{y_1}(t/n)\cdots I_{y_n}(t/n) \\ &\sim e^{-t}(2\pi t/n)^{-n/2}(e^{t/n})^n\sum_y\left(\phi(y)\left\{1-\frac{4y_1^2-1}{8t/n}+O(t^{-2})\right\}\cdot\right. \\ &\quad \cdot\ \left.\cdots\left\{1-\frac{4y_n^2-1}{8t/n}+O(t^{-2})\right\}\right). \end{aligned}$$

Multiplying out we have

$$(2\pi t/n)^{n/2}P_t\phi(0) \sim \sum_y \phi(y)\ \left\{1-\frac{4y_1^2-1}{8t/n} - \cdots - \frac{4y_n^2-1}{8t/n} + O(t^{-2})\right\}.$$

Similarly,

$$\begin{aligned} &(2\pi t/n)^{n/2}P_t\phi(x) \\ &\sim \sum_y \phi(y)\left\{1-\frac{4(y_1-x_1)^2-1}{8t/n} - \cdots - \frac{4(y_n-x_n)^2-1}{8t/n} + O(t^{-2})\right\}. \end{aligned}$$

Subtracting we have

$$\begin{aligned}
&(2\pi t/n)^{n/2}(P_t\phi(0) - P_t(x)) \\
&\sim \sum_y \phi(y)\left\{\frac{4(y_1-x_1)^2-4y_1^2}{8t/n}+\cdots+\frac{4(y_n-x_n)^2-4y_n^2}{8t/n}+O(t^{-2})\right\} \\
&= \sum_y \phi(y)\frac{4}{8t/n}\left\{x_1^2-2x_1y_1+\cdots+x_n^2-2x_ny_n\right\}+O(t^{-2}) \\
&= \frac{1}{t/n}\left\{\frac{x_1^2}{2}\sum_y\phi(y)-x_1\sum_y y_1\phi(y)\right\} \\
&\quad +\cdots+\frac{1}{t/n}\left\{\frac{x_n^2}{2}\sum_y\phi(y)\ -x_n\sum_y y_n\phi(y)\right\}+O(t^{-2}).
\end{aligned}$$

Assuming the center of mass is the origin means $m_i = 0$ for each i; i.e.,

$$\left\langle \frac{\sum_y y_i\phi(y)}{\sum_y \phi(y)} \right\rangle = 0 \quad \text{for each } i$$

or

$$-\frac{1}{2} < \frac{\sum_y y_i\phi(y)}{\sum_y \phi(y)} < \frac{1}{2}.$$

So

$$-\frac{1}{2}\sum_y \phi(y) < \sum_y y_i\phi(y) < \frac{1}{2}\sum_y \phi(y) \quad \text{for each } i.$$

If $0 < \sum_y y_i\phi(y) < \frac{1}{2}\sum_y \phi(y)$, then

$$\begin{aligned}
\frac{x_i^2}{2}\sum_y\phi(y)-x_i\sum_y y_i\phi(y) &> x_i^2\sum_y y_i\phi(y)-x_i\sum_y y_i\phi(y) \\
&= (x_i^2-x_i)\sum_y y_i\phi(y) \\
&\geq 0
\end{aligned}$$

If $-\frac{1}{2}\sum_y \phi(y) < \sum_y y_i\phi(y) < 0$, then

$$\begin{aligned}\frac{x_i^2}{2}\sum_y \phi(y) - x_i\sum_y y_i\phi(y) &> -x_i^2\sum_y y_i\phi(y) - x_i\sum_y y_i\phi(y)\\ &= (x_i^2 + x_i)(-\sum_y y_i\phi(y))\\ &\geq 0.\end{aligned}$$

If $\sum_y y_i\phi(y) = 0$, then

$$\begin{aligned}&\frac{x_i^2}{2}\sum_y \phi(y) - x_i\sum_y y_i\phi(y)\\ &= \frac{x_i^2}{2}\sum_y \phi(y)\\ &\geq 0.\end{aligned}$$

Since some x_i must be nonzero we conclude $P_t\phi(0) > P_t\phi(x)$.

Suppose now that the center of mass is not one point; i.e., some m_i consists of two points.

We may assume $m_i = \{0, 1\}$; i.e.,

$$\frac{\sum_y y_i\phi(y)}{\sum_y \phi(y)} = \frac{1}{2}$$

or

$$\sum_y y_i\phi(y) = \frac{1}{2}\sum_y \phi(y). \tag{2.2}$$

The center of mass consists of two points: the origin and the point e_i whose i^{th} coordinate is 1 with zeros everywhere else. First we show $P_t\phi(0) -$

$P_t\phi(e_i) \sim 0$ for large t.

$$\begin{aligned} P_t\phi(0) - P_t\phi(e_i) &\sim \sum_y \phi(y)\left\{\frac{4(y_i-1)^2}{8t/n} - \frac{4y_i^2}{8t/n}\right\} \\ &= \frac{1}{2t/n}\sum_y \phi(y)(1-2y_i) \\ &= \frac{1}{2t/n}\left\{\sum_y \phi(y) - 2\sum_y y_i\phi(y)\right\} \\ &= 0 \text{ by } (2.2). \end{aligned}$$

Then

$$\frac{x_i^2}{2}\sum_y \phi(y) - x_i\sum_y y_i\phi(y) = (x_i^2 - x_i)\sum_y y_i\phi(y) > 0$$

for $x_i \neq 0$, 1. ∎

Next we prove an analogue in Z^n of Chavel and Karp's "hot potato kugel" theorem and extend the results of "Hot Spots" for R^n by answering a question posed by Chavel and Karp: Is Theorem 2 true for Ω_1, Ω_2 one of which is only assumed to be convex?

Using the usual graph metric in Z^n, i.e., counting edges, the disk with center c and radius r is

$$B(c;r) = \{x : d(x,c) \leq r\} = \{x : \sum_{j=1}^{n} |x_j - c_j| \leq r\}.$$

The Z^n analogue of the R^n theorem is, however, not true for disks as we will show by example below. We must consider instead disks in Z^n defined using the Euclidean metric. The *Euclidean-disk* with center c and radius r is the set

$$\tilde{B}(c;r) = \{x : \sum_{j=1}^{n} |x_j - c_j|^2 \leq r^2\}.$$

The Euclidean-disk of radius r contains the disk of radius r since

$$\sum_{j=1}^{n} |x_j - c_j| \leq r$$

implies

$$\sum_{j=1}^{n} |x_j - c_j|^2 \leq \left(\sum_{j=0}^{n} |x_j - c_j| \right)^2 \leq r^2.$$

We want to emphasize that in Z^n, disks and Euclidean disks are *not* convex. This leads one to believe that in R^n the real issue is not convexity.

We will also need to define *open* sets in Z^n. A set U contained in Z^n is open if some x in U has $2n$ neighbors also in U. The idea is to be able to take a spatial derivative in every direction from at least one point.

Theorem 9 *Let $\tilde{B} = \tilde{B}(c; r)$ be an Euclidean disk in Z^n and Ω a finite set. Suppose*

$$\lim_{t \to \infty} (t/n)^{\frac{n}{2}+1} (P_t 1_\Omega - P_t 1_{\tilde{B}})(x) = 0$$

for all x in an open set $U \subset Z^n \setminus (\tilde{B} \cup \Omega)$. Then $\Omega = \tilde{B}$.

Proof:

$$\begin{aligned} &(t/n)^{\frac{n}{2}+1} (P_t 1_\Omega - P_t 1_{\tilde{B}})(x) \\ &= (t/n)^{\frac{n}{2}+1} e^{-t} \left\{ \sum_{\omega \in \Omega} I_{|\omega_1 - x_1|}(t/n) \cdots I_{|\omega_n - x_n|}(t/n) \right\} \\ &- (t/n)^{\frac{n}{2}+1} e^{-t} \left\{ \sum_{b \in \tilde{B}} I_{|b_1 - x_1|}(t/n) \cdots I_{|b_n - x_n|}(t/n) \right\}. \end{aligned}$$

For large t, this is asymptotic to

$$
\begin{aligned}
&(t/n)^{\frac{n}{2}+1}e^{-t}\cdot(e^{t/n})^n((2\pi t/n)^{-1/2})^n\cdot\\
&\cdot\ \left(\sum_{\omega}\left\{1-\frac{4(\omega_1-x_1)^2-1}{8t/n}-\cdots-\frac{4(\omega_n-x_n)^2-1}{8t/n}+O(t^{-2})\right\}\right.\\
&\qquad\left.-\sum_{b}\left\{1-\frac{4(b_1-x_1)^2-1}{8t/n}-\cdots-\frac{4(b_n-x_n)^2-1}{8t/n}+O(t^{-2})\right\}\right)\\
&= (t/n)\left(\frac{1}{2\pi}\right)^{n/2}\left\{\sum_{\omega}1-\sum_{b}1\right\}\\
&+ (t/n)\left(\frac{1}{2\pi}\right)^{n/2}\left(\frac{n}{8t}\right)\left\{\sum_{b}\sum_{i}(4(b_i-x_i)^2-1)-\sum_{\omega}\sum_{i}(4(\omega_i-x_i)^2-1)\right\}.
\end{aligned}
$$

Our hypothesis is that the limit of this expression as $t\to\infty$ is 0.

This implies $i)$ Ω and $\tilde{B}$ have the same volume (contain the same number of points) and

$$
ii)\qquad \sum_{z\in Z^n}\left\{\sum_{i}(z_i-x_i)^2\{1_\Omega-1_{\tilde{B}}\}(z)\right\}=0\quad\text{for all } x\in U.
$$

$ii)$ is true for some $x=(x_1,x_2,\ldots,x_n)$ and also for $(x_1+1,x_2,\ldots,x_n)$ so we have for x

$$
\sum_{z\in Z^n}\left\{\sum_{i}(z_i^2+x_i^2-2x_iz_i)\{1_\Omega-1_{\tilde{B}}\}(z)\right\}=0 \tag{2.3}
$$

and for $(x_1+1,x_2,\ldots,x_n)$

$$
\sum_{z\in Z^n}\left\{(2x_1+1-2z_1)+\sum_{i}(z_i^2+x_i^2-2x_iz_i)\right\}\{1_\Omega-1_{\tilde{B}}\}(z)=0. \tag{2.4}
$$

Substituting into (2.3) we have

$$\sum_z (2x_1 + 1 - 2z_1)\{1_\Omega - 1_{\tilde{B}}\}(z) = 0$$

which implies

$$\sum_z z_1\{1_\Omega - 1_{\tilde{B}}\}(z) = 0 \tag{2.5}$$

since x is constant.

Similarly for the other coordinates; consequently Ω and $\tilde{B}$ have the same center of mass, which we may assume is the origin. Since (2.5) is true for each coordinate we have

$$\sum_z \sum_i z_i\{1_\Omega - 1_{\tilde{B}}\}(z) = 0 \tag{2.6}$$

which implies

$$\sum_z \sum_i z_i x_i\{1_\Omega - 1_{\tilde{B}}\}(z) = 0. \tag{2.7}$$

Substituting into (2.3) we have

$$\sum_z \left\{ \sum_i z_i^2 \{1_\Omega - 1_{\tilde{B}}\}(z) \right\} = 0$$

or

$$\sum_{\tilde{B}} \left\{ \sum_i b_i^2 \right\} = \sum_\Omega \left\{ \sum_i \omega_i^2 \right\}.$$

Suppose $\Omega \neq \tilde{B}$.

We know $\tilde{B} \not\subset \Omega$ and $\Omega \not\subset \tilde{B}$ (equal volumes) so $\tilde{B} \setminus \Omega \neq \emptyset$ and $\Omega \setminus \tilde{B} \neq \emptyset$.

Since the same set $\tilde{B} \cap \Omega$ is removed from $\tilde{B}$ and from Ω we have

$$vol(\tilde{B} \setminus \Omega) = vol(\Omega \setminus \tilde{B})$$

and

$$\sum_{\tilde{B}\setminus\Omega} \left\{ \sum_i b_i^2 \right\} = \sum_{\Omega\setminus\tilde{B}} \left\{ \sum_i \omega_i^2 \right\}. \tag{2.8}$$

But $\tilde{B} \setminus \Omega$ contains only points that satisfy $\sum_i b_i^2 \leq r^2$ and $\Omega \setminus \tilde{B}$ only points that satisfy $\sum_i \omega_i^2 > r^2$. So we have

$$\begin{aligned} \sum_{\tilde{B}\setminus\Omega} \sum_i b_i^2 &\leq r^2 \cdot \mathrm{vol}(\tilde{B} \setminus \Omega) \\ \sum_{\Omega\setminus\tilde{B}} \sum_i \omega_i^2 &> r^2 \cdot \mathrm{vol}(\Omega \setminus \tilde{B}) \end{aligned}$$

contradicting (2.8). ∎

As mentioned above, this result is not valid for disks. We will present a counterexample in Z^2 and indicate how to find counterexamples in $Z^n, n > 2$. Let B be the disk of radius 8 centered at the origin and let

$$\begin{aligned} \Omega = B &\setminus \{(7,1),(-7,1),(7,-1),(-7,-1)\} \\ &\bigcup \{(5,5),(5,-5),(-5,5),(-5,-5)\}. \end{aligned}$$

Then

$$\lim_{t\to\infty} (t/n)^{\frac{n}{2}+1} \{P_t 1_\Omega - P_t 1_B\}(x) = 0 \quad \forall x \in Z^2 \setminus (B \cup \Omega).$$

To see this, note that we have, as in the proof of Theorem 9, for large t

$$
\begin{aligned}
&(t/n)^{\frac{n}{2}+1}\{P_t 1_\Omega - P_t 1_B\}(x) \\
&\sim \quad (t/n)(2\pi)^{-n/2}\left\{\sum_\omega 1 - \sum_b 1\right\} \\
&+ \quad (t/n)(\frac{1}{2\pi})^{n/2}(\frac{n}{8t})\left\{\sum_b\sum_i(4(b_i - x_i)^2 - 1) - \sum_\omega\sum_i(4(\omega_i - x_i)^2 - 1)\right\}.
\end{aligned}
$$

B and Ω have the same volume so

$$\sum_\omega 1 - \sum_b 1 = 0.$$

B and Ω also have the same center of mass (the origin), and satisfy

$$\sum_B\{\sum_i b_i^2\} = \sum_\Omega\{\sum_i \omega_i^2\}.$$

Therefore

$$\sum_B\{\sum_i(b_i - x_i)^2\} = \sum_\Omega\{\sum_i(\omega_i - x_i)^2\}$$

and the limit is 0. We can use this example to construct examples in higher dimensions. In Z^3 , let B be the disk of radius 8 with center at the origin. For Ω, delete from B the points $(7,1,0),(7,-1,0),(-7,1,0),(-7,-1,0)$ and add the points $(5,5,0),(5,-5,0),(-5,5,0),(-5,-5,0)$. Ω has the same volume as B and, because of the symmetry, the same center of mass.

From the proof of Theorem 9 and the examples above we see that we actually have

Theorem 10 *In Z^n,*

$$\lim_{t\to\infty}(t/n)^{\frac{n}{2}+1}\{P_t 1_{\Omega_1} - P_t 1_{\Omega_2}\}(x) = 0$$

for x in some open set U is equivalent to Ω_1 and Ω_2 satisfying the following three conditions: i) Ω_1 and Ω_2 have the same volume; ii) Ω_1 and Ω_2 have the same center of mass; iii) $\sum_{\Omega_1}\sum_i \omega_i^2 = \sum_{\Omega_2}\sum_i \omega_i^2$.

Turning next to convex sets, Theorem 9 is not valid for Ω_1, Ω_2 one of which is only assumed to be convex. In fact we will show how to find pairs of sets in $Z^n, n \geq 3$, both convex, satisfying

$$\lim_{t\to\infty}(t/n)^{\frac{n}{2}+1}\{P_t 1_{\Omega_1} - P_t 1_{\Omega_2}\}(x) = 0 \tag{2.9}$$

for all x in $Z^n \setminus (\Omega_1 \cup \Omega_2)$ but $\Omega_1 \neq \Omega_2$. For convenience, we will work in Z^3 since the method easily generalizes.

We are assuming Ω_1 and Ω_2 are convex so they are products of intervals, say,

$$\begin{aligned}
\Omega_1 &= [x_1, x_1 + (m-1)] \times [x_2, x_2 + (n-1)] \times [x_3, x_3 + (p-1)] \\
\Omega_2 &= [y_1\,, y_1 + (q-1)] \times [y_2, y_2 + (r-1)] \times [y_3, y_3 + (s-1)].
\end{aligned}$$

By Theorem 10, Ω_1 and Ω_2 have the same volume, so $mnp = qrs$. Ω_1 and Ω_2 also have the same center of mass, which means that the average of the i^{th} coordinates in Ω_1 equals the average of the i^{th} coordinates in Ω_2. Explicitly, for the first coordinates,

$$np \cdot \sum_{j=0}^{m-1}(x_1 + j) = rs \cdot \sum_{j=0}^{q-1}(y_1 + j). \tag{2.10}$$

Equivalently,

$$np\left(mx_1 + \frac{(m-1)m}{2}\right) = rs\left(qy_1 + \frac{(q-1)q}{2}\right)$$

or

$$mnp\left(x_1 + \frac{m-1}{2}\right) = qrs\left(y_1 + \frac{q-1}{2}\right).$$

Since $mnp = qrs$ we have

$$x_1 + \frac{m-1}{2} = y_1 + \frac{q-1}{2}. \tag{2.11}$$

Similarly,

$$x_2 + \frac{n-1}{2} = y_2 + \frac{r-1}{2} \tag{2.12}$$

$$x_3 + \frac{p-1}{2} = y_3 + \frac{s-1}{2}. \tag{2.13}$$

Note that these equations imply that m and q have the same parity, as do n and r, and p and s. Condition (iii) of Theorem 10 says

$$\sum_{\Omega_1}\sum_{i}\omega_i^2 = \sum_{\Omega_2}\sum_{i}\omega_i^2. \tag{2.14}$$

We have

$$\sum_{\Omega_1}\omega_1^2 = np \cdot \{x_1^2 + (x_1+1)^2 + \cdots + (x_1 + (m-1))^2\}$$

$$
\begin{aligned}
&= np\cdot\{x_1^2+x_1^2+2x_1+1+\cdots+x_1^2+\ 2(m-1)x_1+(m-1)^2\}\\
&= np\cdot\left\{mx_1^2+2x_1\sum_{j=0}^{m-1} j+\ \sum_{j=0}^{m-1} j^2\right\}\\
&= np\cdot\left\{mx_1^2+2x_1\frac{(m-1)m}{2}+\ \frac{(m-1)m(2m-1)}{6}\right\}\\
&= mnp\cdot\left\{x_1^2+(m-1)x_1+\frac{(m-1)(2m-1)}{6}\right\}.
\end{aligned}
$$

So (2.14) becomes

$$
\begin{aligned}
& x_1^2+(m-1)x_1+\frac{1}{6}(m-1)(2m-1)\ +x_2^2+(n-1)x_2+\frac{1}{6}(n-1)(2n-1)\\
+ &\ \ x_3^2+(p-1)x_3+\frac{1}{6}(p-1)(2p-1) \qquad (2.15)\\
= &\ \ y_1^2+(q-1)y_1+\frac{1}{6}(q-1)(2q-1)\ +y_2^2+(r-1)y_2+\frac{1}{6}(r-1)(2r-1)\\
+ &\ \ y_3^2+(s-1)y_3+\frac{1}{6}(s-1)(2s-1)
\end{aligned}
$$

From equations (2.11), (2.12), and (2.13) we have

$$
\begin{aligned}
x_1^2+(m-1)x_1+\frac{(m-1)^2}{4} &= y_1^2+(q-1)x_1+\frac{(q-1)^2}{4}\\
x_2^2+(n-1)x_1+\frac{(n-1)^2}{4} &= y_2^2+(r-1)x_1+\frac{(r-1)^2}{4}\\
x_3^2+(p-1)x_1+\frac{(p-1)^2}{4} &= y_3^2+(s-1)x_1+\frac{(s-1)^2}{4}.
\end{aligned}
$$

Substituting into (2.15)

$$
\begin{aligned}
&\frac{1}{6}(m-1)(2m-1)-\frac{1}{4}(m-1)^2+\frac{1}{6}(n-1)(2n-1)-\frac{1}{4}(n-1)^2\\
&\qquad +\frac{1}{6}(p-1)(2p-1)-\frac{1}{4}(p-1)^2\\
= &\ \frac{1}{6}(q-1)(2q-1)-\frac{1}{4}(q-1)^2+\frac{1}{6}(r-1)(2r-1)-\frac{1}{4}(r-1)^2
\end{aligned}
$$

$$+\frac{1}{6}(s-1)(2s-1)-\frac{1}{4}(s-1)^2.$$

This is equivalent to

$$\begin{aligned}(m-1)(m+1)+(n-1)(n+1)+(p-1)(p+1)\\ = \ (q-1)(q+1)+(r-1)(r+1)+(s-1)(s+1)\end{aligned}$$

or

$$m^2+n^2+p^2=q^2+r^2+s^2.$$

So we seek two triples of integers m, n, p and q, r, s such that $mnp = qrs$ and $m^2+m^2+p^2 = q^2+r^2+s^2$ and corresponding parities match. One solution is to take for q, r, s an allowable permutation of m, n, p. In that case, Ω_2 is a rotation of Ω_1. There are also nontrivial solutions. One is $12, 10, 1$ and $4, 2, 15$. Explicitly, we could take

$$\begin{aligned}\Omega_1 &= [-5,6]\times[-4,5]\times[0,0]\\ \Omega_2 &= [-1,2]\times[0,1]\times[-7,7].\end{aligned}$$

Since we worked coordinate by coordinate, the discussion generalizes. In Z^n we want two rectangular solids Ω_1, Ω_2 of dimensions $m_1, m_2, \ldots, m_n$ and $q_1, q_2, \ldots, q_n$, respectively, such that

$$\begin{aligned}m_1m_2\cdots m_n &= q_1q_2\cdots q_n\\ m_1^2+m_2^2+\cdots+m_n^2 &= q_1^2+q_2^2+\cdots+q_n^2.\end{aligned}$$

The Z^3 example extends to an example in Z^n by taking

$$\begin{aligned} m_1, m_2, \ldots, m_n &= 12, 10, 1, v, v, \ldots, v \\ q_1, q_2, \ldots, q_n &= 4, 2, 15, v, v, \ldots, v \end{aligned}$$

where v is any integer.

In Z^2, the situation is different. We want pairs of integers m, n and q, r such that $mn = qr$ and $m^2 + n^2 = q^2 + r^2$. If m and n are given, then q and r are determined; either $q = m$ and $r = n$, so $\Omega_2 = \Omega_1$ or $q = n$ and $r = m$, so Ω_2 is a rotation of Ω_1

Turning now to R^n, Chavel and Karp ask if Theorem (2) is true for Ω_1, Ω_2, one of which is only assumed to be convex. Our results in Z^n show us how to find sets Ω_1, Ω_2 satisfying (2.9) for all x in $R^n \setminus (\Omega_1 \cup \Omega_2)$, both convex, but $\Omega_1 \neq \Omega_2$. The proof of Theorem (2) shows that (2.9) implies Ω_1 and Ω_2 : i) have the same volume; ii)have the same center of mass; and iii) satisfy

$$\int_{\Omega_1} d^2(x,y)dy = \int_{\Omega_2} d^2(x,y)dy \text{ for all } x \text{ in } U.$$

Running the proof backwards, we can see that conditions (i), (ii), and (iii) imply (2.9) for all x in U. So we have

Theorem 11 *In R^n,*

$$\lim_{t\to\infty} (t/n)^{\frac{n}{2}+1}\{P_t 1_{\Omega_1} - P_t 1_{\Omega_2}\}(x) = 0$$

for x in some open set $U \subset R^n \setminus (\Omega_1 \cup \Omega_2)$ is equivalent to Ω_1 and Ω_2 satisfying the following three conditions: i) Ω_1 and Ω_2 have the same volume; ii) Ω_1 and Ω_2 have the same center of mass; iii)$\int_{\Omega_1} d^2(x,y)dy = \int_{\Omega_2} d^2(x,y)dy$

for all x in U.

Condition (iii) says

$$\int_{\Omega_1} \sum_{j=1}^{n} (x_j^2 - 2x_j y_j + y_j^2) dy = \int_{\Omega_2} \sum_{j=1}^{n} (x_j^2 - 2x_j y_j + y_j^2) dy.$$

This is equivalent to, using (i) and (ii), $\int_{\Omega_1} \sum_{j=1} y_j^2 dy = \int_{\Omega_2} \sum_{j=1} y_j^2 dy$. The natural analogue to consider in R^n of a rectangular solid in Z^n is an ellipsoid. So we ask can we find two ellipsoids satisfying these three conditions. Again, for convenience, we will first present an example in three dimensions. The volume of the ellipsoid

$$\Omega = \left\{ y \in R^3 : \frac{y_1^2}{a^2} + \frac{y_2^2}{b^2} + \frac{y_3^2}{c^2} \leq 1 \right\}$$

is $\frac{4}{3}\pi abc$, its center of mass is the origin, and

$$\int_{\Omega} \sum_{j=1}^{3} y_j^2 dy = \frac{4}{15} \pi abc (a^2 + b^2 + c^2).$$

Therefore, we again want solutions to the system

$$mnp = abc \qquad (2.16)$$

$$m^2 + n^2 + p^2 = a^2 + b^2 + c^2 \qquad (2.17)$$

but we are no longer restricted to integers. In fact, given any ellipsoid, except a ball, there are infinitely many other ellipsoids satisfying conditions (i), (ii), and (iii) and, therefore, (2.9). Any solution to the system, where a, b, and c are given, corresponds to an ellipsoid with the same volume and center of mass as Ω that also satisfies condition (iii). In R^n, given an ellipsoid

$$\Omega_1 = \left\{ y : \frac{y_1^2}{a_1^2} + \cdots + \frac{y_n^2}{a_n^2} \leq 1 \right\}$$

any solution to the system

$$\begin{aligned} m_1 m_2 \cdots m_n &= a_1 a_2 \cdots a_n \\ m_1^2 + m_2^2 + \cdots + m_n^2 &= a_1^2 + a_2^2 + \cdots + a_n^2. \end{aligned}$$

corresponds to an ellipsoid

$$\Omega_2 = \left\{ y : \frac{y_1^2}{m_1^2} + \cdots + \frac{y_n^2}{m_n^2} \leq 1 \right\}$$

such that (2.9) holds.

If Ω_1 were a ball,

$$\Omega_1 = \left\{ y : \sum_{j=1}^{n} y_j^2 \leq a^2 \right\}$$

the system would be

$$\begin{aligned} m_1 m_2 \cdots m_n &= a^n \\ m_1^2 + m_2^2 + \cdots + m_n^2 &= n a^2. \end{aligned}$$

This system has only one positive solution.

Chapter 3

Trees

3.1 Heat Kernel for Trees

We recall that a path in a graph $G = (V, E)$ is a sequence $x_0, x_1, \ldots, x_n$ of elements of V such that (x_i, x_{i+1}) is in E for $i = 0, 1, \ldots, n-1$. The path is *closed* if $x_n = x_0$. A closed path is a *cycle* if the vertices $x_j, j = 1, 2, \ldots, n$ are distinct. A *tree* is a connected graph with no cycles. A tree with q edges at each vertex is called *q-regular*. We will consider only infinite trees.

Let T be an infinite $(p+1)$-regular tree. Its *adjacency matrix* A is the infinite square matrix whose rows and columns are labeled by the vertices of T, and whose a_{xy} entry is 1 if x and y are neighbors and 0 if they are not. Each row and column has only $p+1$ nonzero entries. Powers of the adjacency matrix count the number of paths between each pair of vertices: a^k_{xy}, the xy entry in A^k, is the number of paths of length k joining x and y. We can view the matrix A as a linear operator acting on functions defined on the vertices of T. For $f \in L_0^2(T)$

$$\begin{aligned} Af(x) &= \sum_{y \in T} a_{xy} f(y) \\ &= \sum_{y \sim x} f(y). \end{aligned}$$

The identity matrix I also acts on functions:

$$\begin{aligned} If(x) &= \sum_{y \in T} i_{xy} f(y) \\ &= f(x). \end{aligned}$$

Since

$$\Delta f(x) = \frac{1}{p+1} \sum_{y \sim x} f(y) - f(x)$$

we have

$$\Delta = \frac{1}{p+1} A - I. \tag{3.1}$$

Now suppose we are given a nonnegative function ϕ defined on a finite subset of the vertices of T. We seek the solution to the heat equation on T, with continuous time parameter, and initial data ϕ. That is, we want

$$u : T \times [0, \infty) \to R$$

such that

$$\Delta u(x,t) = \frac{\partial}{\partial t} u(x,t)$$

and

$$\lim_{t \to 0} u(x,t) = \phi(x).$$

The Laplacian is a bounded linear operator on the Banach space $L_0^2(T)$ so a formal solution is

$$u(x,t) = (e^{t\Delta}\phi)(x).$$

By (3.1) we have

$$(e^{t\Delta}\phi)(x) = (e^{t(\frac{1}{p+1}A-I)}\phi)(x).$$

Since

$$(e^{\frac{1}{p+1}At}\phi)(x) = \sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{1}{p+1}\right)^k t^k(A^k\phi)(x)$$

our formal solution is

$$u(x,t) = e^{-t}\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{1}{p+1}\right)^k t^k(A^k\phi)(x)$$

or

$$u(x,t) = e^{-t}\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{1}{p+1}\right)^k t^k\sum_{y\sim x}a_{xy}^k\phi(y). \tag{3.2}$$

Now we begin to study the matrices A^k. Following M. Burger [2], we define the following functions on pairs of vertices of T :

$$\delta_0(x,y) = \begin{cases} 1 & \text{if } x=y \\ 0 & \text{otherwise} \end{cases}$$

and

$$\delta_n(x,y) = \begin{cases} 1 & \text{if } d(x,y)=n \\ 0 & \text{otherwise.} \end{cases}$$

We also define the operation * as follows:

$$(\delta_r * \delta_s)(x,y) = \sum_z \delta_r(x,z)\delta_s(z,y).$$

We have

$$\begin{aligned}(\delta_n * \delta_0)(x,y) &= \sum_z \delta_n(x,z)\delta_0(z,y) \\ &= \delta_n(x,y)\end{aligned}$$

and

$$\begin{aligned}(\delta_1 * \delta_1) &= \sum_z \delta_1(x,z)\delta_1(z,y) \\ &= \begin{cases} p+1 & \text{if } d(x,y)=0 \\ 1 & \text{if } d(x,y)=2 \\ 0 & \text{otherwise} \end{cases}\end{aligned}$$

$$\begin{aligned}(\delta_1 * \delta_n) &= \sum_z \delta_1(x,z)\delta_n(z,y) \\ &= \begin{cases} p & \text{if } d(x,y)=n-1 \\ 1 & \text{if } d(x,y)=n+1 \\ 0 & \text{otherwise.} \end{cases}\end{aligned}$$

Note that

$$\delta_1 * \delta_1 = \delta_2 + (p+1)\delta_0 \tag{3.3}$$

$$\delta_1 * \delta_n = \delta_{n+1} + p\delta_{n-1}. \tag{3.4}$$

Let $\delta_1^k = \delta_1 * \delta_1^{k-1}$. We want to point out the relationship between the entries in the matrices A^k and the functions δ_1^k. Note first that $a_{xy} = \delta_1(x,y)$.

Then

$$\begin{aligned} a^2_{xy} &= \sum_z a_{xz}a_{zy} \\ &= \sum_z \delta_1(x,z)\delta_1(z,y) \\ &= (\delta_1 * \delta_1)(x,y) \\ &= \delta_1^2(x,y) \end{aligned}$$

and

$$\begin{aligned} a^k_{xy} &= \sum_z a_{xz}a^{k-1}_{zy} \\ &= \sum_z \delta_1(x,z)\delta_1^{k-1}(z,y) \\ &= (\delta_1 * \delta_1^{k-1})(x,y) \\ &= \delta_1^k(x,y). \end{aligned}$$

So our formal solution (3.2) is now

$$u(x,t) = e^{-t}\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{1}{p+1}\right)^k t^k \sum_y \delta_1^k(x,y)\phi(y).$$

Since $\delta_1^k(x,y)$ is the number of paths of length k joining x and y, it is a function of k and of p. To derive explicit expressions for $\delta_1^k(x,y)$ we begin by expanding the first few using the relations (3.3) and (3.4):

$$\delta_1 = \delta_1$$

$$\delta_1^2 = \delta_1 * \delta_1$$

$$= \delta_2 + (p+1)\delta_0$$

$$\begin{aligned}
\delta_1^3 &= \delta_1 * \delta_1^2 \\
&= \delta_1 * \{\delta_2 + (p+1)\delta_0\} \\
&= \delta_1 * \delta_2 + (p+1)(\delta_1 * \delta_0) \\
&= \delta_3 + p\delta_1 + (p+1)\delta_1 \\
&= \delta_3 + (2p+1)\delta_1
\end{aligned}$$

$$\begin{aligned}
\delta_1^4 &= \delta_1 * \delta_1^3 \\
&= \delta_1 * \{\delta_3 + (2p+1)\delta_1\} \\
&= \delta_1 * \delta_3 + (2p+1)(\delta_1 * \delta_1) \\
&= \delta_4 + p\delta_2 + (2p+1)\{\delta_2 + (p+1)\delta_0\} \\
&= \delta_4 + (3p+1)\delta_2 + (2p+1)(p+1)\delta_0.
\end{aligned}$$

Let $C(k,d)$ be the coefficient of δ_d in the expansion of δ_1^k.

Remarks:

1) δ_1^k is expressible in terms of δ_j, where j and k have the same parity, $j \leq k$. The proof is by induction on k. We see above that it is true for $k = 1, 2, 3, 4$. Assume it is true for k, i.e.

$$\delta_1^k = C(k,k)\delta_k + C(k,k-2)\delta_{k-2} + \cdots + C(k,k-r)\delta_{k-r}$$

where

$$k - r = \begin{cases} 0 & \text{if k is even} \\ 1 & \text{if k is odd.} \end{cases}$$

Now use $\delta_1 * \delta_n = \delta_{n+1} + p\delta_{n-1}$.

2)When $\delta_1^k(x,y)$ is evaluated, only the δ_d term, where $d = d(x,y)$, is nonzero. Since $\delta_d(x,y) = 1$, $\delta_1^k(x,y) = C(k,d)$. Therefore, $C(k,d)$ is the number of paths of length k joining any pair of vertices that are distance d apart.

We now have

$$u(x,t) = e^{-t}\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{1}{p+1}\right)^k t^k \sum_y C(k,d(x,y))\phi(y).$$

Now we shift our focus to find explicit formulas for $C(k,d)$. To begin, we show how to obtain the coefficients in the expansion of δ_1^{k+1} from the coefficients in the expansion of δ_1^k. For k even we have

$$\delta_1^k = C(k,k)\delta_k + C(k,k-2)\delta_{k-2} + \cdots + C(k,0)\delta_0$$

and

$$\begin{aligned}
\delta_1^{k+1} &= \delta_1 * \delta_1^k \\
&= C(k,k)(\delta_1 * \delta_k) + C(k,k-2)(\delta_1 * \delta_{k-2}) + \cdots + C(k,0)(\delta_1 * \delta_0) \\
&= C(k,k)\delta_{k+1} + pC(k,k)\delta_{k-1} \\
&+ C(k,k-2)\delta_{k-1} + pC(k,k-2)\delta_{k-3} \\
&\vdots \\
&+ C(k,2)\delta_3 + pC(k,2)\delta_1 \\
&+ C(k,0)\delta_1.
\end{aligned}$$

Comparing coefficients we have

$$C(k+1,k+1) = C(k,k)$$

and

$$\begin{aligned}
C(k+1,k-1) &= C(k,k-2) + pC(k,k) \\
C(k+1,k-3) &= C(k,k-4) + pC(k,k-2) \\
&\vdots \\
C(k+1,1) &= C(k,0) + pC(k,2).
\end{aligned}$$

If k is odd we have

$$\delta_1^k = C(k,k)\delta_k + C(k,k-2)\delta_{k-2} + \cdots + C(k,1)\delta_1$$

and

$$\begin{aligned}
\delta_1^{k+1} &= C(k,k)(\delta_1 * \delta_k) + C(k,k-2)(\delta_1 * \delta_{k-2}) + \cdots + C(k,0)(\delta_1 * \delta_1) \\
&= C(k,k)\delta_{k+1} + pC(k,k)\delta_{k-1} \\
&+ C(k,k-2)\delta_{k-1} + pC(k,k-2)\delta_{k-3} \\
&\vdots \\
&+ C(k,1)\delta_2 + (p+1)C(k,1)\delta_0
\end{aligned}$$

So again

$$C(k+1,k+1) = C(k,k)$$

and for $r = 1, 3, \ldots, k-2$,

$$C(k+1, k-r) = C(k, k-r-1) + pC(k, k-r+1)$$

but

$$C(k+1, 0) = (p+1)C(k, 1).$$

To summarize, we have, for all k,

$$C(k+1, k+1) = C(k, k)$$

which implies $C(k,k) = 1$ for all k since $C(1,1) = 1$. Note that all this says is if x and y are distance k apart then the number of paths of length k joining them is 1. We also have $C(k,d) = 0$ if k and d have different parities, or if $d > k$. If k and d have the same parity then, for $d \neq 0$,

$$C(k,d) = C(k-1, d-1) + pC(k-1, d+1) \tag{3.5}$$

and, for k even,

$$C(k, 0) = (p+1)C(k-1, 1) \tag{3.6}$$

Using (3.5) and (3.6) we can derive explicit formulas for the coefficients $C(k,d)$. For example:

$$\begin{aligned} C(k, k-2) &= C(k-1, k-3) + pC(k-1, k-1) \\ &= C(k-1, k-3) + p \\ &= C(k-2, k-4) + pC(k-2, k-2) + p \\ &= C(k-2, k-4) + 2p \end{aligned}$$

$$\begin{aligned} &\vdots \\ &= C(2,0) + (k-2)p \\ &= (k-1)p + 1 \end{aligned}$$

i.e.,

$$C(k, k-2) = (k-1)p + 1. \tag{3.7}$$

Proposition 6 *$C(k, d)$ is a polynomial in p of degree $s = \frac{k-d}{2}$.*

Proof: Changing notation we want to show

$$C(d+2s, d) = 1 + A_1 p + A_2 p^2 + \cdots + A_s p^s.$$

The proof is by induction on s. We've already shown

$$C(d, d) = 1 \tag{3.8}$$

and

$$C(d+2, d) = 1 + (d+1)p. \tag{3.9}$$

Assume true for $s-1$; i.e.

$$C(d+2(s-1), d) = 1 + A_1 p + \cdots + A_{s-1} p^{s-1}. \tag{3.10}$$

By (3.5),

$$C(d+2s, d) = C(d+2s-1, d-1) + pC(d+2s-1, d+1).$$

The second term on the right side can be written $pC(d+1+2(s-1), d+1)$.

Applying the induction hypothesis (3.10), we have

$$C(d+2s,d) = C(d+2s-1,d-1) + p(1+B_1p+\cdots+B_{s-1}p^{s-1}).$$

Now apply (3.5) to the first term on the right side to get

$$\begin{aligned} C(d+2s,d) &= C(d+2s-2,d-2) + pC(d+2s-2,d) \\ &+ p(1+B_1p+\cdots+B_{s-1}p^{s-1}). \end{aligned}$$

The middle term on the right side can be written $pC(d+2(s-1),d)$. Applying (3.10) we have

$$\begin{aligned} C(d+2s,d) &= C(d+2s-2,d-2) + p(1+E_1p+\cdots+E_{s-1}p^{s-1}) \\ &+ p(1+B_1p+\cdots+B_{s-1}p^{s-1}) \\ &= C(d+2s-2,d-2) + p(2+F_1p+\cdots+F_{s-1}p^{s-1}). \end{aligned}$$

Continue alternately applying (3.5) and (3.10). After d steps we have

$$C(d+2s,d) = C(2s,0) + p(d+L_1p+\cdots+L_{s-1}p^{s-1}). \tag{3.11}$$

By (3.6),

$$\begin{aligned} C(2s,0) &= (p+1)C(2s-1,1) \\ &= (p+1)C(1+2(s-1),1) \\ &= (p+1)(1+M_1p+\cdots+M_{s-1}p^{s-1}). \end{aligned}$$

Substituting into (3.11) we have

$$C(d+2s,d) = 1 + R_1 p + \cdots + R_s p^s. \quad \blacksquare$$

Since $C(k,d)$ counts the number of paths of length k joining any pair of vertices that are distance d apart, we expect it to decrease as d increases. In fact, $C(k,d)$ is not only greater than $C(k,d+2)$ but the first $\frac{k-(d+2)}{2}$ terms of $C(k,d)$ constitute the polynomial $C(k,d+2)$. We have

Proposition 7 *$C(k,d) = C(k,d+2) +$ the $p^{\frac{k-d}{2}}$ term of $C(k,d)$.*

Proof: Change notation to $C(k,k-r)$. The proof is by induction on r, r even. We want to show

$$C(k,k-r) = C(k,k-r+2) + \tilde{A}p^{\frac{r}{2}}.$$

For $r=0$, $C(k,k)=1$. For $r=2$, we have already shown (3.7)

$$C(k,k-2) = 1 + (k-1)p = C(k,k) + (k-1)p.$$

Assume true for $r-2$, i.e.

$$C(k,k-(r-2)) = C(k,k-(r-2)+2) + Ap^{\frac{r-2}{2}}. \qquad (3.12)$$

From (3.5) we have

$$\begin{aligned} &C(k,k-r) - C(k,k-r+2) \\ &= \quad C(k-1,k-r-1) + pC(k-1,k-r+1) \\ &\qquad -\{C(k-1,k-r+1) + pC(k-1,k-r+3)\} \end{aligned}$$

$$= C(k-1,k-r-1) - C(k-1,k-r+1)$$
$$+p\{C(k-1,k-r+1) - C(k-1,k-r+3)\}.$$

From the induction hypothesis (3.12) the last expression in the brackets is equal to $Ap^{\frac{r-2}{2}}$ since $C(k-1,k-r+1) = C(k-1,k-1-(r-2))$. So we have

$$C(k,k-r) - C(k,k-r+2) = C(k-1,k-r-1) - C(k-1,k-r+1) + Ap^{\frac{r}{2}}.$$

Applying (3.5) again, the right side is equal to

$$\begin{aligned} &C(k-2,k-r-2) + pC(k-2,k-r) \\ &\quad -\{C(k-2,k-r) + pC(k-2,k-r+2)\} + Ap^{\frac{r}{2}} \\ &= C(k-2,k-r-2) - C(k-2,k-r) \\ &\quad +p\{C(k-2,k-r) - C(k-2,k-r+2)\} + Ap^{\frac{r}{2}}. \end{aligned}$$

Since $C(k-2,k-r) = C(k-2,k-2-(r-2))$, the expression in brackets is equal to $Bp^{\frac{r}{2}}$. So we now have

$$\begin{aligned} &C(k,k-r) - C(k,k-r+2) \\ &= C(k-2,k-r-2) - C(k-2,k-r) + (A+B)p^{\frac{r}{2}}. \end{aligned}$$

Continuing, we have

$$\begin{aligned} &C(k,k-r) - C(k,k-r+2) \\ &= C(r,0) - C(r,2) + Fp^{\frac{r}{2}}. \end{aligned}$$

$$\begin{aligned}
&= (p+1)C(r-1,1) - \{C(r-1,1) + pC(r-1,3)\} + Fp^{\frac{r}{2}}. \\
&= p\{C(r-1,1) - C(r-1,3)\} + Fp^{\frac{r}{2}}. \\
&= pGp^{\frac{r-2}{2}} + Fp^{\frac{r}{2}} \\
&= \tilde{A}p^{\frac{r}{2}}. \quad \blacksquare
\end{aligned}$$

Proposition 7 says that the coefficient of p^s in $C(k,d)$, $1 \le s \le \frac{k-d}{2}$ does not depend on d since it is also the coefficient of p^s in $C(k,0)$, if k is even, or $C(k,1)$, if k is odd. We derive explicit formulas for these coefficients, and these formulas will be functions of s and of k. We know

$$\begin{aligned}
C(k,k) &= 1 \\
C(k,k-2) &= 1 + (k-1)p \\
C(k,k-4) &= 1 + (k-1)p + A_2p^2.
\end{aligned}$$

To find A_2, write

$$A_2p^2 = C(k,k-4) - C(k,k-2)$$

and apply (3.5) to get

$$\begin{aligned}
A_2p^2 &= C(k-1,k-5) + pC(k-1,k-3) \\
&\quad -\{C(k-1,k-3) + pC(k-1,k-1)\} \\
&= C(k-1,k-5) - C(k-1,k-3) \\
&\quad +p\{C(k-1,k-3) - C(k-1,k-1)\}. \\
&= C(k-1,k-5) - C(k-1,k-3) \\
&\quad +p\{(k-2)p + 1 - 1\} \quad \text{by (3.9) and (3.8)}
\end{aligned}$$

$$= C(k-1,k-5) - C(k-1,k-3) + (k-2)p^2.$$

Applying (3.5) again we have

$$\begin{aligned}
A_2p^2 &= C(k-2,k-6) + pC(k-2,k-4) \\
&\quad -\{C(k-2,k-4) + pC(k-2,k-2)\} + (k-2)p^2 \\
&= C(k-2,k-6) - C(k-2,k-4) \\
&\quad +p\{C(k-2,k-4) - C(k-2,k-2)\} + (k-2)p^2 \\
&= C(k-2,k-6) - C(k-2,k-4) \\
&\quad +p\{(k-3)p + 1 - 1\} + (k-2)p^2 \\
&= C(k-2,k-6) - C(k-2,k-4) + (k-3)p^2 + (k-2)p^2.
\end{aligned}$$

After applying (3.5) $k-4$ times, we have

$$\begin{aligned}
A_2p^2 &= C(4,0) - C(4,2) + 3p^2 + 4p^2 + \cdots + (k-2)p^2 \\
&= (p+1)C(3,1) - \{C(3,1) + pC(3,3)\} + 3p^2 + \cdots + (k-2)p^2 \\
&= p\{C(3,1) - C(3,3)\} + 3p^2 + \cdots + (k-2)p^2 \\
&= p\{2p + 1 - 1\} + 3p^2 + \cdots + (k-2)p^2 \\
&= 2p^2 + 3p^2 + \cdots + (k-2)p^2
\end{aligned}$$

i.e.,

$$A_2p^2 = C(k,k-4) - C(k,k-2) = p^2 \sum_{j=2}^{k-2} j. \tag{3.13}$$

To find the coefficient of p^3 we start with

$$A_3p^3 = C(k,k-6) - C(k,k-4)$$

and, as before, apply (3.5):

$$\begin{aligned} A_3p^3 &= C(k,k-6) - C(k,k-4) \\ &= C(k-1,k-7) + pC(k-1,k-5) \\ &\quad -\{C(k-1,k-5) + pC(k-1,k-3)\} \\ &= C(k-1,k-7) - C(k-1,k-5) \\ &\quad +p\{C(k-1,k-5) - C(k-1,k-3)\}. \end{aligned}$$

The last expression in brackets can be written

$$C(k-1,k-1-4) - C(k-1,k-1-2)$$

and, by (3.13), is equal to $p^2\sum_{j=2}^{k-3} j$. We have

$$A_3p^3 = C(k-1,k-7) - C(k-1,k-5) + p^3\sum_{j=2}^{k-3} j.$$

By (3.5) the right side is equal to

$$\begin{aligned} &C(k-2,k-8) + pC(k-2,k-6) \\ &\quad -\{C(k-2,k-6) + pC(k-2,k-4)\} + p^3\sum_{j=2}^{k-3} j \\ &= C(k-2,k-8) - C(k-2,k-6) \\ &\quad +p\{C(k-2,k-6) - C(k-2,k-4)\} + p^3\sum_{j=2}^{k-3} j \\ &= C(k-2,k-8) - C(k-2,k-6) + p\cdot p^2\sum_{j=2}^{k-4} j + p^3\sum_{j=2}^{k-3} j. \end{aligned}$$

We continue applying (3.5) and (3.13) until we have

$$A_3 p^3 \quad = \quad C(6,0) - C(6,2) + p^3 \sum_{j=2}^{4} j + p^3 \sum_{j=2}^{5} j \; + \cdots + p^3 \sum_{j=2}^{k-3} j.$$

By (3.6),

$$\begin{aligned} C(6,0) - C(6,2) &= (p+1)C(5,1) - \{C(5,1) + pC(5,3)\} \\ &= p\{C(5,1) - C(5,3)\} \\ &= p^3 \sum_{j=2}^{3} j. \end{aligned}$$

Therefore,

$$A_3 = \sum_{i=3}^{k-3} \sum_{j=2}^{i} j$$

i.e.

$$C(k, k-6) - C(k, k-4) = p^3 \sum_{i=3}^{k-3} \sum_{j=2}^{i} j.$$

Proposition 8 *The coefficient of p^s in $C(k, k-2s)$ is*

$$\sum_{l=s}^{k-s} \sum_{m=s-1}^{l} \cdots \sum_{i=3}^{h} \sum_{j=2}^{i} j.$$

Proof: The proof is by induction on s.

Assume true for $s-1$, i.e.,

$$C(k, k-2(s-1)) - C(k, k-2(s-1)+2) = p^{s-1} \sum_{l=s-1}^{k-(s-1)} \cdots \sum_{j=2}^{i} j. \quad (3.14)$$

By (3.5)

$$\begin{aligned} C(k,k-2s)-C(k,k-2s+2) &= C(k-1,k-2s-1)+pC(k-1,k-2s+1) \\ &\quad -\{C(k-1,k-2s+1)+pC(k-1,k-2s+3)\} \\ &= C(k-1,k-2s-1)-C(k-1,k-2s+1) \\ &\quad +p\{C(k-1,k-2s+1)-C(k-1,k-2s+3)\}. \end{aligned}$$

The last expression in brackets can be written

$$C(k-1,k-1-2(s-1))-C(k-1,k-1-2(s-1)+2)$$

and by the induction hypothesis (3.14) is equal to

$$p^{s-1}\sum_{r=s-1}^{k-1-(s-1)}\sum_{m=s-2}^{r}\cdots\sum_{j=2}^{i}j.$$

We have

$$\begin{aligned} C(k,k-2s)-C(k,k-2s+2) &= C(k-1,k-2s-1)-C(k-1,k-2s+1) \\ &\quad +p^{s}\sum_{r=s-1}^{k-s}\sum_{m=s-2}^{r}\cdots\sum_{j=2}^{i}j. \end{aligned}$$

Continue applying (3.5) and the induction hypothesis (3.14) until we have

$$\begin{aligned} C(k,k-2s)-C(k,k-2s+2) &= C(2s,0)-C(2s,2) \\ &\quad +p^{s}\sum_{r=s-1}^{2s-(s-1)}\cdots\sum_{j=2}^{i}j \\ &\quad \vdots \end{aligned}$$

$$+p^s \sum_{r=s-1}^{k-s} \cdots \sum_{j=2}^{i} j.$$

From (3.5),(3.6) and (3.14)

$$\begin{aligned}
&C(2s,0)-C(2s,2)\\
&= (p+1)C(2s-1,1)-\{C(2s-1,1)+pC(2s-1,3)\}\\
&= p\{C(2s-1,1)-C(2s-1,3)\}\\
&= p\cdot p^{s-1}\sum_{r=s-1}^{2s-1-(s-1)} \cdots \sum_{j=2}^{i} j\\
&= p^s \sum_{r=s-1}^{s} \cdots \sum_{j=2}^{i} j.
\end{aligned}$$

Consequently

$$C(k,k-2s)-C(k,k-2s+2)=p^s\sum_{l=s}^{k-s}\sum_{r=s-1}^{l}\cdots\sum_{j=2}^{i} j. \quad \blacksquare$$

Since $C(k,d)=0$ if k and d have different parities or if $k<d$, our solution is

$$u(x,t)=e^{-t}\sum_{y}\left\{\sum_{k=0}^{\infty}\frac{1}{(d+2k)!}\left(\frac{1}{p+1}\right)^{d+2k} t^{d+2k}C(d+2k,d)\phi(y)\right\}$$

where $d=d(x,y)$. We have shown

$$\begin{aligned}
C(d+2k,d) &= 1+p(d+2k-1)+p^2\sum_{j=2}^{d+2k-2} j\\
&\quad +p^3\sum_{i=3}^{d+2k-3}\sum_{j=2}^{i} j+\cdots+p^k\sum_{l=k}^{d+k}\sum_{r=k-1}^{l}\cdots\sum_{j=2}^{i} j.
\end{aligned}$$

Theorem 12 *The heat kernel for the $(p+1)-$regular tree is*

$$p(x,y,t) = e^{-t}\sum_{k=0}^{\infty}\frac{1}{(d+2k)!}\left(\frac{1}{p+1}\right)^{d+2k} t^{d+2k}C(d+2k,d)$$

where $d = d(x,y)$.

Proof: For convenience, write $p(x,y,t)$ as $e^{-t}g(t,d)$, where $d = d(x,y)$. Each vertex $x \neq y$ in T has one neighbor one unit closer to y and p neighbors one unit further from y. Therefore

$$\begin{aligned}
&\Delta_x p(x,y,t)\\
&= \frac{1}{p+1}\sum_{z\sim x} p(z,y,t) - p(x,y,t)\\
&= e^{-t}\frac{1}{p+1}g(t,d-1) + e^{-t}\frac{p}{p+1}g(t,d+1) - e^{-t}g(t,d)\\
&= e^{-t}\frac{1}{p+1}\sum_{k=0}^{\infty}\frac{1}{(d-1+2k)!}\left(\frac{1}{p+1}\right)^{d-1+2k} t^{d-1+2k}C(d-1+2k,d-1)\\
&\quad +e^{-t}\frac{p}{p+1}\sum_{k=0}^{\infty}\frac{1}{(d+1+2k)!}\left(\frac{1}{p+1}\right)^{d+1+2k} t^{d+1+2k}C(d+1+2k,d+1)\\
&\quad -e^{-t}g(t,d).
\end{aligned}$$

We also have

$$\begin{aligned}
\frac{\partial}{\partial t}p(x,y,t) &= \frac{\partial}{\partial t}\{e^{-t}g(t,d)\}\\
&= e^{-t}\frac{\partial}{\partial t}g(t,d) - e^{-t}g(t,d)\\
&= e^{-t}\frac{\partial}{\partial t}\sum_{k=0}^{\infty}\frac{1}{(d+2k)!}\left(\frac{1}{p+1}\right)^{d+2k} t^{d+2k}C(d+2k,d) - e^{-t}g(t,d)\\
&= e^{-t}\sum_{k=0}^{\infty}\frac{1}{(d+2k-1)!}\left(\frac{1}{p+1}\right)^{d+2k} t^{d+2k-1}C(d+2k,d)
\end{aligned}$$

$$
\begin{aligned}
&-e^{-t}g(t,d)\\
=\;& e^{-t}\frac{1}{(d-1)!}\left(\frac{1}{p+1}\right)^{d} t^{d-1}C(d,d)\\
&+e^{-t}\sum_{k=1}^{\infty}\frac{1}{(d+2k-1)!}\left(\frac{1}{p+1}\right)^{d+2k} t^{d+2k-1}C(d+2k,d)\\
&-e^{-t}g(t,d).
\end{aligned}
$$

Now apply (3.5) to the middle expression to obtain

$$
\begin{aligned}
& e^{-t}\frac{1}{(d-1)!}\left(\frac{1}{p+1}\right)^{d} t^{d-1}C(d,d)\\
+\;& e^{-t}\sum_{k=1}^{\infty}\frac{1}{(d+2k-1)!}\left(\frac{1}{p+1}\right)^{d+2k} t^{d+2k-1}C(d+2k-1,d-1)\\
+\;& pe^{-t}\sum_{k=1}^{\infty}\frac{1}{(d+2k-1)!}\left(\frac{1}{p+1}\right)^{d+2k} t^{d+2k-1}C(d+2k-1,d+1)\\
-\;& e^{-t}g(t,d).
\end{aligned}
$$

Combining the first two expressions and re-indexing the third we have

$$
\begin{aligned}
& e^{-t}\sum_{k=0}^{\infty}\frac{1}{(d+2k-1)!}\left(\frac{1}{p+1}\right)^{d+2k} t^{d+2k-1}C(d+2k-1,d-1)\\
+\;& pe^{-t}\sum_{k=0}^{\infty}\frac{1}{(d+2k+1)!}\left(\frac{1}{p+1}\right)^{d+2k+1} t^{d+2k+1}C(d+2k+1,d+1)\\
-\;& e^{-t}g(t,d)\\
=\;& \Delta_x p(x,y,t)
\end{aligned}
$$

To show $\lim_{t\to 0} p(x,y,t) = \delta_y(x)$ write

$$
p(x,y,t) \;=\; e^{-t}\frac{1}{d!}\left(\frac{1}{p+1}\right)^{d} t^{d}
$$

$$+e^{-t}\sum_{k=1}^{\infty}\frac{1}{(d+2k)!}\left(\frac{1}{p+1}\right)^{d+2k}t^{d+2k}C(d+2k,d).$$

For $d \neq 0$, clearly $\lim_{t\to 0} p(x,y,t) = 0$.

For $d = 0$,

$$\lim_{t\to 0} p(x,y,t) = \lim_{t\to 0} e^{-t}t^0 = 1. \quad \blacksquare$$

Theorem 13 *i) $p(x,y,t)$ is symmetric in the space variables. ii) $p(x,y,t)$ satisfies the conservation of heat property.*

Proof: i) $p(x,y,t)$ depends only on t and the distance between x and y.

ii) We will show that $\sum_x p(x,y,t)$ is constant as a function of t and we already have $\sum_x p(x,y,0) = 1$. For a fixed vertex y, there are $p+1$ vertices at distance 1 from y, $p(p+1)$ vertices at distance 2, and $p^{n-1}(p+1)$ vertices at distance n. Therefore,

$$\begin{aligned}
\frac{\partial}{\partial t}\sum_x p(x,y,t) &= \sum_x \frac{\partial}{\partial t}p(x,y,t) \\
&= \sum_x \Delta p(x,y,t) \\
&= \Delta\left\{e^{-t}g(t,0) + e^{-t}\sum_{n=1}^{\infty}p^{n-1}(p+1)g(t,n)\right\} \\
&= e^{-t}\left\{\frac{1}{p+1}(p+1)g(t,1) - g(t,0)\right\} \\
&\quad +e^{-t}\left\{\sum_{n=1}^{\infty}p^{n-1}(p+1)\left(\frac{1}{p+1}g(t,n-1) + \frac{p}{p+1}g(t,n+1)\right)\right\} \\
&\quad -e^{-t}\left\{\sum_{n=1}^{\infty}p^{n-1}(p+1)\ g(t,n)\right\} \\
&= e^{-t}\{g(t,1) - g(t,0)\} \\
&\quad +e^{-t}\left\{g(t,0) + p\ g(t,1) + \sum_{n=3}^{\infty}p^{n-1}g(t,n-1)\right\}
\end{aligned}$$

$$
\begin{aligned}
& +e^{-t}\left\{\sum_{n=1}^{\infty} p^n g(t,n+1)\right\} \\
& -e^{-t}\left\{(p+1)g(t,1)+\sum_{n=2}^{\infty} p^{n-1}(p+1)g(t,n)\right\} \\
= \; & e^{-t}\sum_{2}^{\infty} p^n g(t,n) + e^{-t}\sum_{2}^{\infty} p^{n-1} g(t,n) \\
& -e^{-t}\sum_{2}^{\infty} p^{n-1}(p+1)g(t,n) \\
= \; & 0. \quad \blacksquare
\end{aligned}
$$

Next we show that $C(d+2k,d)$ can also be expressed in terms of binomial coefficients. We need the following easy lemma.

Lemma 3

$$\sum_{j=r}^{n} B(j,r) = B(n+1,r+1).$$

Proof: The proof is by induction.

For $n = r : B(r,r) = B(r+1,r+1)$.

For $n = r+1 :$

$$
\begin{aligned}
B(r,r)+B(r+1,r) &= 1+r+1 \\
&= r+2 \\
&= B(r+2,r+1)
\end{aligned}
$$

Assume true for $n-1$. Then

$$
\begin{aligned}
\sum_{j=r}^{n} B(j,r) &= \sum_{j=r}^{n-1} B(j,r) + B(n,r) \\
&= B(n,r+1) + B(n,r)
\end{aligned}
$$

$$\begin{aligned} &= \frac{n!}{(r+1)!(n-r-1)!} + \frac{n!}{r!(n-r)!} \\ &= \frac{(n+1)!}{(r+1)!(n-r-1)!} \\ &= B(n+1, r+1). \quad \blacksquare \end{aligned}$$

Proposition 9 *The coefficient of p^s in $C(d+2k, d)$, for $1 \leq s \leq k$, is*

$$B(d+2k, s) - B(d+2k, s-1).$$

Proof: Let $n = d + 2k$.

For $s = 1$, we have $n - 1 = B(n, 1) - B(n, 0)$.

For $s = 2$, we want to show

$$\sum_{j=2}^{n-2} j = B(n,2) - B(n,1).$$

$$\begin{aligned} \sum_{j=2}^{n-2} j &= \sum_{j=1}^{n-2} j - 1 \\ &= \frac{(n-2)(n-1)}{2} - 1 \\ &= \frac{n(n-3)}{2} \end{aligned}$$

and

$$\begin{aligned} B(n,2) - B(n,1) &= \frac{n!}{2!(n-2)!} - \frac{n!}{1!(n-1)!} \\ &= \frac{n(n-3)}{2}. \end{aligned}$$

For $s = 3$, we want to show

$$\sum_{i=3}^{n-3} \sum_{j=2}^{i} j = B(n,3) - B(n,2).$$

We have

$$\begin{aligned}
\sum_{i=3}^{n-3} \sum_{j=2}^{i} j &= \sum_{j=2}^{3} j + \sum_{j=2}^{4} j + \cdots + \sum_{j=2}^{n-3} j \\
&= B(5,2) - B(5,1) \\
&\quad + B(6,2) - B(6,1) \\
&\quad \vdots \\
&\quad + B(n-1,2) - B(n-1,1) \\
&= \sum_{j=5}^{n-1} B(j,2) - \sum_{j=5}^{n-1} B(j,1) \\
&= B(n,3) - B(n,2) \qquad \text{by Lemma 3.}
\end{aligned}$$

Assume true for $s - 1$: i.e.,

$$\sum_{l=s-1}^{n-(s-1)} \cdots \sum_{j=2}^{i} j = B(n, s-1) - B(n, s-2).$$

Then

$$\begin{aligned}
\sum_{r=s}^{n-s} \sum_{l=s-1}^{r} \cdots \sum_{j=2}^{i} j &= \sum_{l=s-1}^{s} \cdots \sum_{j=2}^{i} j + \sum_{l=s-1}^{s+1} \cdots \sum_{j=2}^{i} j + \cdots + \sum_{l=s-1}^{n-s} \cdots \sum_{j=2}^{i} j \\
&= B(2s-1, s-1) - B(2s-1, s-2) \\
&\quad + B(2s, s-1) - B(2s, s-2) \\
&\quad \vdots \\
&\quad + B(n-1, s-1) - B(n-1, s-2)
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{j=2s-1}^{n-1} B(j, s-1) - \sum_{j=2s-1}^{n-1} B(j, s-2) \\
&= B(n, s) - B(n, s-1) \qquad \text{by Lemma 3.} \blacksquare
\end{aligned}
$$

Lemma 4 *For n even, we have, for*

$$C(n,0) = 1 + A_1 p + A_2 p^2 + \cdots + A_{\frac{n}{2}} p^{\frac{n}{2}}$$

and

$$C(n+1,1) = 1 + F_1 p + F_2 p^2 + \cdots + F_{\frac{n}{2}} p^{\frac{n}{2}},$$

i) $s \cdot A_s > 1 + A_1 + A_2 + \cdots + A_{s-1} \qquad 1 \le s < \frac{n}{2}$

ii) $\frac{n}{2} \cdot A_{\frac{n}{2}} = 1 + A_1 + A_2 + \cdots + A_{\frac{n-2}{2}}$

iii) $s \cdot F_s > 1 + F_1 + F_2 + \cdots + F_{s-1} \qquad 1 \le s < \frac{n}{2}$

iv) $\frac{n}{2} \cdot F_{\frac{n}{2}} = 2(1 + F_1 + F_2 + \cdots + F_{\frac{n-2}{2}})$.

Proof:

$$
\begin{aligned}
s \cdot A_s &= s\{B(n,s) - B(n,s-1)\} \\
&= s\left\{\frac{n!}{s!(n-s)!} - \frac{n!}{(s-1)!(n-s+1)!}\right\} \\
&= \frac{n!(n-2s+1)}{(s-1)!(n-s+1)!}
\end{aligned}
$$

and

$$
\begin{aligned}
1 + A_1 + A_2 + \cdots + A_{s-1} &= 1 + B(n,1) - B(n,0) \\
&\quad + B(n,2) - B(n,1) \\
&\quad \vdots
\end{aligned}
$$

$$
\begin{aligned}
&\qquad + B(n, s-1) - B(n, s-2) \\
&= B(n, s-1) \\
&= \frac{n!}{(s-1)!(n-s+1)!}.
\end{aligned}
$$

But

$$\frac{n!(n-2s+1)}{(s-1)!(n-s+1)!} \geq \frac{n!}{(s-1)!(n-s+1)!}$$

with equality if and only if $s = \frac{n}{2}$. This gives (i) and (ii).

For (iii) and (iv),

$$
\begin{aligned}
s \cdot F_s &= s\{B(n+1, s) - B(n+1, s-1)\} \\
&= s\left\{\frac{(n+1)!}{s!(n+1-s)!} - \frac{(n+1)!}{(s-1)!(n-s+2)!}\right\} \\
&= \frac{(n+1)!(n-2s+2)}{(s-1)!(n-s+2)!}
\end{aligned}
$$

and

$$
\begin{aligned}
1 + F_1 + F_2 + \cdots + F_{s-1} &= B(n+1, s-1) \\
&= \frac{(n+1)!}{(s-1)!(n-s+2)!}.
\end{aligned}
$$

We have

$$\frac{(n+1)!(n-2s+2)}{(s-1)!(n-s+2)!} > \frac{(n+1)!}{(s-1)!(n-s+2)!}$$

for $1 \leq s \leq \frac{n}{2}$, and for $s = \frac{n}{2}$ the right side is twice the left side. ∎

Lemma 5 *For $A > 0, B_j > 0$, and $p \geq 1$, $A \geq B_0 + B_1 + \cdots + B_{s-1}$ implies $Ap^s \geq B_0 + B_1 p + \cdots + B_{s-1}p^{s-1}$. The inequality is strict for $p > 1$.*

Proof: For $s = 1$, $A \geq B_0$ implies $Ap \geq B_0$, and for $p > 1$, $Ap > B_0$.

For $s = 2$, we want to show $A \geq B_0 + B_1$ implies

$$Ap^2 \geq B_0 + B_1 p. \tag{3.15}$$

For $p = 1$, there is nothing to show.

For $p > 1$, note that

$$\frac{d}{dp}[Ap^2] = 2Ap \geq 2p(B_0 + B_1) \geq B_1 = \frac{d}{dp}[B_0 + B_1 p].$$

Therefore, the left side of (3.15) increases faster than the right side.

Assume true for $s - 1$.

Then we want to show $A \geq B_0 + B_1 + \cdots + B_{s-1}$ implies

$$Ap^s \geq B_0 + B_1 p + \cdots + B_{s-1} p^{s-1} \tag{3.16}$$

Again, for $p = 1$, there is nothing to show.

For $p > 1$, $\frac{d}{dp}[Ap^s] = sAp^{s-1}$ and

$$\begin{aligned} sA &\geq s(B_0 + B_1 + \cdots + B_{s-1}) \\ &> B_1 + 2B_2 + \cdots + (s-1)B_{s-1}. \end{aligned}$$

Therefore, by the induction hypothesis,

$$\begin{aligned} sAp^{s-1} &> B_1 + 2B_2 p + \cdots + (s-1)B_{s-1}p^{s-2} \\ &= \frac{d}{dp}[B_0 + B_1 p + \cdots + B_{s-1}p^{s-2}] \end{aligned}$$

so the left side of (3.16) increases faster than the right side. ∎

Theorem 14 *For t fixed, $p(x,y,t)$ decreases as the distance between x and y increases.*

Proof: We want to show $e^{-t}g(t,d) > e^{-t}g(t,d+1)$ or, equivalently, $g(t,d) > g(t,d+1)$ for all d. For convenience, let $m = p+1$. Write

$$g(t,d) = \frac{1}{d!}\left(\frac{1}{m}\right)^{d} t^{d} + \frac{1}{(d+2)!}\left(\frac{1}{m}\right)^{d+2} t^{d+2}C(d+2,d) + \cdots$$

as

$$A_0t^d + A_1t^{d+2} + A_2t^{d+4} + \cdots + A_kt^{d+2k} + \cdots$$

and

$$g(t,d+1) = \frac{1}{(d+1)!}\left(\frac{1}{m}\right)^{d+1} t^{d+1} + \frac{1}{(d+3)!}\left(\frac{1}{m}\right)^{d+3} t^{d+3}C(d+3,d+1) + \cdots$$

as

$$B_0t^{d+1} + B_1t^{d+3} + B_2t^{d+5} + \cdots + B_kt^{d+1+2k} + \cdots$$

We will show

1) $A_0t^d + \frac{1}{2}A_1t^{d+2} > B_0t^{d+1}$

2) $\frac{1}{2}A_kt^{d+2k} + \frac{1}{2}A_{k+1}t^{d+2k+2} > B_kt^{d+1+2k}$.

1) We want

$$\frac{1}{d!}\left(\frac{1}{m}\right)^{d} t^{d} + \frac{1}{(d+2)!}\left(\frac{1}{m}\right)^{d+2} t^{d+2}C(d+2,d) > \frac{1}{(d+1)!}\left(\frac{1}{m}\right)^{d+1} t^{d+1}$$

or equivalently (multiply by $2(d+2)!\ m^{d+2}$, rearrange)

$$t^d\{C(d+2,d)t^2 - 2m(d+2)t + 2m^2(d+2)(d+1)\} > 0. \tag{3.17}$$

The discriminant is

$$\begin{aligned} & 4m^2(d+2)^2 - 4\cdot 2m^2(d+2)(d+1)C(d+2,d) \\ = & \ 4m^2(d+2)\{d+2-2(d+1)C(d+2,d)\} \\ = & \ 4m^2(d+2)\{d+2-2(d+1)(1+(d+1)p)\} \\ < & \ 0. \end{aligned}$$

Therefore, since (3.17) is true for $t = 1$, (3.17) is true for all $t > 0$.

2) We want

$$\frac{1}{2}\frac{1}{(d+r)!}\left(\frac{1}{m}\right)^{d+r} t^{d+r}C(d+r,d)+\frac{1}{(d+r+2)!}\left(\frac{1}{m}\right)^{d+r+2} t^{d+r+2}C(d+r+2,d)$$

$$> \frac{1}{(d+r+1)!}\left(\frac{1}{m}\right)^{d+r+1} t^{d+r+1}C(d+r+1,d+1)$$

or equivalently (multiply by $2(d+r+2)!\ m^{d+r+2}$, rearrange)

$$\begin{aligned} t^{d+r}\{C(d+r+2,d)t^2 & - 2m(d+r+2)C(d+r+1,d+1)t \\ & + (d+r+2)(d+r+1)m^2C(d+r,d)\} > 0. \end{aligned}$$

Here, r is even and $r \geq 2$. We will show that the expression in the brackets is always positive by showing that its minimum value is positive. The minimum occurs at

$$t = \frac{2m(d+r+2)C(d+r+1,d+1)}{2C(d+r+2,d)}$$

and the minimum is

$$(d+r+2)(d+r+1)m^2C(d+r,d) - \frac{m^2(d+r+2)^2\ C^2(d+r+1,d+1)}{C(d+r+2,d)}.$$

So we want to show

$$(d+r+1)C(d+r,d)C(d+r+2,d)-(d+r+2)C^2(d+r+1,d+1) > 0. \quad (3.18)$$

Using (3.5), we have

$$C(d+r+1,d+1) = C(d+r,d) + pC(d+r,d+2)$$

and, for $d \geq 2$,

$$\begin{aligned} C(d+r+2,d) &= C(d+r+1,d-1) + pC(d+r+1,d+1) \\ &= C(d+r,d-2) + pC(d+r,d) \\ &\quad +p\{C(d+r,d) + pC(d+r,d)\} \\ &= C(d+r,d-2) + 2pC(d+r,d) + p^2C(d+r,d+2). \end{aligned}$$

Therefore, (3.18) is equivalent to

$$(d+r+1)C(d+r,d)\{C(d+r,d-2) + 2pC(d+r,d) + p^2C(d+r,d+2)\}$$

$$-\ (d+r+2)\{C(d+r,d) + pC(d+r,d+2)\}^2 > 0$$

or

$$\begin{aligned} & p^2C(d+r,d+2)\{(d+r+1)C(d+r,d) - (d+r+2)C(d+r,d+2)\} \\ + \quad & 2pC(d+r,d)\{(d+r+1)C(d+r,d) - (d+r+2)C(d+r,d+2)\} \\ + \quad & C(d+r,d)\{(d+r+1)C(d+r,d-2) - (d+r+2)C(d+r,d)\} > 0. \end{aligned}$$

We will show that the expressions in the brackets are positive.

$$i) \qquad (d+r+1)C(d+r,d) > (d+r+2)C(d+r,d+2): \qquad (3.19)$$

From Proposition 7,

$$C(d+r,d) = C(d+r,d+2) + \text{the } p^{\frac{r}{2}} \text{ term of } C(d+r,d).$$

Therefore, (3.19) is equivalent to

$$(d+r+1)\{\text{the } p^{\frac{r}{2}} \text{ term of } C(d+r,d)\} > C(d+r,d+2)$$

or, letting $s = \frac{r}{2}$

$$(d+2s+1)A_s p^s > 1 + A_1 p + \cdots + A_{s-1}p^{s-1}.$$

Since $s < \frac{d+r}{2}$ and $d+2s+1 > s$, Lemma 4 implies

$$(d+2s+1)A_s p^s > 1 + A_1 + \cdots + A_{s-1}$$

and the result follows from Lemma 5.

$$ii) \qquad (d+r+1)C(d+r,d-2) > (d+r+2)C(d+r,d): \qquad (3.20)$$

From Proposition 7,

$$C(d+r,d-2) = C(d+r,d) + \text{the } p^{\frac{r+2}{2}} \text{ term of } C(d+r,d-2).$$

Therefore, (3.20) is equivalent to

$$(d+r+1)\{\text{the } p^{\frac{r+2}{2}} \text{ term of } C(d+r,d-2)\} > C(d+r,d)$$

or, letting $s = \frac{r+2}{2}$

$$(d+2s-1)A_s p^s > 1 + A_1 p + \cdots + A_{s-1}p^{s-1}.$$

Since $s \leq \frac{d+r}{2}$ and $d+2s-1 > s$, this follows from Lemma 4 and Lemma 5.

There are two cases left: $d = 0$ and $d = 1$. For $d = 0$, we want, from (3.18),

$$(r+1)C(r,0)C(r+2,0) > (r+2)C^2(r+1,1). \qquad (3.21)$$

By (3.6), $C(r+2,0) = (p+1)C(r+1,1)$ so (3.21) is equivalent to

$$(r+1)(p+1)C(r,0) > (r+2)C(r+1,1)$$

or

$$(r+1)\{(p+1)C(r,0) - C(r+1,1)\} > C(r+1,1). \qquad (3.22)$$

By (3.5), $C(r+1,1) = C(r,0) + pC(r,2)$ so (3.22) is equivalent to

$$(r+1)\{(p+1)C(r,0) - C(r,0) - pC(r,2)\} > C(r,0) + pC(r,2)$$

or

$$(r+1)p\{C(r,0) - C(r,2)\} > C(r,0) + pC(r,2).$$

Using Proposition 7, this becomes

$$(r+1)p\ \{\text{the } p^{\frac{r}{2}} \text{ term of } C(r,0)\} > C(r,0) + pC(r,2).$$

Letting $s = \frac{r}{2}$, we want to show

$$\begin{aligned}(2s+1)pA_sp^s &> 1 + A_1p + \cdots + A_sp^s \\ &\quad +p(1 + A_1p + \cdots + A_{s-1}p^{s-1})\end{aligned}$$

or

$$(2s+1)pA_sp^s > 1 + (1 + A_1)p + (A_1 + A_2)p^2 \cdots + (A_{s-1} + A_s)p^s.$$

But by Lemma 4

$$(2s+1)A_s = 1 + 1 + A_1 + A_1 + A_2 + \cdots + A_{s-1} + A_s$$

and the inequality follows from Lemma 5 for $p > 1$.

For $d = 1$, we want, from (3.18),

$$(r+2)C(r+1,1)C(r+3,1) > (r+3)C^2(r+2,2). \tag{3.23}$$

From (3.6), $C(r+2,0) = (p+1)C(r+1,1)$. Substituting into (3.23) we now want

$$(r+2)C(r+2,0)C(r+3,1) > (r+3)(p+1)C^2(r+1,1). \tag{3.24}$$

From Proposition 7,

$$C(r+2,0) = C(r+2,2) + \text{the } p^{\frac{r+2}{2}} \text{ term of } C(r+2,0)$$

i.e., letting $s = \frac{r+2}{2}$,

$$C(2s,0) = C(2s,2) + A_s p^s.$$

From (3.5)

$$\begin{aligned} C(r+3,1) &= C(r+2,0) + pC(r+2,2) \\ &= C(2s,2) + A_s p^s + pC(2s,2) \\ &= (p+1)C(2s,2) + A_S p^s. \end{aligned}$$

Therefore, the left side of (3.24) is equal to

$$(2s)\{(p+1)C^2(2s,2) + (p+2)C(2s,2)A_s p^s + (A_s p^s)^2\}$$

and the right side is

$$(2s+1)(p+1)C^2(2s,2).$$

Subtracting $(2s)(p+1)C^2(2s,2)$ from each side, we now want to show

$$(2s)A_s p^s\{(p+2)C(2s,2) + A_s p^s\} > (p+1)C^2(2s,2)$$

or

$$(2s)A_s p^s\{(p+2)(1 + A_1 p + \cdots + A_{s-1}p^{s-1}) + A_s p^s\}$$

$$> (p+1)(1 + A_1 p + \cdots + A_{s-1} p^{s-1})^2. \tag{3.25}$$

From Lemma 4

$$(2s)A_s > 1 + A_1 + \cdots + A_{s-1}$$

so by Lemma 5 ,

$$(2s)A_s p^s > 1 + A_1 p + \cdots + A_{s-1} p^{s-1}.$$

Therefore we have (3.25) and the result follows. ∎

3.2 Hot Spots on Trees

Regular trees are in some ways discrete analogues of hyperbolic spaces. One expects the movement of hot spots on trees to mimic the movement of hot spots on hyperbolic spaces. We show that the hot spots are contained in the convex hull of the support of the initial data and, as in the case of hyperbolic spaces, the hot spots do not necessarily tend to one fixed point.

Let T be a regular tree. A set $C \subset T$ is convex if it contains all minimal paths from x to y for all pairs of vertices x, y in C. Since minimal paths in T are unique, a set will be convex if and only if it is connected. The convex hull C_B of a set $B \subset T$ is the smallest connected set containing B. If C is convex and $x \notin C$ then there is a unique $y_0 \in C$ such that $d(x, C) = d(x, y_0)$.

Theorem 15 *Suppose $\phi \geq 0$ is defined on a finite set $S \subset T$. Let C_S be the convex hull of S and let $H(t; \phi) = \{x \in T : P_t\phi(x) = \max_{z \in T} P_t\phi(z)\}$. Then $H(t; \phi) \subset C_S$ for all t.*

Proof: For $x \notin C_S$, let $y_0 \in C_S$ be the unique vertex such that $d(x, C_S) =$

$d(x, y_0)$. Then for any $y \in C_S, d(y_0, y) < d(x, y)$. Therefore by Theorem 14

$$\begin{aligned} P_t\phi(x) &= e^{-t} \sum_{y \in C_S} g(t, d(x, y))\phi(y) \\ &< e^{-t} \sum_{y \in C_S} g(t, d(y_0, y))\phi(y) \\ &= P_t\phi(y_0). \quad \blacksquare \end{aligned}$$

We turn next to the question of the nonuniqueness of hot spots. We have

Theorem 16 *Let T be an $m-$regular tree. If $m \geq 4$ and if the initial temperature distribution consists of two point sources distance 4 apart, then there are two distinct hot spots. If $m = 3$, starting with point sources distance 8 apart guarantees distinct hot spots.*

Proof: Let support $\phi = \{p, q\}$ with $\phi(p) = \phi(q) = 1$.

The convex hull C of the support of ϕ is the unique minimal path joining p and q. For the $m \geq 4$ case, we will write this path as $\{p, y, x, z, q\}$.

Clearly, $P_t\phi(p) = P_t\phi(q)$ for all t and $P_t\phi(y) = P_t\phi(z)$ for all t so we only have to show that x is not the hot spot.

$P_t\phi(p) = P_t\phi(q) = e^{-t}\{g(t, 0) + g(t, 4)\}$ and $P_t\phi(x) = e^{-t}\{2g(t, 2)\}$. We will show that $g(t, 0) + g(t, 4) > 2g(t, 2)$ for all t.

Recall

$$\begin{aligned} g(t,0) + g(t,4) &= 1 + \frac{1}{2!}\frac{1}{m^2}C(2,0)t^2 + \frac{1}{4!}\frac{1}{m^4}C(4,0)t^4 + \cdots \\ &+ \frac{1}{4!}\frac{1}{m^4}C(4,4)t^4 + \frac{1}{6!}\frac{1}{m^6}C(6,4)t^6 + \cdots \end{aligned}$$

and

$$2g(t,2) = 2\{\frac{1}{2!}\frac{1}{m^2}C(2,2)t^2 + \frac{1}{4!}\frac{1}{m^4}C(4,2)t^4 + \cdots\}.$$

Comparing the coefficients of t^2, we have

$$C(2,0) > 2C(2,2)$$

since $C(2,0) = m$ and $C(2,2) = 1$.

Comparing the coefficients of t^4 we want

$$C(4,0) + C(4,4) > 2C(4,2).$$

This is equivalent to, with $p = m - 1$,

$$1 + 3p + 2p^2 + 1 > 2(1 + 3p)$$

or $p > 3/2$, i.e., $m \geq 3$.

For t^{2n} we want

$$C(2n,0) + C(2n,4) > 2C(2n,2).$$

From Proposition 6 we have

$$\begin{aligned} C(2n,0) &= 1 + A_1 p + A_2 p^2 + \cdots + A_n p^n. \\ C(2n,2) &= 1 + A_1 p + A_2 p^2 + \cdots + A_{n-1} p^{n-1}. \\ C(2n,4) &= 1 + A_1 p + A_2 p^2 + \cdots + A_{n-2} p^{n-2}. \end{aligned}$$

We want

$$\begin{aligned} 1 + A_1 p + \cdots + A_n p^n + \\ 1 + A_1 p + \cdots + A_{n-2} p^{n-2} &> 2(1 + A_1 p + \cdots + A_{n-1} p^{n-1}) \end{aligned}$$

or

$$A_n p^n > A_{n-1} p^{n-1}$$

or

$$p > \frac{A_{n-1}}{A_n}. \tag{3.26}$$

From Proposition 9

$$A_n = B(2n, n) - B(2n, n-1) = \frac{(2n)!}{n!(n+1)!}$$

and

$$A_{n-1} = B(2n, n-1) - B(2n, n-2) = \frac{3(2n)!}{(n-1)!(n+2)!}$$

so (3.26) is equivalent to

$$p > \frac{3(2n)!}{(n-1)!(n+2)!} \cdot \frac{n!}{(n+1)!}$$

or

$$p > \frac{3n}{n+2}.$$

Since p must be an integer (3.26) is true for $p \geq 3$, i.e., $m \geq 4$.

For the $m = 3$ case we start with p and q distance 8 apart and show $P_t\phi(p) = P_t\phi(q) > P_t\phi(x)$ where x is the vertex that is distance 4 from p and distance 4 from q. We have $P_t\phi(p) = P_t\phi(q) = e^{-t}\{g(t,0) + g(t,8)\}$ and

$P_t\phi(x) = e^{-t}\{2g(t,4)\}$ with

$$\begin{aligned} g(t,0)+g(t,8) &= 1+\frac{1}{2!}\frac{1}{m^2}C(2,0)t^2+\frac{1}{4!}\frac{1}{m^4}C(4,0)t^4+\cdots \\ &+ \frac{1}{8!}\frac{1}{m^8}C(8,8)t^8+\frac{1}{10!}\frac{1}{m^{10}}C(10,8)t^{10}+\cdots \end{aligned}$$

and

$$2g(t,4) = 2\{\frac{1}{4!}\frac{1}{m^4}C(4,4)t^4+\frac{1}{6!}\frac{1}{m^6}C(6,4)t^6+\cdots\}.$$

Comparing the coefficients of t^4 we have $C(4,0) > 2C(4,4)$ since

$$C(4,0) = 1+3\cdot 2+2\cdot 2^2 \text{ and } C(4,4) = 1.$$

Comparing the coefficients of t^6 we have $C(6,0) > 2C(6,4)$ since

$$C(6,0) = 1+5\cdot 2+9\cdot 2^2+5\cdot 2^3 \text{ and } C(6,4) = 1+5\cdot 2.$$

For $t^{2n}, n \geq 4$, we want

$$C(2n,0)+C(2n,8) > 2C(2n,4).$$

That is, with $p = 2$,

$$\begin{aligned} &1+A_1p+\cdots+A_np^n+ \\ &1+A_1p+\cdots+A_{n-4}p^{n-4} \quad > \quad 2(1+A_1p+\cdots+A_{n-2}p^{n-2}) \end{aligned}$$

or

$$A_{n-1}2^{n-1}+A_n2^n = A_{n-3}2^{n-3}+A_{n-2}2^{n-2}. \qquad (3.27)$$

Using $A_j = B(2n,j) - B(2n,j-1)$ (Proposition 9), we have

$$\begin{aligned}
A_n &= \frac{(2n)!}{n!(n+1)!} \\
A_{n-1} &= \frac{3(2n)!}{(n-1)!(n+2)!} \\
A_{n-2} &= \frac{5(2n)!}{(n-2)!(n+3)!} \\
A_{n-3} &= \frac{7(2n)!}{(n-3)!(n+4)!}
\end{aligned}$$

so 3.27 is equivalent to

$$\frac{3(2n)!\cdot 2^{n-1}}{(n-1)!(n+2)!} + \frac{(2n)!\cdot 2^{n}}{n!(n+1)!} > \frac{7(2n)!\cdot 2^{n-3}}{(n-3)!(n+4)!} + \frac{5(2n)!\cdot 2^{n-2}}{(n-2)!(n+3)!}$$

or

$$3\cdot 2^2\cdot n(n+4)(n+3)+2^3\cdot(n+4)(n+3)(n+2) > 7\cdot n(n-1)(n-2)+5\cdot 2\cdot n(n-1)(n+4)$$

or

$$(n+4)(n+3)(20n+16) > n(n-1)(17n+26)$$

which is easily seen to be true for $n \geq 4$. ∎

Note that for $m = 2$ the "tree" is Z^1 and in that case, for large t, the hot spot is always the center of mass (Theorem 8).

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