Generalized Linear Polyominoes, Green functions and Green matrices

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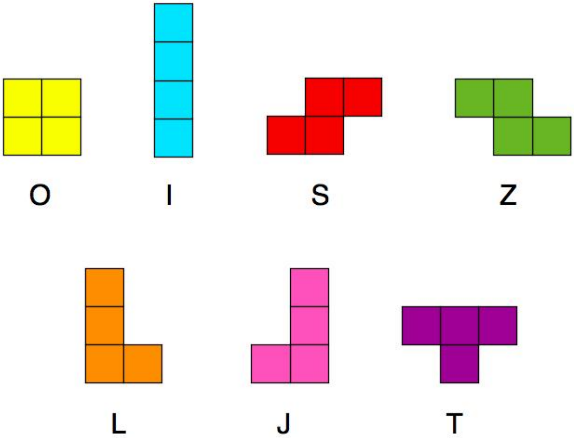
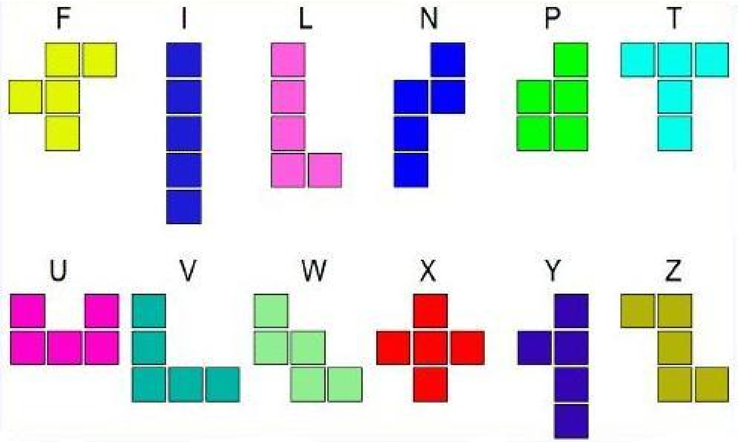
- $$\mathcal{G}^{H} = \mathcal{G} - \sum_{i,j=1}^{n} b_{ij} \mathcal{P}_{\mathcal{G}(\sigma_i)\mathcal{G}(\sigma_j)}$$

Tetrominoes

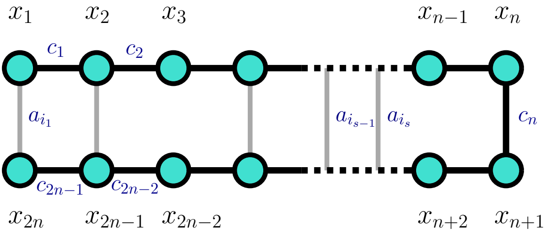


Pentaminoes



Generalized linear Polyominoes: $\mathbb{L}_n$

- $V = \{x_1, \dots, x_{2n}\}$



- $c_i = c(x_i, x_{i+1}) > 0,\ i = 1, \dots, 2n-1$

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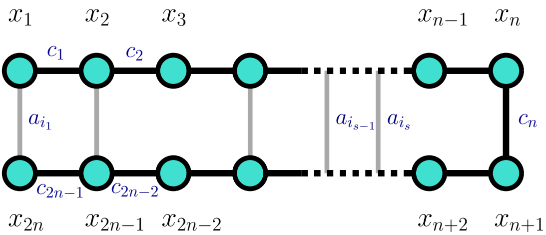

- $c_i = c(x_i, x_{i+1}) > 0,\ i = 1, \dots, 2n-1$
- $a_i = c(x_i, x_{2n+1-i}) \geq 0,\ i = 1, \dots, n-1$

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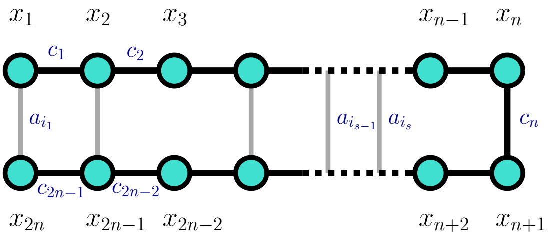

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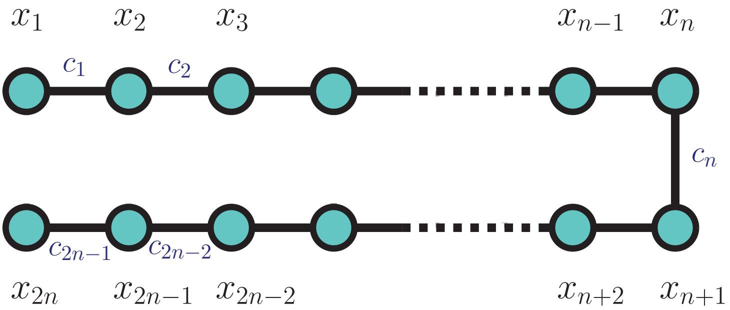
- $a_i = c(x_i, x_{2n+1-i}) \geq 0,\ i = 1, \dots, n-1$
- Link number $\mathcal{P} \in \mathbb{L}_n$: $s = \#\{i : a_i > 0\}$

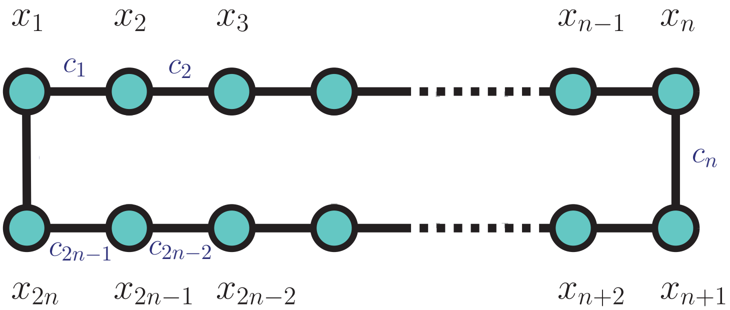
Generalized linear Polyominoes: $\mathbb{L}_n$

- Path



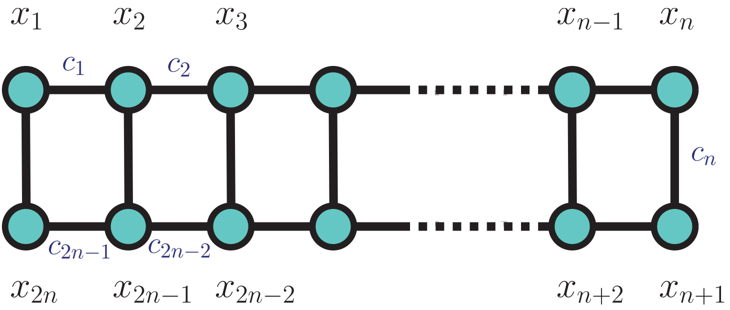
Generalized linear Polyominoes: $\mathbb{L}_n$

- Cycle



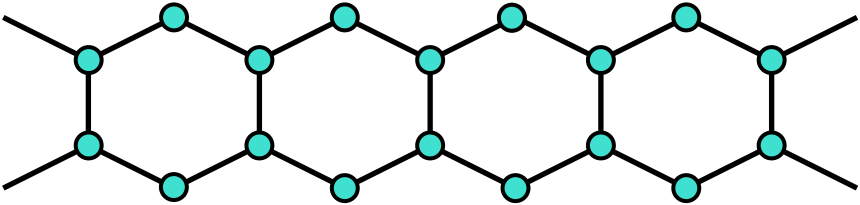
Generalized linear Polyominoes: $\mathbb{L}_n$

- Linear chain



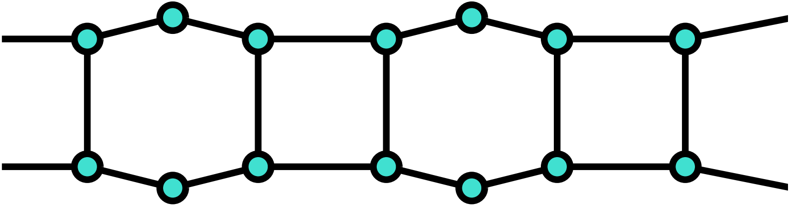
Generalized linear Polyominoes: $\mathbb{L}_n$

- Linear hexagonal chain

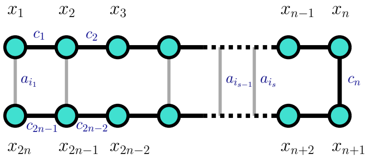


Generalized linear Polyominoes: $\mathbb{L}_n$

- Phenylene

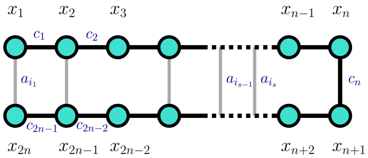


Combinatorial Laplacian



- *Laplacian operator*: $\mathcal{L}(u)(x) = \sum_{y \in V} c(x,y)\big(u(x) - u(y)\big)$

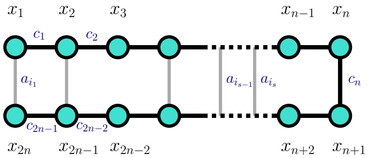
Combinatorial Laplacian



Combinatorial Laplacian: L

- $$\mathsf{L} = \begin{bmatrix} c_1 + a_{i_1} & -c_1 & & & -a_{i_1} \\ -c_1 & c_1 + c_2 + a_{i_2} & -c_2 & -a_{i_2} & \\ & \ddots & \ddots & \ddots & \\ & -a_{i_2} & -c_{2n-2} & c_{2n-2} + c_{2n-1} + a_{i_2} & -c_{2n-1} \\ -a_{i_1} & & & -c_{2n-1} & c_{2n-1} + a_{i_1} \end{bmatrix}$$

Combinatorial Laplacian



- $\mathcal{L}$ is positive semi–definite, singular and $\mathcal{L}(v) = 0$ iff $v =$ cte

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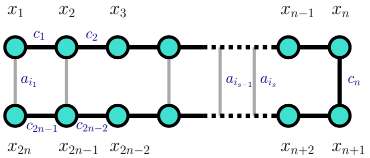
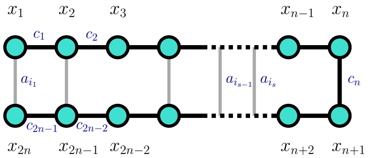


- $\mathcal{L}$ is positive semi–definite, singular and $\mathcal{L}(v) = 0$ iff $v =$ cte
- *Green operator and Green function*: $\mathcal{G}$ and $G(x, y)$
- If $\langle f, 1\rangle = 0$, then $u = \mathcal{G}(f)$ is the unique solution of the Poisson $\mathcal{L}(u) = f$ such that $\langle u, 1\rangle = 0$

Combinatorial Laplacian



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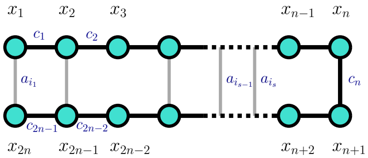

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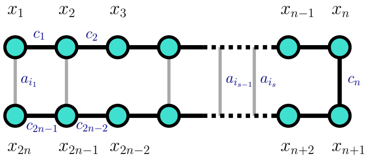

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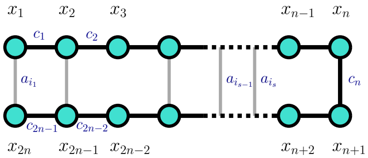
- $\mathcal{G} \circ \mathcal{L} = \mathcal{L} \circ \mathcal{G} = \mathcal{I} - \frac{1}{n}\langle \cdot, 1\rangle \Longrightarrow \mathsf{G} = \mathsf{L}^{\dagger}$

Dipole Perturbation



- We obtain the *Polyominoe*, **by adding s edges**

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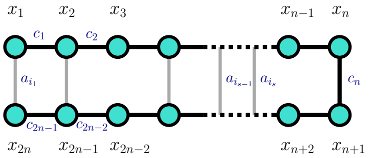

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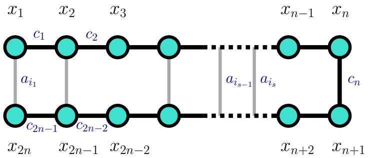

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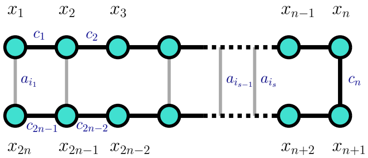
- $$\mathcal{L} = \mathcal{L}^{\text{path}} + \sum_{j=1}^{s} \mathcal{P}_{\sigma_j}, \text{ where } \mathcal{P}_{\sigma_j}(u) = \sigma_j \langle \sigma_j, u \rangle$$

Dipole Perturbation



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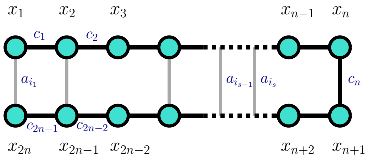

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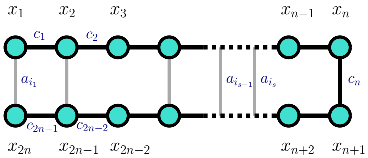

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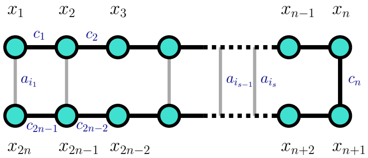
- $$\boxed{\mathcal{G} = \mathcal{G}^{\text{path}} - \sum_{k,m=1}^{s} b_{km} \mathcal{P}_{\mathcal{G}^{\text{path}}(\sigma_m)\mathcal{G}^{\text{path}}(\sigma_k)}, \; \mathcal{P}_{\sigma\tau}(u) = \sigma\langle \tau, u\rangle}$$

Dipole Perturbation



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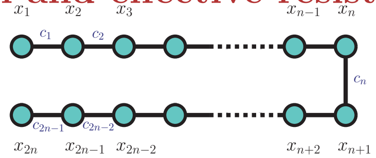
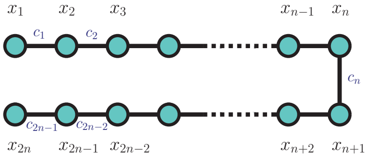
- $\Lambda = \left(\langle \mathcal{G}^{\text{path}}(\sigma_m), \sigma_k \rangle\right) \Longrightarrow$ $\boxed{(b_{km}) = (\mathsf{I} + \Lambda)^{-1}}$
- $$\boxed{G(x,y) = G^{\text{path}}(x,y) - \sum_{k,m=1}^{s} b_{km}\mathcal{G}^{\text{path}}(\sigma_m)(x)\mathcal{G}^{\text{path}}(\sigma_k)(y)}$$

Green function and effective resistance



- The Green function of a path on $2n$ vertices is
- $$G^{\text{path}}(x_i,x_j) = \frac{1}{4n^2}\left[\sum_{\ell=1}^{\min\{i,j\}-1}\frac{\ell^2}{c_\ell} + \sum_{\ell=\max\{i,j\}}^{2n-1}\frac{(2n-\ell)^2}{c_\ell} - \sum_{\ell=\min\{i,j\}}^{\max\{i,j\}-1}\frac{k(2n-\ell)}{c_\ell}\right]$$

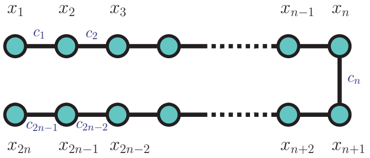
Green function and effective resistance



- *Effective resistance*

$$R(x_i, x_j) = G(x_i, x_i) + G(x_j, x_j) - 2G(x_i, x_j)$$

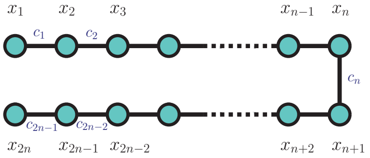
Green function and effective resistance



- *Effective resistance*

$$R(x_i, x_j) = G(x_i, x_i) + G(x_j, x_j) - 2G(x_i, x_j)$$
$$= \sum_{j=2}^{2n} \frac{1}{\lambda_j} (u(x_j) - u(x_i))^2$$

Green function and effective resistance



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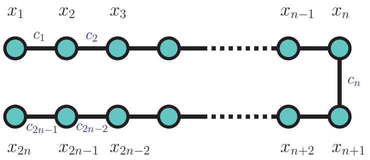
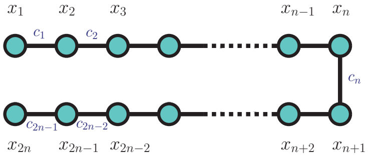
Green function and effective resistance



- *Kirchhoff index*

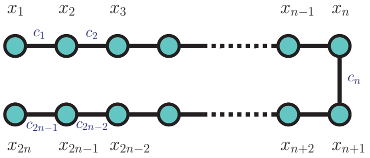
$$\mathrm{k} = \frac{1}{2}\sum_{x,y\in V} R(x,y) = 2n\sum_{x\in V} G(x,x)$$

Green function and effective resistance



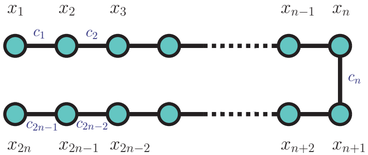
- *Kirchhoff index* $$\mathrm{k}^{\mathrm{path}} = \sum_{\ell=1}^{2n-1} \frac{\ell(2n-\ell)}{c_\ell}$$

Green function and effective resistance



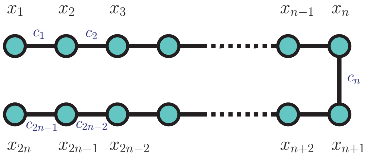
- $$\mathcal{G}^{\text{path}}(\sigma_k)(x_j) = 2n\sqrt{a_{i_k}}\left[\sum_{\ell=\max\{j,i_k\}}^{2n-i_k} \frac{1}{c_\ell} - \sum_{\ell=i_k}^{2n-i_k} \frac{1}{c_\ell}\right]$$

Green function and effective resistance



- $$\langle \mathcal{G}^{\text{path}}(\sigma_k), \sigma_m \rangle = \sqrt{a_{i_k} a_{i_m}}\, R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})$$

Green function and effective resistance



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- **OBJECTIVE:** Determine $(\mathsf{I}+\Lambda)^{-1}$, $\Lambda = \left(\langle \mathcal{G}^{\text{path}}(\sigma_m), \sigma_k \rangle\right)$

Inverse of $\mathsf{I} + \Lambda$

- $\Lambda = \left(\sqrt{a_{i_k} a_{i_m}}\, R(x_{\max\{i_k, i_m\}}, x_{2n+1-\max\{i_k, i_m\}}) \right)$

Inverse of $\mathsf{I} + \Lambda$

- $\Lambda = \left(\sqrt{a_{i_k} a_{i_m}}\, R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\right)$
- D: *Diagonal matrix* with entries $a_{i_1}, \ldots, a_{i_s}$

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- D: *Diagonal matrix* with entries $a_{i_1}, \ldots, a_{i_s}$
- $\mathsf{I} + \Lambda = \mathsf{D}^{\frac{1}{2}} \left[\mathsf{D}^{-1} + \mathsf{A}\right] \mathsf{D}^{\frac{1}{2}}$, where

$$\mathsf{A} = \begin{bmatrix} R(x_{i_1}, x_{2n+1-i_1}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ R(x_{i_2}, x_{2n+1-i_2}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ \vdots & \vdots & \ddots & \vdots \\ R(x_{i_s}, x_{2n+1-i_s}) & R(x_{i_s}, x_{2n+1-i_s}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \end{bmatrix}$$

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- $\left(\mathsf{I}+\Lambda\right)^{-1} = \mathsf{I} - \mathsf{D}^{\frac{1}{2}}\left[\mathsf{D}+\mathsf{A}^{-1}\right]^{-1}\mathsf{D}^{\frac{1}{2}}$

Inverse of $\mathsf{I} + \Lambda$

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- D: *Diagonal matrix* with entries $a_{i_1}, \ldots, a_{i_s}$
- $\mathsf{I} + \Lambda = \mathsf{D}^{\frac{1}{2}} \left[\mathsf{D}^{-1} + \mathsf{A}\right] \mathsf{D}^{\frac{1}{2}}$, where

$$\mathsf{A} = \begin{bmatrix} R(x_{i_1}, x_{2n+1-i_1}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ R(x_{i_2}, x_{2n+1-i_2}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ \vdots & \vdots & \ddots & \vdots \\ R(x_{i_s}, x_{2n+1-i_s}) & R(x_{i_s}, x_{2n+1-i_s}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \end{bmatrix}$$

- If $\alpha_j = R(x_{i_j}, x_{2n+1-i_j}) = \displaystyle\sum_{\ell=i_j}^{2n-i_j} \frac{1}{c_\ell}$

Inverse of $\mathsf{I}+\Lambda$

- $\Lambda = \left(\sqrt{a_{i_k} a_{i_m}}\, R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\right)$
- D: *Diagonal matrix* with entries $a_{i_1}, \ldots, a_{i_s}$
- $\mathsf{I}+\Lambda = \mathsf{D}^{\frac{1}{2}}\left[\mathsf{D}^{-1}+\mathsf{A}\right]\mathsf{D}^{\frac{1}{2}}$, where

$$\mathsf{A} = \begin{bmatrix} R(x_{i_1}, x_{2n+1-i_1}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ R(x_{i_2}, x_{2n+1-i_2}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ \vdots & \vdots & \ddots & \vdots \\ R(x_{i_s}, x_{2n+1-i_s}) & R(x_{i_s}, x_{2n+1-i_s}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \end{bmatrix}$$

- If $\alpha_j = R(x_{i_j}, x_{2n+1-i_j}) = \sum_{\ell=i_j}^{2n-i_j} \frac{1}{c_\ell} \Longrightarrow \mathsf{A} = \left(\alpha_{\max\{k,m\}}\right)$

Properties $\mathsf{A} = \left(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\right)$

- *Parameters:* $\alpha_1, \ldots, \alpha_s$

Properties $\mathsf{A} = \left(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\right)$

- *Parameters:* $\alpha_1, \ldots, \alpha_s$
- *Weak type D matrix*: $\Sigma = \left(\alpha_{\min\{k,m\}}\right)$

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$$\mathsf{A} = \begin{bmatrix} \alpha_1 & \alpha_1 & \cdots & \alpha_1 \\ \alpha_1 & \alpha_2 & \cdots & \alpha_2 \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_1 & \alpha_2 & \cdots & \alpha_s \end{bmatrix}$$

Properties $\mathsf{A} = \left(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}}) \right)$

- *Parameters:* $\alpha_1, \ldots, \alpha_s$
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- *Type D matrix*: If moreover $\alpha_1 < \cdots < \alpha_s$

Properties $A = \left(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}}) \right)$

- *Parameters:* $\alpha_1, \ldots, \alpha_s$
- *Weak type D matrix*: $\Sigma = \left(\alpha_{\min\{k,m\}}\right)$
- *Type D matrix*: If moreover $\alpha_1 < \cdots < \alpha_s$
- *Flipped weak type D matrix*: $\Sigma = \left(\alpha_{\max\{k,m\}}\right)$

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- *Flipped type D matrix*: If moreover $\alpha_1 > \cdots > \alpha_s$

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- *Flipped type D matrix*: If moreover $\alpha_1 > \cdots > \alpha_s$
- *Green matrix*: $\mathsf{G} = \left(\alpha_{\min\{k,m\}} \right) \circ \left(\beta_{\max\{k,m\}} \right)$

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- *Green matrix*: $G = \left(\alpha_{\min\{k,m\}}\right) \circ \left(\beta_{\max\{k,m\}}\right)$
- $$g_{km} = \alpha_{\min\{k,m\}}\beta_{\max\{k,m\}} = \begin{cases} \alpha_k\beta_m, & \text{if } k \leq m, \\ \alpha_m\beta_k, & \text{if } k \geq m \end{cases}$$

Properties $\mathsf{A} = \left(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}}) \right)$

- *Parameters:* $\alpha_1, \ldots, \alpha_s$
- *Weak type D matrix*: $\Sigma = \left(\alpha_{\min\{k,m\}}\right)$
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- *Green matrix*: $\mathsf{G} = \left(\alpha_{\min\{k,m\}}\right) \circ \left(\beta_{\max\{k,m\}}\right)$
- G is a non singular Green matrix iff G^{-1} is a tridiagonal and irreducible matrix. [GK 40's]

Properties of $\mathsf{A} = \left(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\right)$

- *Parameters:* $\alpha_1, \ldots, \alpha_s$ ($\alpha_{s+1} = 0$)
- *Flipped weak type D matrix*: $\Sigma = \left(\alpha_{\max\{k,m\}}\right)$
- *Flipped type D matrix*: If moreover $\alpha_1 > \cdots > \alpha_s$

Properties of A $= \Big(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}}) \Big)$

- *Parameters:* $\alpha_1, \dots, \alpha_s$ ($\alpha_{s+1} = 0$)
- *Flipped weak type D matrix*: $\Sigma = \big(\alpha_{\max\{k,m\}}\big)$
- *Flipped type D matrix*: If moreover $\alpha_1 > \cdots > \alpha_s$
- Σ is invertible iff $\alpha_i \neq \alpha_{i+1}$. Moreover, if $\gamma_j = (\alpha_j - \alpha_{j+1})^{-1}$

$$\Sigma^{-1} = \begin{bmatrix} \gamma_1 & -\gamma_1 & 0 & \cdots & 0 \\ -\gamma_1 & \gamma_1 + \gamma_2 & -\gamma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \gamma_{s-2} + \gamma_{s-1} & -\gamma_{s-1} \\ 0 & 0 & \cdots & -\gamma_{s-1} & \gamma_{s-1} + \gamma_s \end{bmatrix}$$

Properties of $\mathsf{A} = \left(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\right)$

- *Parameters:* $\alpha_j = R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})$
- $\alpha_1 > \cdots > \alpha_s > 0$

Properties of A $= \left(R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})\right)$

- Parameters: $\alpha_j = R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})$
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- Parameters: $\alpha_j = R(x_{\max\{i_k,i_m\}}, x_{2n+1-\max\{i_k,i_m\}})$
- $\alpha_1 > \cdots > \alpha_s > 0 \Longrightarrow$ A is a flypped type D matrix
- $$\mathsf{A}^{-1} = \begin{bmatrix} \gamma_1 & -\gamma_1 & 0 & \cdots & 0 \\ -\gamma_1 & \gamma_1+\gamma_2 & -\gamma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \gamma_{s-2}+\gamma_{s-1} & -\gamma_{s-1} \\ 0 & 0 & \cdots & -\gamma_{s-1} & \gamma_{s-1}+\gamma_s \end{bmatrix}$$
  $$\gamma_s = R(x_{i_s}, x_{2n+1-i_s})^{-1},$$
  $$\gamma_k = \left[R(x_{i_k}, x_{i_{k+1}}) + R(x_{2n+1-i_{k+1}}, x_{2n+1-i_k})\right]^{-1}$$

Computing $(b_{km}) = (\mathsf{I} + \Lambda)^{-1}$, $s \geq 3$

- $\left(\mathsf{I} + \Lambda\right)^{-1} = \mathsf{I} - \mathsf{D}^{\frac{1}{2}}(\mathsf{A}^{-1} + \mathsf{D})^{-1}\mathsf{D}^{\frac{1}{2}}$

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- $\mathsf{A}^{-1} + \mathsf{D}$ is tridiagonal and therefore, $\left(\mathsf{A}^{-1} + \mathsf{D}\right)^{-1}$ is a Green matrix, that is determined by the green function of a discrete Sturm–Liouville problem.

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$$\begin{bmatrix} a_{i_1}+\gamma_1 & -\gamma_1 & 0 & \cdots & 0 \\ -\gamma_1 & a_{i_2}+\gamma_1+\gamma_2 & -\gamma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{i_{s-1}}+\gamma_{s-2}+\gamma_{s-1} & -\gamma_{s-1} \\ 0 & 0 & \cdots & -\gamma_{s-1} & a_{i_s}+\gamma_{s-1}+\gamma_s \end{bmatrix}$$

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- $(a_{i_k}+\gamma_{k-1}+\gamma_k)z_k - \gamma_{k-1}z_{k-1} - \gamma_k z_{k+1} = 0$

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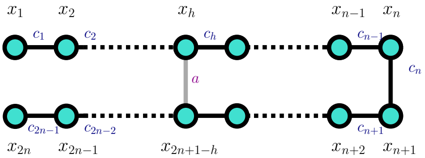
- $(a_{i_k}+\gamma_{k-1}+\gamma_k)z_k - \gamma_{k-1}z_{k-1} - \gamma_k z_{k+1} = 0,\ 2 \leq k \leq s-1$
- If $\{u_k\}_{k=1}^s$, $\{v_k\}_{k=1}^s$ are two solutions satisfying

  $$u_1 = \gamma_1,\ u_2 = a_{i_1}+\gamma_1,\ \ v_{s-1} = a_{i_s}+\gamma_{s-1}+\gamma_s,\ v_s = \gamma_{s-1},$$

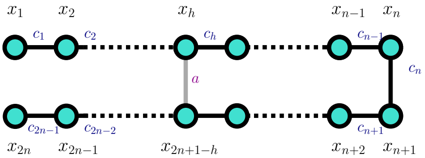
  $$b_{km} = \delta_{km} - \frac{\sqrt{a_{i_k}a_{i_m}}}{\gamma_1\big((a_{i_1}+\gamma_1)v_1 - \gamma_1 v_2\big)}\, u_{\min\{k,m\}} v_{\max\{k,m\}}$$

$s = 1$ and $i_1 = h$



$c_{2n} = a_h > 0$

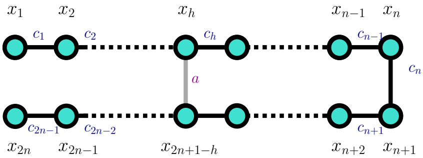
$s = 1$ and $i_1 = h$



$$c_{2n} = a_h > 0$$

- $$(\mathsf{I} + \Lambda)^{-1} = \frac{1}{c_{2n}}\left[\frac{1}{c_{2n}} + \sum_{j=h}^{2n-h}\frac{1}{c_j}\right]^{-1}$$

$s = 1$ and $i_1 = h$



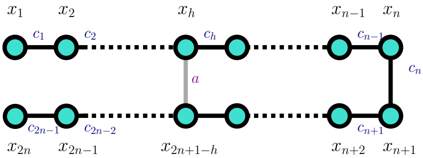
$$c_{2n} = a_h > 0$$

$$G(x_i, x_j) = \frac{1}{4n^2}\left[\sum_{k=1}^{\min\{i,j\}-1}\frac{k^2}{c_k} + \sum_{k=\max\{i,j\}}^{2n-1}\frac{(2n-k)^2}{c_k} - \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1}\frac{k(2n-k)}{c_k}\right]$$

$$- \frac{1}{4n^2}\left[\frac{1}{c_{2n}} + \sum_{k=h}^{2n-h}\frac{1}{c_k}\right]^{-1}\left[\sum_{k=h}^{2n-h}\frac{k}{c_k} - 2n\sum_{k=\phi_h(i)}^{2n-h}\frac{1}{c_k}\right]$$

$$\times\left[\sum_{k=h}^{2n-h}\frac{k}{c_k} - 2n\sum_{k=\phi_h(j)}^{2n-h}\frac{1}{c_k}\right]$$

$s = 1$ and $i_1 = h$



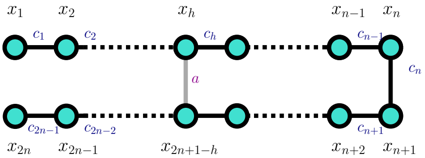
$c_{2n} = a_h > 0$

$$R(x_i, x_j) = \sum_{k=\min\{h,i,j\}}^{\min\{h,\max\{i,j\}\}-1} \frac{1}{c_k} + \sum_{k=\max\{2n+1-h,\min\{i,j\}\}}^{\max\{2n+1-h,i,j\}-1} \frac{1}{c_k}$$

$$+ \left[\frac{1}{c_{2n}} + \sum_{k=h}^{2n-h} \frac{1}{c_k}\right]^{-1} \left[\sum_{k=\phi_h(\min\{i,j\})}^{\phi_h(\max\{i,j\})-1} \frac{1}{c_k}\right]$$

$$\times \left[\frac{1}{c_{2n}} + \sum_{k=h}^{\phi_h(\min\{i,j\})-1} \frac{1}{c_k} + \sum_{k=\phi_h(\max\{i,j\})}^{2n-h} \frac{1}{c_k}\right]$$

$s = 1$ and $i_1 = h$

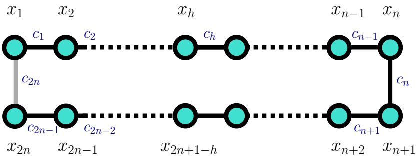


$$c_{2n} = a_h > 0$$

$$\mathrm{k} = \sum_{k=1}^{2n} \frac{k(2n-k)}{c_k} + \left[\frac{1}{c_{2n}} + \sum_{k=h}^{2n-h} \frac{1}{c_k}\right]^{-1}$$

$$\times \left[\left[\sum_{k=h}^{2n-h} \frac{k}{c_k}\right]^2 - 2n \sum_{k=h}^{2n-h} \left[\sum_{m=k}^{2n-h} \frac{1}{c_m}\right]^2 - 2n(h-1) \left[\sum_{k=h}^{2n-h} \frac{1}{c_k}\right]^2\right]$$

$s = 1$ and $i_1 = h = 1$


x_1
x_2
x_h
x_{n-1}
x_n
c_1
c_2
c_h
c_{n-1}
c_{2n}
c_n
c_{2n-1}
c_{2n-2}
c_{n+1}
x_{2n}
x_{2n-1}
x_{2n+1-h}
x_{n+2}
x_{n+1}

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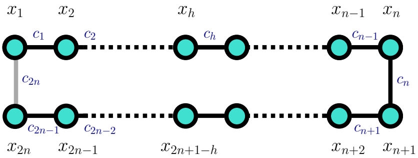

- $$(\mathsf{I} + \Lambda)^{-1} = \frac{1}{c_{2n}} \left[\sum_{j=1}^{2n} \frac{1}{c_j} \right]^{-1}$$

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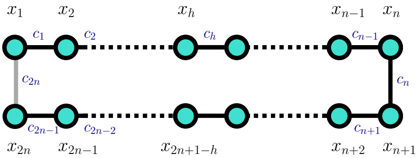
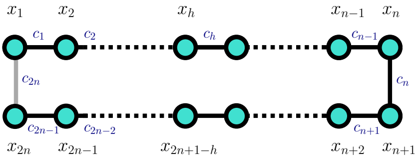


$$G(x_i,x_j) = \frac{1}{4n^2}\left[\sum_{k=1}^{\min\{i,j\}-1}\frac{k^2}{c_k} + \sum_{k=\max\{i,j\}}^{2n}\frac{(2n-k)^2}{c_k} - \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1}\frac{k(2n-k)}{c_k}\right]$$

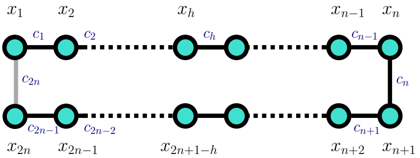
$$-\frac{1}{4n^2}\left[\sum_{k=1}^{2n}\frac{1}{c_k}\right]^{-1}\left[\sum_{k=1}^{2n}\frac{k}{c_k} - 2n\sum_{k=i}^{2n}\frac{1}{c_k}\right]\left[\sum_{k=1}^{2n}\frac{k}{c_k} - 2n\sum_{k=j}^{2n}\frac{1}{c_k}\right]$$

$s = 1$ and $i_1 = h = 1$



$$R(x_i, x_j) = \left[\sum_{k=1}^{2n} \frac{1}{c_k}\right]^{-1} \left[\sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{1}{c_k}\right] \left[\sum_{k=1}^{\min\{i,j\}-1} \frac{1}{c_k} + \sum_{k=\max\{i,j\}}^{2n} \frac{1}{c_k}\right]$$

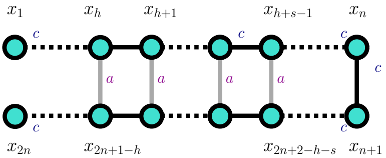
$s = 1$ and $i_1 = h = 1$



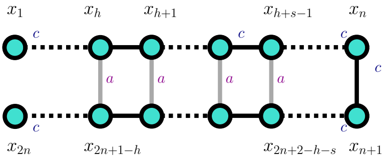
$$R(x_i,x_j) = \left[\sum_{k=1}^{2n}\frac{1}{c_k}\right]^{-1}\left[\sum_{k=\min\{i,j\}}^{\max\{i,j\}-1}\frac{1}{c_k}\right]\left[\sum_{k=1}^{\min\{i,j\}-1}\frac{1}{c_k}+\sum_{k=\max\{i,j\}}^{2n}\frac{1}{c_k}\right]$$

$$\mathrm{k} = \sum_{k=1}^{2n}\frac{k(2n-k)}{c_k}+\left[\sum_{k=1}^{2n}\frac{1}{c_k}\right]^{-1}\left[\left[\sum_{k=1}^{2n-1}\frac{k}{c_k}\right]^2-2n\sum_{j=1}^{2n-1}\left[\sum_{k=j}^{2n-1}\frac{1}{c_k}\right]^2\right]$$

$s \geq 3$, $a_{i_j} = a > 0$ and $c_j = c$

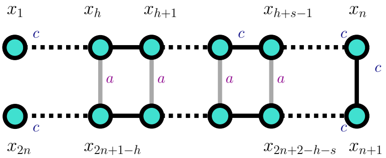


$s \geq 3$, $a_{i_j} = a > 0$ and $c_j = c$



- $$2qz_k - z_{k+1} - z_{k-1} = 0, \quad k = 2, \dots, s-1 \qquad q = 1 + \frac{a}{c}$$

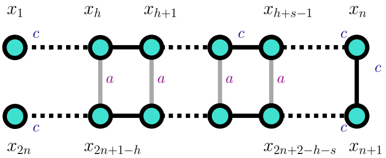
$s \geq 3$, $a_{i_j} = a > 0$ and $c_j = c$



- $$2qz_k - z_{k+1} - z_{k-1} = 0, \quad k = 2, \ldots, s-1 \qquad q = 1 + \frac{a}{c}$$

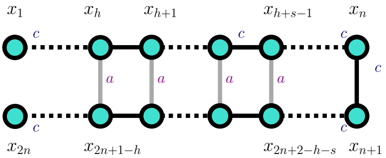
- $$Q_k(q) = \begin{cases} \big(2(n-h-s)+1\big)V_k(q) + 2U_k(q), & k \geq 0, \\ 2(n-h-s+k)+3 & k \leq 0. \end{cases}$$

$s \geq 3$, $a_{i_j} = a > 0$ and $c_j = c$



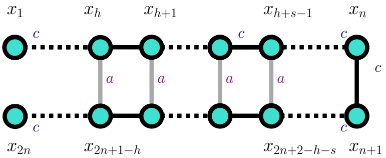
$$(\mathsf{I} + \Lambda)^{-1}_{ij} = \delta_{ij} - \frac{aV_{\min\{i,j\}-1}(q)Q_{s-\max\{i,j\}}(q)}{cV_s(q) + a\big(2(n-s-h)+1\big)U_{s-1}(q)}$$

$s \geq 3$, $a_{i_j} = a > 0$ and $c_j = c$



$$\mathsf{v}_{j,m} = \frac{\sqrt{a}}{c}\Big(2\big(n - \phi_{h+m-1}(j)\big) + 1\Big), \qquad \mathsf{u} = (\mathsf{I} + \Lambda)^{-1}\mathsf{v}$$

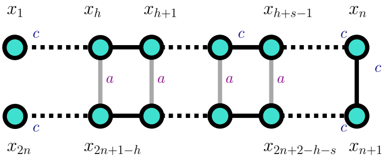
$s \geq 3$, $a_{i_j} = a > 0$ and $c_j = c$



$$\mathsf{v}_{j,m} = \frac{\sqrt{a}}{c}\Big(2\big(n - \phi_{h+m-1}(j)\big) + 1\Big), \qquad \mathsf{u} = (\mathsf{I} + \Lambda)^{-1}\mathsf{v}$$

$$\mathsf{u}_{j,m} = \frac{\sqrt{a}V_{\min\{\phi_h(j)-h,m-1\}}(q)Q_{s-1-\max\{\phi_h(j)-h,m-1\}}(q)}{cV_s(q) + a\big(2(n-s-h)+1\big)U_{s-1}(q)}$$

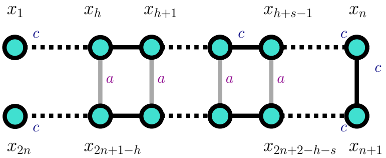
$s \geq 3$, $a_{i_j} = a > 0$ and $c_j = c$



$$G(x_i, x_j) = G(x_{2n+1-i}, x_{2n+1-j}) = G^{\text{path}}(x_i, x_j) - \frac{1}{4}\langle \mathsf{u}_i, \mathsf{v}_j \rangle,$$

$$G(x_i, x_{2n+1-j}) = G(x_{2n+1-i}, x_j) = G^{\text{path}}(x_i, x_{2n+1-j}) + \frac{1}{4}\langle \mathsf{u}_i, \mathsf{v}_j \rangle$$

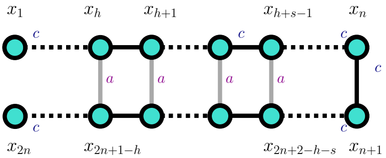
$s \geq 3$, $a_{i_j} = a > 0$ and $c_j = c$



$$R(x_i, x_j) = R^{\text{path}}(x_i, x_j) - \frac{1}{4}\Big[\langle \mathsf{u}_i, \mathsf{v}_i\rangle + \langle \mathsf{u}_j, \mathsf{v}_j\rangle - 2\langle \mathsf{u}_i, \mathsf{v}_j\rangle\Big]$$

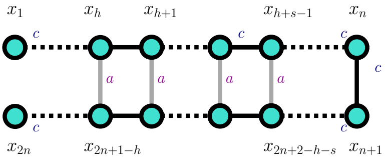
$$R(x_i, x_{2n+1-j}) = R^{\text{path}}(x_i, x_{2n+1-j}) - \frac{1}{4}\Big[\langle \mathsf{u}_i, \mathsf{v}_i\rangle + \langle \mathsf{u}_j, \mathsf{v}_j\rangle + 2\langle \mathsf{u}_i, \mathsf{v}_j\rangle\Big]$$

$s \geq 3$, $a_{i_j} = a > 0$ and $c_j = c$



$$\mathrm{k} = \frac{n}{3c}(4n^2 - 1) - \frac{1}{2}\sum_{j=1}^{n} \langle \mathsf{u}_j, \mathsf{v}_j \rangle$$

$s \geq 3$, $a_{i_j} = a > 0$ and $c_j = c$



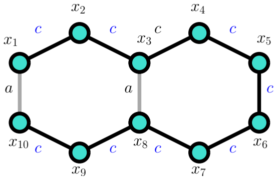
$$\mathrm{k} = \frac{n(4n^2-1)}{3c} - \frac{n}{c}\left[(h+s-1)\big(2(n-h)+1\big) - s(s-1)\right]$$

$$+ \frac{n\big(n-h-s+1\big)\Big[6c^2 - a(a+2c)\big(2(n-h-s)+1\big)\big(2(n-h-s)+3\big)\Big]}{3c(a+2c)\Big[cV_s(q) + a\big(2(n-h-s)+1\big)U_{s-1}(q)\Big]} U_{s-1}(q)$$

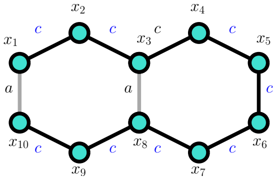
$$+ \frac{n\Big[(h-1)(a+2c)Q_{s-1}(q) + cs\Big[\big(2(n-h-s)+1\big)T_s(q) + W_s(q)\Big]\Big]}{(a+2c)\Big[cV_s(q) + a\big(2(n-h-s)+1\big)U_{s-1}(q)\Big]}$$

Naphtalene $s = 2$

$$(I+\Lambda)^{-1} = \begin{bmatrix} 1+\frac{9a}{c} & \frac{5a}{c} \\ \frac{5a}{c} & 1+\frac{5a}{c} \end{bmatrix}^{-1}$$



Naphtalene $s = 2$



$$(I+\Lambda)^{-1} = \begin{bmatrix} 1+\frac{9a}{c} & \frac{5a}{c} \\ \frac{5a}{c} & 1+\frac{5a}{c} \end{bmatrix}^{-1}$$

$G(x_i, x_j) =$

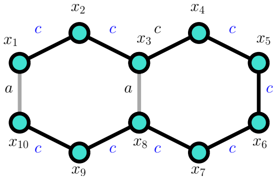
$$= \frac{77}{20} + \frac{1}{20} i\,(i-11) + \frac{1}{20} j(j-11) - \frac{1}{2}|j-i|$$

$$-\frac{1}{400}(10|i-10| - 10|i-1|)\Big(\frac{12}{7}|j-10| - \frac{12}{7}|j-1| - \frac{10}{7}|j-8| + \frac{10}{7}|j-3|\Big)$$

$$-\frac{1}{400}(10|i-8| - 10|i-3|)\Big(-\frac{10}{7}|j-10| + \frac{10}{7}|j-1| + \frac{20}{7}|j-8| - \frac{10}{7}|j-3|\Big)$$

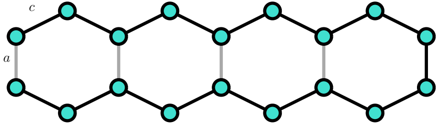
Naphtalene $s = 2$

$$(I+\Lambda)^{-1} = \begin{bmatrix} 1+\frac{9a}{c} & \frac{5a}{c} \\ \frac{5a}{c} & 1+\frac{5a}{c} \end{bmatrix}^{-1}$$

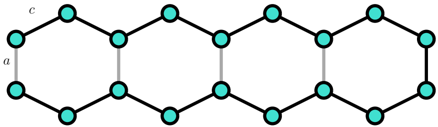


$$\mathrm{k} = \frac{33}{2c} - \frac{5a(44a+25c)}{c(c^2+14ca+20a^2)}$$

Hexagonal Chain. $s \geq 3$



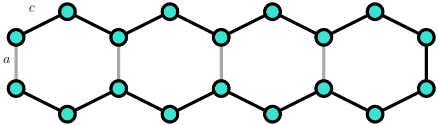
Hexagonal Chain. $s \geq 3$



$$(I+\Lambda)^{-1} = \begin{bmatrix} \frac{a}{2n}+\frac{c}{8n} & -\frac{c}{8n} & 0 & \cdots & 0 \\ -\frac{c}{8n} & \frac{a}{2n}+\frac{c}{4n} & -\frac{c}{8n} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{a}{2n}+\frac{c}{4n} & -\frac{c}{8n} \\ 0 & 0 & \cdots & -\frac{c}{8n} & \frac{a}{2n}+\frac{c}{8n}+\frac{9c}{40n} \end{bmatrix}^{-1}$$

$$2\left(1+\frac{2a}{c}\right)z_k - z_{k-1} - z_{k+1} = 0$$

Hexagonal Chain. $s \geq 3$

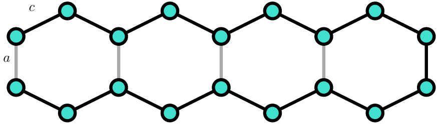


$$(I+\Lambda)^{-1} = \begin{bmatrix} \frac{a}{2n}+\frac{c}{8n} & -\frac{c}{8n} & 0 & \cdots & 0 \\ -\frac{c}{8n} & \frac{a}{2n}+\frac{c}{4n} & -\frac{c}{8n} & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{a}{2n}+\frac{c}{4n} & -\frac{c}{8n} \\ 0 & 0 & \cdots & -\frac{c}{8n} & \frac{a}{2n}+\frac{c}{8n}+\frac{9c}{40n} \end{bmatrix}^{-1}$$

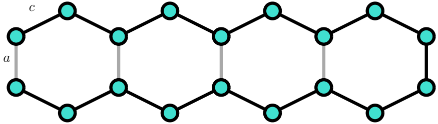
$$\boxed{2\left(1+\frac{2a}{c}\right)z_k - z_{k-1} - z_{k+1} = 0}$$

$$u_1 = \frac{c}{8n},\ u_2 = \frac{a}{2n}+\frac{c}{8n},\ v_{s-1} = \frac{a}{2n}+\frac{9c}{40n},\ v_s = \frac{c}{8n}.$$

Hexagonal Chain. $s \geq 3$



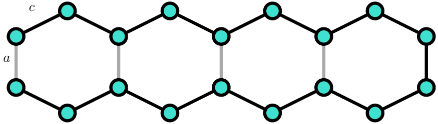
Hexagonal Chain. $s \geq 3$



$$u(k) = \frac{1}{8n}\left[cU_k(q) - (4a+c)U_{k-1}(q)\right]$$

$$v(k) = \frac{c}{40n}\left[5U_{s-k}(q) - U_{s-k-1}(q)\right]$$

Hexagonal Chain. $s \geq 3$

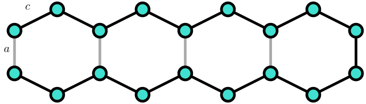


$$u(k) = \frac{1}{8n}\left[cU_k(q) - (4a+c)U_{k-1}(q)\right]$$

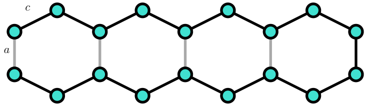
$$v(k) = \frac{c}{40n}\left[5U_{s-k}(q) - U_{s-k-1}(q)\right]$$

$$\left((\mathsf{I}+\Lambda)^{-1}\right)_{km} = \delta_{km} - \frac{320n^2}{c(cV_{s-1}(q) + 5aU_{s-1}(q))} u_{\min\{k,m\}} v_{\max\{k,m\}}$$

Hexagonal Chain. $s = 4$



Hexagonal Chain. $s = 4$



$$k = \frac{323}{6c} - \frac{2a(6080a^3 + 609c^3 + 9864ca^2 + 4692c^2a)}{c(320a^4 + 544ca^3 + 280c^2a^2 + 44c^3a + c^4)}$$