Lemma III.1.5 For any $u \neq v$, we have

$$r'_{u,v}(0) \geq 0.$$

Proof: Since $r_{u,v}'(t) = \frac{d}{dt} \frac{p_t(u,v)}{p_t(v,v)} = \frac{p'_t(u,v)\, p_t(v,v) - p_t(u,v)\, p'_t(v,v)}{p_t(v,v)^2}$,

it remains to show

$$p_t'(u,v)\, p_t(v,v) \geq p_t(u,v)\, p_t'(v,v) \quad \text{at } t=0$$

We have $p_0(v,v) = \frac{1}{d_v}$, $p_0(u,v) = 0$, since $p_0(u,v) = \langle P_0 \delta_v, \delta_u \rangle \frac{1}{d_u}$
$= \frac{\delta_{uv} d_u}{d_u} = \delta_{uv}$

Moreover,
$$p_t'(u,v)\Big|_{t=0} = \Delta_u\, p_t(u,v)\Big|_{t=0} = (\Delta_u \delta_v)(u)$$
$$= \frac{1}{d_u} \sum_{z \sim u} \left(\delta_v(z) - \delta_v(u)\right)$$
$$= \frac{1}{d_u} \sum_{z \sim u} \delta_v(z) = \begin{cases} \frac{1}{d_u} & v \sim u \\ 0 & v \not\sim u \end{cases} \geq 0.$$

Therefore $p_t'(u,v)\, p_t(v,v)\Big|_{t=0} = p_t'(u,v)\Big|_{t=0} \geq 0 = p_0(u,v)\, p_t'(v,v)\Big|_{t=0}$ □.

Proof of Nica's Theorem:

Observe first that we need to show

$$h(t) := p_t'(u,v)\, p_t(v,v) - p_t(u,v)\, p_t'(v,v) \geq 0, \quad \forall t \geq 0.$$

Recall that $p_t(u,v) = \langle P_t \delta_v, \delta_u \rangle \frac{1}{d_u} = (P_t \delta_v)(u)$

We use the spectral decomposition of P_t. Let us denote the 3 distinct eigenvalues by $0, \theta_1, \theta_2$.

Then $P_t = I_0 + e^{-\theta_1 t} I_{\theta_1} + e^{-\theta_2 t} I_{\theta_2}$

where I_{θ_i} is the projection operator to the eigenspace of θ_i.

I_0 is the projection to the space spanned by const. fct.

That is $I_0(u,v) = \phi_0(u)\phi_0(v)\, d_v = \dfrac{d_v}{\mathrm{vol}(V)}$.

For regular graph, we have $I_0(u,v) = \dfrac{d}{|V|\cdot d} = \dfrac{1}{|V|} = \dfrac{1}{N}$.

Then $h(t) = p_t'(u,v)\,p_t(v,v) - p_t(u,v)\,p_t'(v,v)$

$$= P_t'(u,v)\,P_t(v,v) - \underbrace{P_t(u,v)}_{(u,v)\text{-entry of the matrix } P_t}\,P_t'(v,v)$$

$$= \left(-\theta_1 e^{-t\theta_1} I_{\theta_1}(u,v) - \theta_2 e^{-t\theta_2} I_{\theta_2}(u,v)\right)\left(\frac{1}{N} + e^{-t\theta_1} I_{\theta_1}(v,v) + e^{-t\theta_2} I_{\theta_2}(v,v)\right)$$

$$- \left(\frac{1}{N} + e^{-t\theta_1} I_{\theta_1}(u,v) + e^{-t\theta_2} I_{\theta_2}(u,v)\right)\left(-\theta_1 e^{-t\theta_1} I_{\theta_1}(v,v) - \theta_2 e^{-t\theta_2} I_{\theta_2}(v,v)\right)$$

$$= \frac{\theta_1 e^{-t\theta_1}}{N}\left(-I_{\theta_1}(u,v) + I_{\theta_1}(v,v)\right) + \frac{\theta_2 e^{-t\theta_2}}{N}\left(-I_{\theta_2}(u,v) + I_{\theta_2}(v,v)\right)$$

$$+ \theta_1 e^{-2t\theta_1}\left(-I_{\theta_1}(u,v) I_{\theta_1}(v,v) \overset{=0}{+} I_{\theta_1}(v,v) I_{\theta_1}(u,v)\right)$$

$$+ \theta_2 e^{-2t\theta_2}\left(I_{\theta_2}(u,v) I_{\theta_2}(v,v) \overset{=0}{-} I_{\theta_2}(u,v) I_{\theta_2}(v,v)\right)$$

$$+ e^{-t(\theta_1+\theta_2)}\Big(-\theta_1 I_{\theta_1}(u,v) I_{\theta_2}(v,v) - \theta_2 I_{\theta_2}(u,v) I_{\theta_1}(v,v)$$
$$+ \theta_2 I_{\theta_2}(v,v) I_{\theta_1}(u,v) + \theta_1 I_{\theta_1}(v,v) I_{\theta_2}(u,v)\Big)$$

$$= \frac{\theta_1}{N}\left(I_{\theta_1}(v,v) - I_{\theta_1}(u,v)\right) e^{-t\theta_1} + \frac{\theta_2}{N}\left(I_{\theta_2}(v,v) - I_{\theta_2}(u,v)\right)$$

$$+ (\theta_1 - \theta_2)\left(I_{\theta_1}(v,v) I_{\theta_2}(u,v) - I_{\theta_1}(u,v) I_{\theta_2}(v,v)\right) e^{-t(\theta_1+\theta_2)}$$

Then we have

$$g(t) := e^{t(\theta_1+\theta_2)} h(t) = \underbrace{\frac{\theta_1}{N}\left(I_{\theta_1}(v,v)-I_{\theta_1}(u,v)\right)}_{A} e^{t\theta_2} + \underbrace{\frac{\theta_2}{N}\left(I_{\theta_2}(v,v)-I_{\theta_2}(u,v)\right)}_{B} e^{t\theta_1} + R$$

where R is independent of t.

<u>Lemma</u> III.1.6. We have $I_{\theta_1}(v,v) \geq I_{\theta_1}(u,v)$

and $I_{\theta_2}(v,v) \geq I_{\theta_2}(u,v)$

With the help of Lemma III.1.6, we see

$$g(t) = Ae^{t\theta_2} + Be^{t\theta_1} + R \quad \text{with } A, B \geq 0.$$

Then $g'(t) = A\theta_2 e^{t\theta_2} + B\theta_1 e^{t\theta_1} \geq 0$. ~~since~~

Recall that we have by Lemma III.1.5 that

$$g(0) = h(0) \geq 0.$$

We derive $g(t) \geq 0, \ \forall t. \Rightarrow h(t) \geq 0, \ \forall t.$ □

<u>Proof of Lemma III.1.6</u> :

The two projections I_{θ_1}, I_{θ_2} satisfy

$$I_{\theta_1} + I_{\theta_2} = P_0 - I_0 = I_d - I_0$$

and $\theta_1 I_{\theta_1} + \theta_2 I_{\theta_2} = -\Delta$

Solving it leads to

$$I_{\theta_1} = \frac{(-\Delta) - \theta_2(I_d - I_0)}{\theta_1 - \theta_2}, \quad I_{\theta_2} = \frac{(-\Delta) - \theta_1(I_d - I_0)}{\theta_2 - \theta_1}$$

Therefore, $I_{\theta_1}(v,v) - I_{\theta_1}(u,v) = \dfrac{(-\Delta)(v,v) - \theta_2(1-\frac{1}{N}) - (-\Delta)(u,v) + \theta_2(0-\frac{1}{N})}{\theta_1-\theta_2}$

$$= \frac{(-\Delta)(v,v) - \theta_2 - (-\Delta)(u,v)}{\theta_1 - \theta_2} = \frac{\cancel{d}1 - \theta_2 + \frac{a_{uv}}{d_u}}{\theta_1 - \theta_2}$$

Recall from Lemma III.1.4., $\theta_2 \geq \frac{d+1}{d} = 1 + \frac{1}{d}$

That is, $1 - \theta_2 + \frac{a_{uv}}{d} \leq 0$

Therefore $I_{\theta_1}(v,v) - I_{\theta_1}(u,v) \geq 0$.

Similarly, $I_{\theta_2}(v,v) - I_{\theta_2}(u,v) = \dfrac{(-\Delta)(v,v) - \theta_1(1-\frac{1}{N}) - (-\Delta)(u,v) + \theta_1(0 - \frac{1}{N})}{\theta_2 - \theta_1}$

$$= \frac{1 - \theta_1 + \frac{a_{uv}}{d_u}}{\theta_2 - \theta_1} \geq 0.$$

In the last inequality, we use $\theta_1 \leq 1$. $\square$

(III.2) Heat kernel on locally finite infinite graphs.

Consider a locally finite infinite graph $G = (V, E)$, and the vertex measure $\mu(x) = d_x$, $\forall x \in V$.

Recall $\ell^2(V) = \{ f: V \to \mathbb{R} : \sum_{x \in V} f(x)^2 d_x < \infty \}$.

__Prop__ III.2.1 $\Delta: \ell^2(V) \to \ell^2(V)$ is a bounded operator.

__Proof__. This follows from the calculation that for any $f \in \ell^2(V)$,

$$\sum_{x \in V} (\Delta f(x))^2 d_x = \sum_{x \in V} \frac{1}{d_x^2} \Big(\sum_{y: y \sim x} (f(y) - f(x)) \Big)^2 d_x$$

$$= \sum_{x \in V} \frac{1}{d_x} \cdot \Big(\sum_{y: y \sim x} (f(y) - f(x)) \Big)^2 \overset{C\text{-}S}{\leq} \sum_{x \in V} \sum_{y: y \sim x} (f(y) - f(x))^2 \overset{C\text{-}S}{\leq} 2 \sum_x \sum_{y \sim x} (f(y)^2 + f(x)^2)$$

$$\cancel{= 2 \sum_{\{x,y\} \in E} (f(y) - f(x))^2 \overset{C\text{-}S}{\leq} 4 \sum_{\{x,y\}} (f(y)^2 + f(x)^2)} = 2 \sum_x \sum_{y \sim x} f(y)^2 + 2 \|f\|_2^2$$

$$\overset{\text{Fubini}}{=} 2 \sum_y \sum_{x \sim y} f(y)^2 + 2 \|f\|_2^2 = 4 \|f\|_2^2$$

$= \cancel{4} \sum_x f(x)^2 d_x = \cancel{4} \|f\|_{\ell_2}^2$, That is. $\|\Delta f\|_2 \leq 2 \|f\|_2$. $\square$

i.e. $\|\Delta\| \leq 2$.

Prop III.2.2. $\Delta : \ell^2(V) \to \ell^2(V)$ is a self-adjoint operator.

Proof: This can been as follows: for any $f, g \in \ell^2(V)$, we have

$$\langle \Delta f, g \rangle = \sum_{x \in V} \frac{1}{d_x} \sum_{y : y \sim x} (f(y) - f(x))\, g(x) \cdot d_x$$

$$= \sum_{x \in V} \sum_{y : y \sim x} (f(y) g(x) - f(x) g(x)) \quad (1)$$

Notice that, we have

$$\sum_{x \in V} \sum_{y : y \sim x} | f(y) g(x) - f(x) g(x) | \leq \sum_{x \in V} \sum_{y : y \sim x} |f(y) g(x)| + \sum_{x \in V} |f(x) g(x)| d_x$$

$$\leq \sqrt{\sum_{x \in V} \sum_{y : y \sim x} f(y)^2} \sqrt{\sum_{x \in V} \sum_{y : y \sim x} g(x)^2} + \cancel{\langle f, g \rangle}\, \|f\|_2 \|g\|_2$$

$$\overset{\text{Fubini}}{=} \sqrt{\sum_{y} \sum_{x : x \sim y} f(y)^2} \sqrt{\sum_{x \in V} g(x)^2 d_x} + \|f\|_2 \|g\|_2$$

$$= 2 \|f\|_2 \|g\|_2 < \infty$$

By Fubini, we can interchage the order of summation in (1).

Therefore

$$\sum_{x \in V} \sum_{y : y \sim x} (f(y) g(x) - f(x) g(x))$$

$$= \sum_{y \in V} \sum_{x : x \sim y} (f(y) g(x) - f(x) g(x))$$

$$= \sum_{x \in V} \sum_{y : y \sim x} (f(x) g(y) - f(y) g(y))$$

This yields

$$\langle \Delta f, g \rangle = \frac{1}{2} \sum_{x \in V} \sum_{y : y \sim x} \left(f(y) g(x) - f(x) g(x) + f(x) g(y) - f(y) g(y) \right)$$

$$= -\frac{1}{2} \sum_{x \in V} \sum_{y : y \sim x} (f(y) - f(x)) (g(y) - g(x))$$

Similarly,

$$\langle f, \Delta g \rangle = -\frac{1}{2} \sum_{x \in V} \sum_{y : y \sim x} (g(y) - g(x)) (f(y) - f(x))$$

That is $\langle \Delta f, g \rangle = \langle f, \Delta g \rangle$, $\forall f, g \in \ell^2(V)$. $\square$

We consider the heat equation:

$$\begin{cases} \dfrac{\partial u(x,t)}{\partial t} = \Delta u(x,t) \\ u(x,0) = f(x) \end{cases}$$

Since Δ is bounded, we can define P_t via the exponential of Δ by

$$P_t = e^{t\Delta} = \sum_{n=0}^{\infty} \frac{t^n \Delta^n}{n!}$$

(The series converges in norm. (Reed-Simon I. pp. 264.)

We then can define the kernel by, $\forall\ x, y \in V$

$$p_t(x,y) = \left\langle P_t \frac{\delta_y}{d_y}, \delta_x \right\rangle.$$

Then for any $f \in \ell^2(V)$, we have

$$P_t f(x) = P_t\Big(\sum_y f(y)\delta_y\Big) = \sum_y f(y)\, P_t(\delta_y)(x)$$

$$= \sum_y f(y) \frac{P_t \delta_y(x)}{d_y} \cdot d_y$$

$$= \sum_y f(y)\, p_t(x,y)\, d_y.$$

Next, we consider a finite, connected subgraph of G. The following is an analogue of Green's Thm:

<u>Lemma III.2.3</u>: For any $f, g: V \to \mathbb{R}$, we have

$$\sum_{x\in D} \Delta f(x) g(x) d_x = -\sum_{\{x,y\}\in E_D} (f(y)-f(x))(g(y)-g(x))$$

$$- \sum_{\substack{\cancel{x\in D} \\ \{x,z\}\in E \\ x\in D,\, z\notin D}} (f(x)-f(z))\, g(x).$$

Proof: $\sum_{x\in D} \Delta f(x) g(x)\, dx = \sum_{x\in D} \sum_{y: y\sim x} (f(y)-f(x))\, g(x)$

Every edge $\{x,y\} \in E_D$ contributes

$$(f(y)-f(x))g(x) \text{ and } (f(x)-f(y))\,g(y)$$

~~Every edge~~ which adds up to $-(f(y)-f(x))(g(y)-g(x))$

Every edge $\{x,z\}\in E$, $x\in D$, $z\notin D$ contributes

$$(f(z)-f(x))\,g(x)$$

$\square$.

Notations: A vertex x is said in the boundary of D, ~~and~~ if $x\in D$ and $\exists\, z\notin D$ s.t. $x\sim z$. Otherwise, x_D is said to be in the interior of D.

Observe that, if either f or g are zero on $V\setminus \mathrm{int}\, D$, we have by the above lemma that

$$\langle \Delta f, g\rangle_D = \langle f, \Delta g\rangle_D .$$

Moreover, if one of f and g is finitely supported, it is true that $\langle \Delta f, g\rangle = \langle f, \Delta g\rangle$.

We next discuss the weak and strong maximum principles for heat equations:

Lemma III 2.4: Suppose D is a finite, connected subgraph of G. and $u: D\times [0,T] \to \mathbb{R}$

is continuous for $t\in[0,T]$ and C^1 for $t\in(0,T)$, and satisfies $\frac{\partial u}{\partial t}(x,t) = \Delta u(x,t)$ on $\mathrm{int}\, D \times (0,T)$

Then.

(1) If $\exists\ (x_0, t_0) \in \operatorname{int} D \times (0,T)$ s.t. (x_0, t_0) is a maximum (or minimum) for u on $D \times [0,T]$, then

$$u(x, t_0) = u(x_0, t_0) \quad \text{for all } x \in D.$$

(ii)

$$\max_{D \times [0,T]} u = \max_{D \times \{0\} \cup \partial D \times [0,T]} u$$

$$\min_{D \times [0,T]} u = \min_{D \times \{0\} \cup \partial D \times [0,T]} u.$$

Proof: (1) At a maximum (or minimum) we have

$$\frac{\partial}{\partial t} u(x_0, t_0) = 0$$

The heat equation then implies

$$\Delta u(x_0, t_0) = \frac{1}{d_{x_0}} \sum_{y : y \sim x_0} \Big(\underbrace{u(y, t_0) - u(x_0, t_0)}_{\leq 0} \Big) = 0$$

Therefore $u(y, t_0) = u(x_0, t_0)$, $\forall y \sim x_0$.

By iterating the above argument, the assumption that D is connected yields the statement of (1).

(2). Consider $v = u - \varepsilon t$ for $\varepsilon > 0$.

Then $\dfrac{\partial v}{\partial t} - \Delta v = \dfrac{\partial u}{\partial t} - \Delta u - \varepsilon = -\varepsilon < 0$. in $\operatorname{int} D \times (0,T)$.

If v has a maximum at $(x_0, t_0) \in \operatorname{int} D \times (0,T]$, then

$$\frac{\partial v}{\partial t}(x_0, t_0) \geq 0 \quad \text{and} \quad \Delta v(x_0, t_0) \leq 0.$$

Therefore we obtain $0 \leq -\varepsilon < 0$ a contradiction.

Hence $\displaystyle\max_{D \times [0,T]} v = \max_{D \times \{0\} \cup \partial D \times [0,T]} v$.

We then estimate

$$\max_{D\times[0,T]} u = \max_{D\times[0,T]} (v + \varepsilon t)$$

$$\leq \max_{D\times[0,T]} v + \varepsilon T$$

$$= \max_{D\times\{0\}\cup\partial D\times[0,T]} v + \varepsilon T.$$

$$\leq \max_{D\times\{0\}\cup\partial D\times[0,T]} u + \varepsilon T$$

Letting $\varepsilon \to 0$ we derive that

$$\max_{D\times[0,T]} u \leqslant \max_{D\times\{0\}\cup\partial D\times[0,T]} u$$

That is, $\max_{D\times[0,T]} u = \max_{D\times\{0\}\cup\partial D\times[0,T]} u$.

The claim for the minimum follows by applying the above argument to $-u$. $\square$

<u>Remark</u>: ~~B~~ From the above proof, it follows that.

(i) if u satisfies $-\Delta u + \frac{\partial u}{\partial t} \leqslant 0$ on $\operatorname{int} D \times (0,T)$

then $\max_{D\times[0,T]} u = \max_{D\times\{0\}\cup\partial D\times[0,T]} u.$

(ii) if u satisfies $-\Delta u + \frac{\partial u}{\partial t} \geqslant 0$ on $\operatorname{int} D \times (0,T)$

then $\min_{D\times[0,T]} u = \min_{D\times\{0\}\cup\partial D\times[0,T]} u$. $\square$.