International Conference
Inverse Problem and Related Topics
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# Spectra of graphs with pendants

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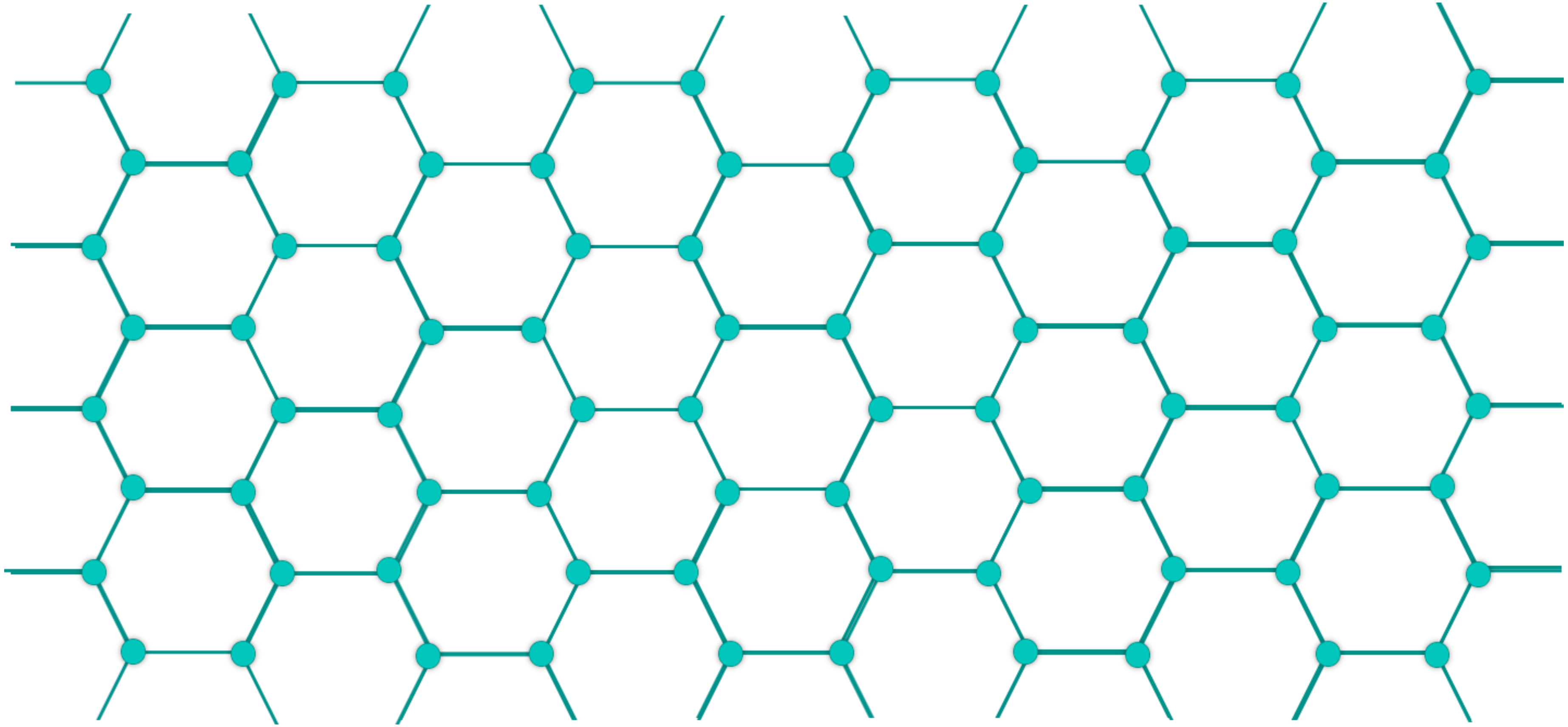
**Related papers:**

1. A. Suzuki, Spectrum of the Laplacian on a covering graph with pendant edges I, Linear Algebra Appl. **439**, 3464–3489, 2013.
2. I. Sasaki, A. Suzuki, Essential spectrum of the discrete Laplacian on a deformed lattice, in preparation.

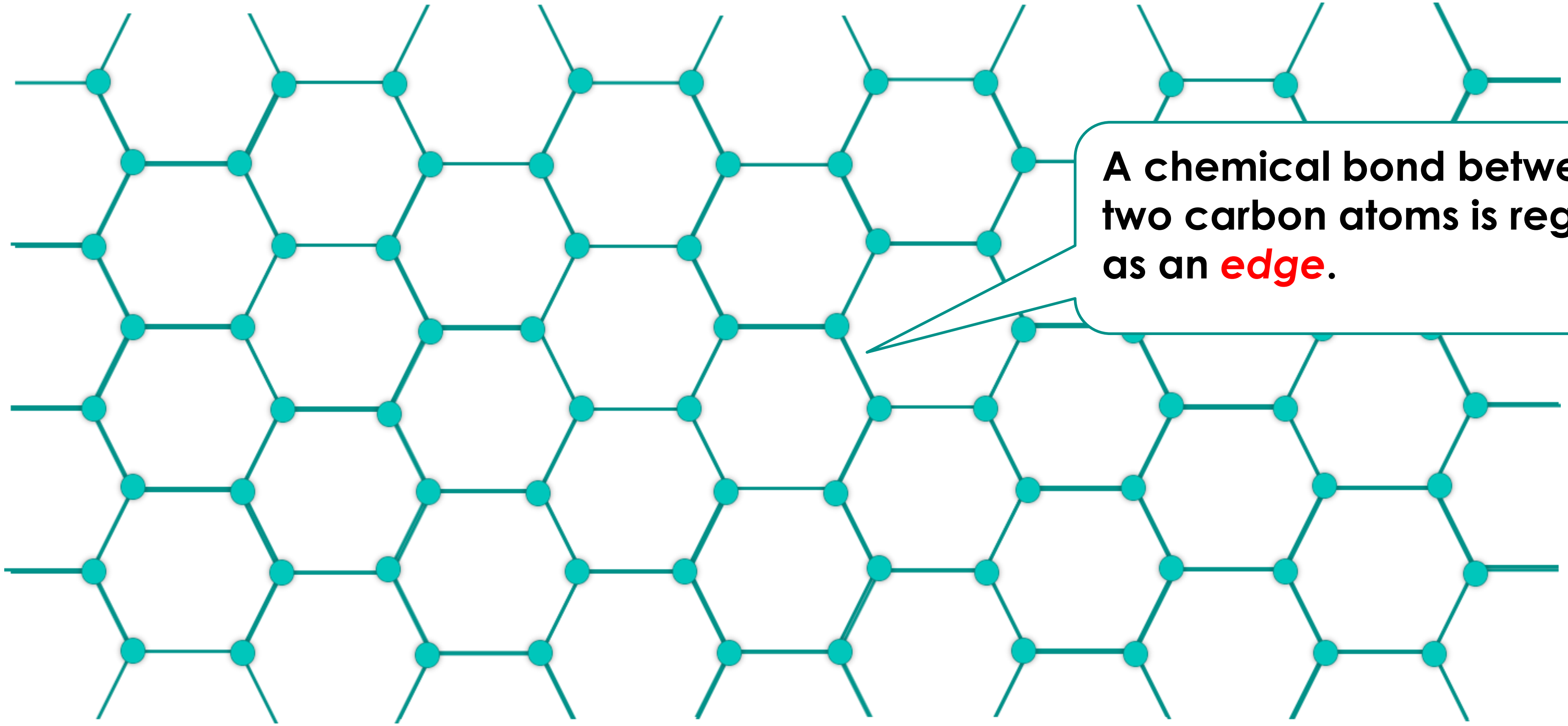
# 1. Graphs with pendants

# Graphene: hexagonal lattice  consisting of carbon atoms



: A carbon atom

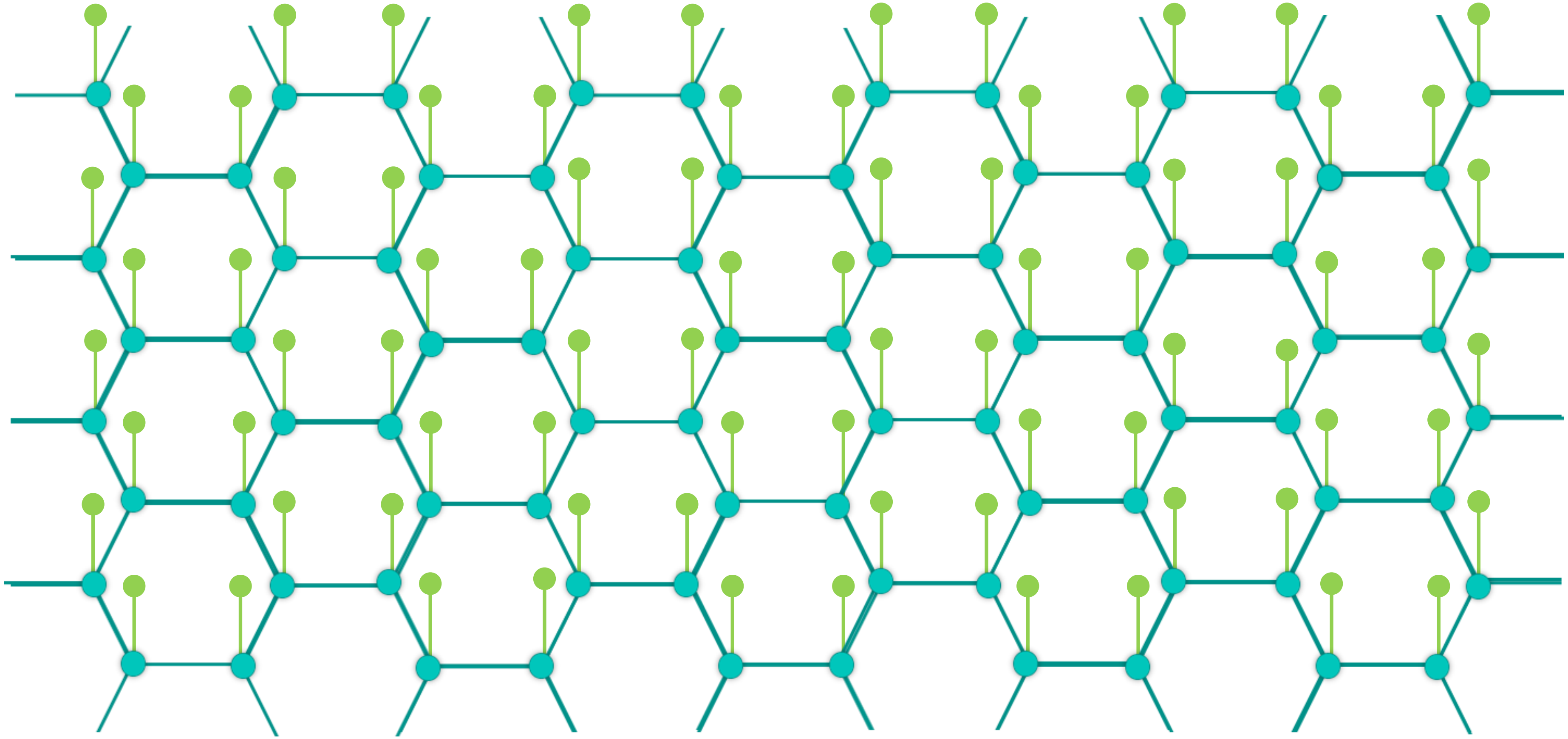
# Graphene: hexagonal lattice consisting of carbon atoms



A chemical bond between two carbon atoms is regarded as an *edge*.

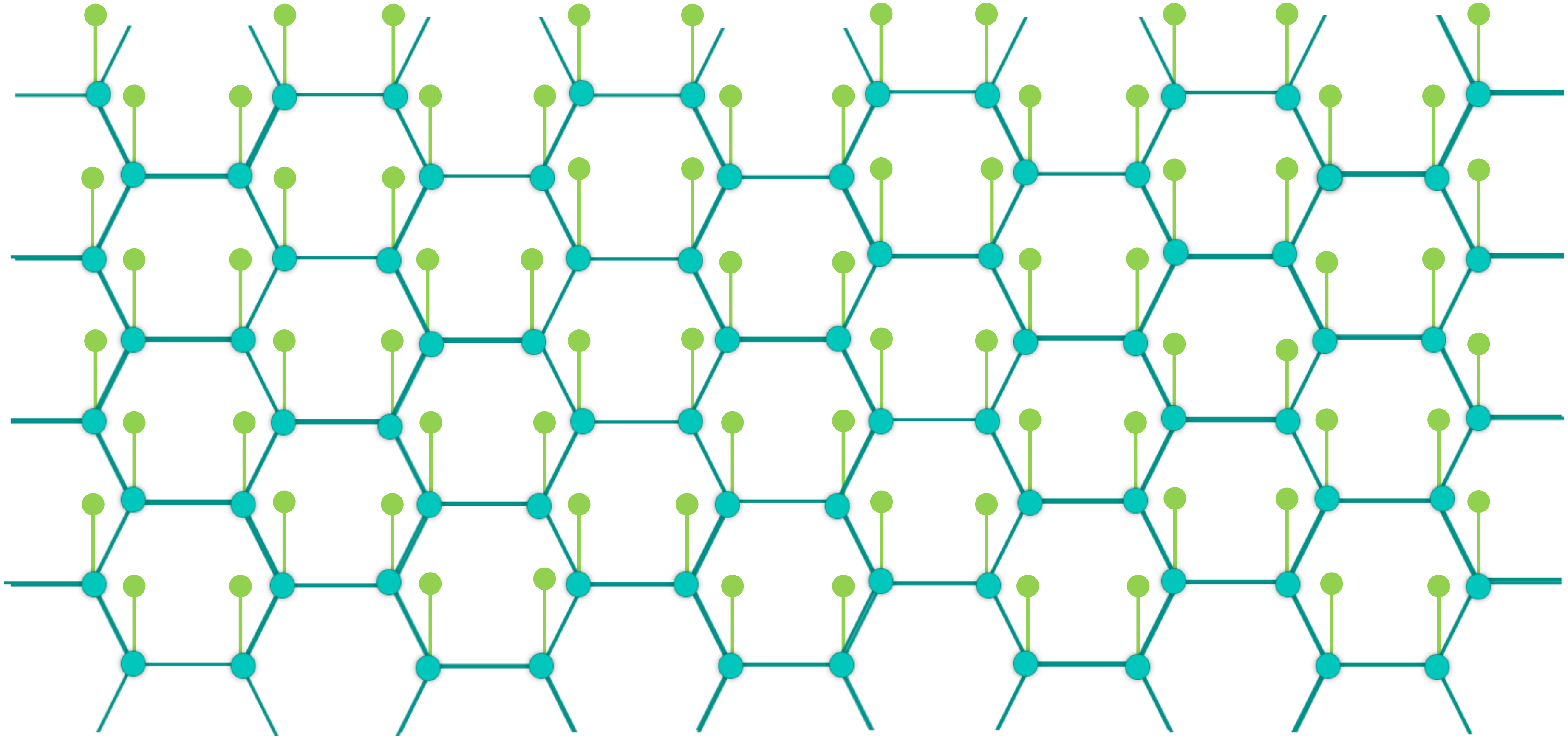
: A carbon atom is regarded as a *vertex* with a degree of 3.

# Graphane (with an *a*): Fully hydrogenated graphene



- : A carbon atom
- : A hydrogen atom

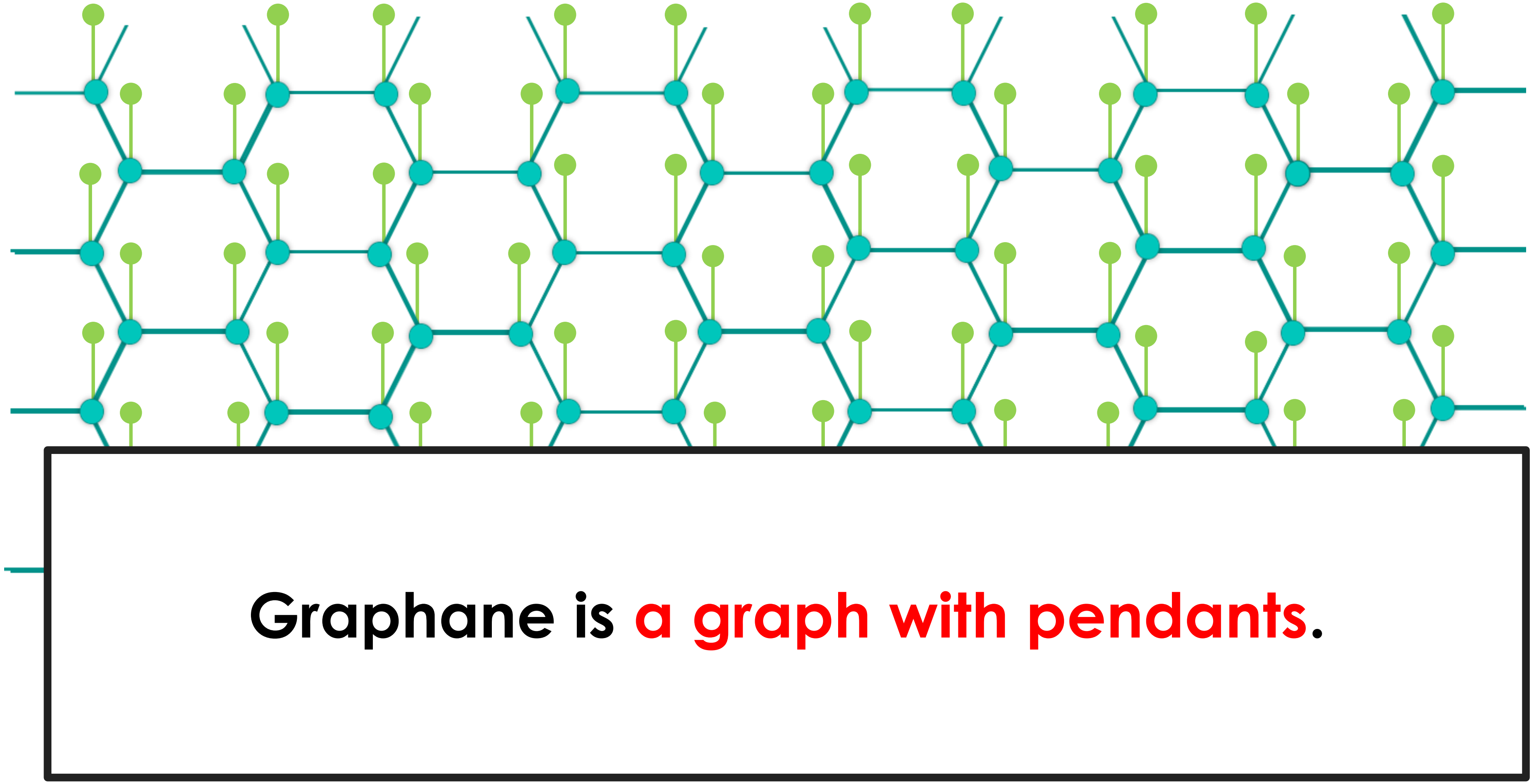
# Graphane (with an *a*): Fully hydrogenated graphene



 : A carbon atom corresponds to a vertex with a **degree of 4**.

 : A hydrogen atom corresponds to a vertex with a **degree of 1**. → a ***pendant vertex***

# Graphane (with an *a*): Fully hydrogenated graphene

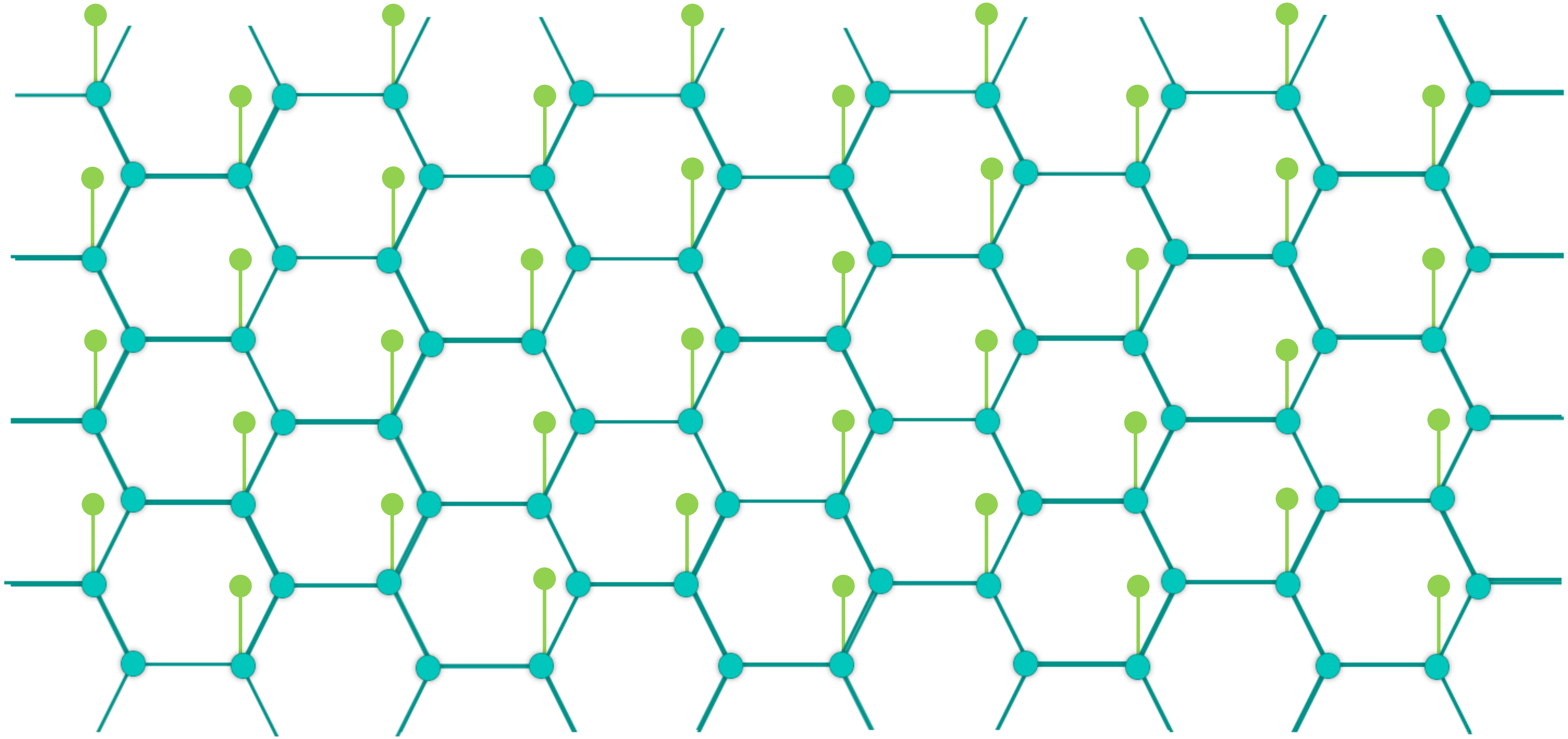


**Graphane is a graph with pendants.**

● : A carbon atom corresponds to a vertex with a degree of 4.

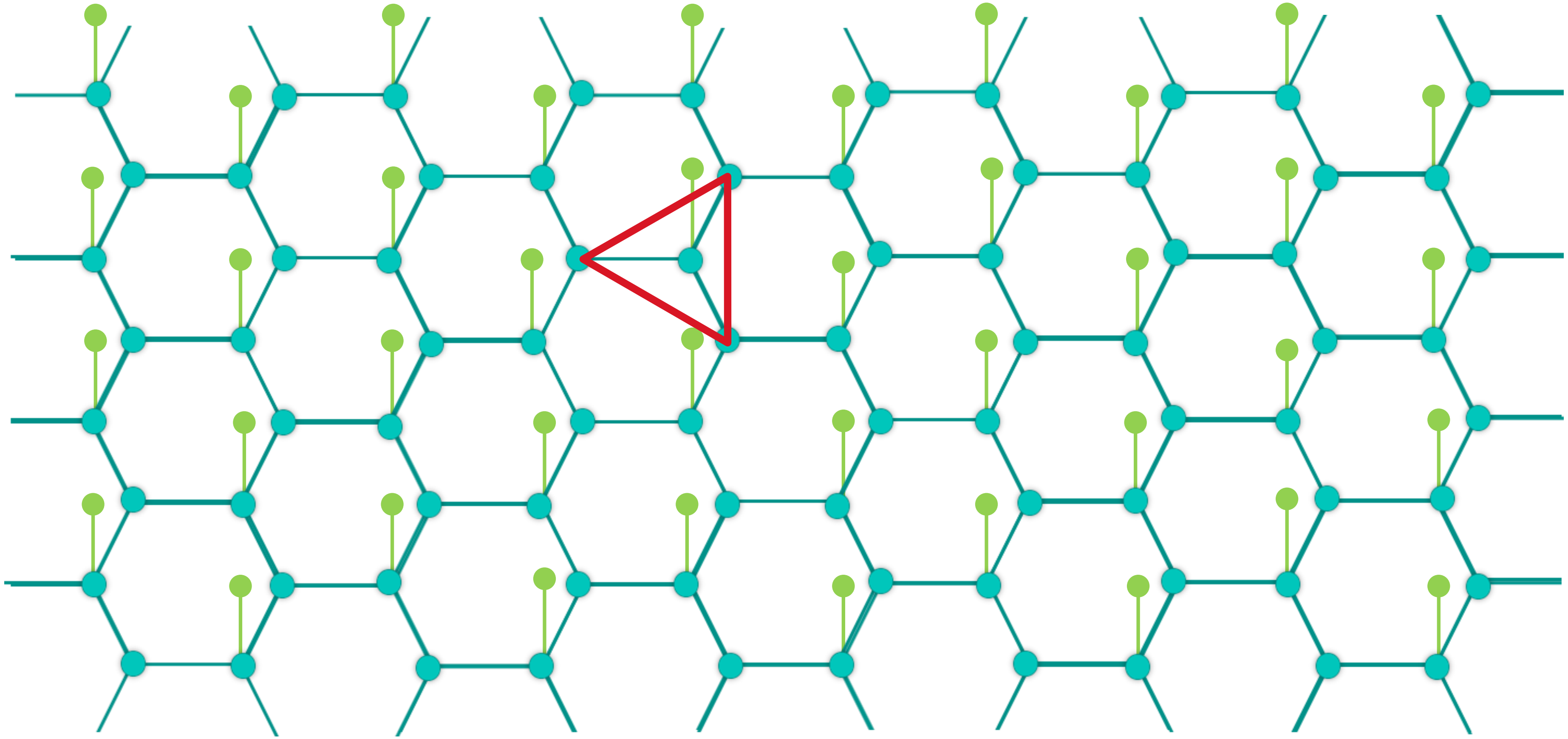
● : A hydrogen atom corresponds to a vertex with a degree of 1. → a *pendant vertex*

# Graphone: Half hydrogenated graphene (triangle type)



: A carbon atom
: A hydrogen atom

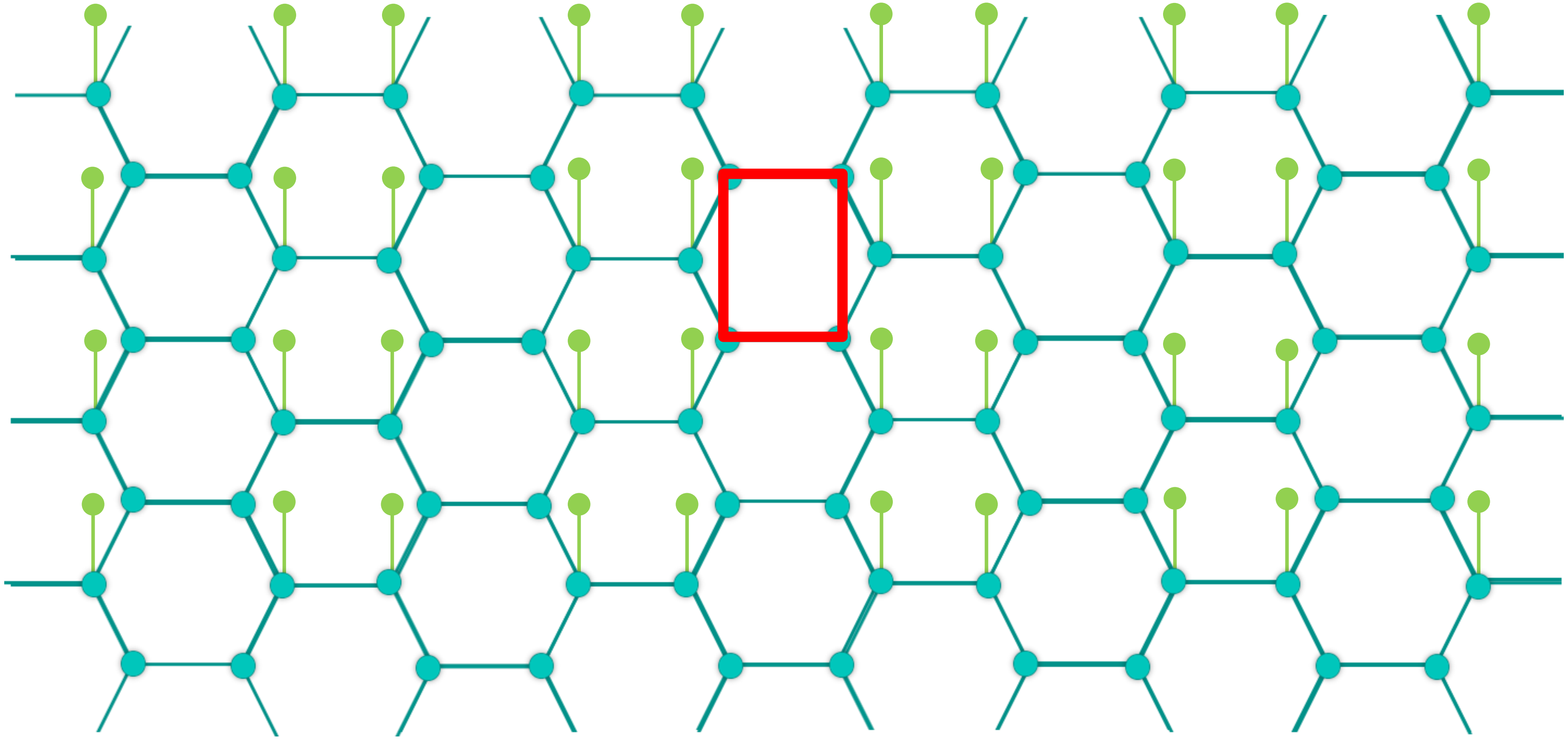
# Graphone: Half hydrogenated graphene (triangle type)



: A carbon atom corresponds to a vertex with a degree of 3 or 4.

: A hydrogen atom corresponds to a pendant vertex.

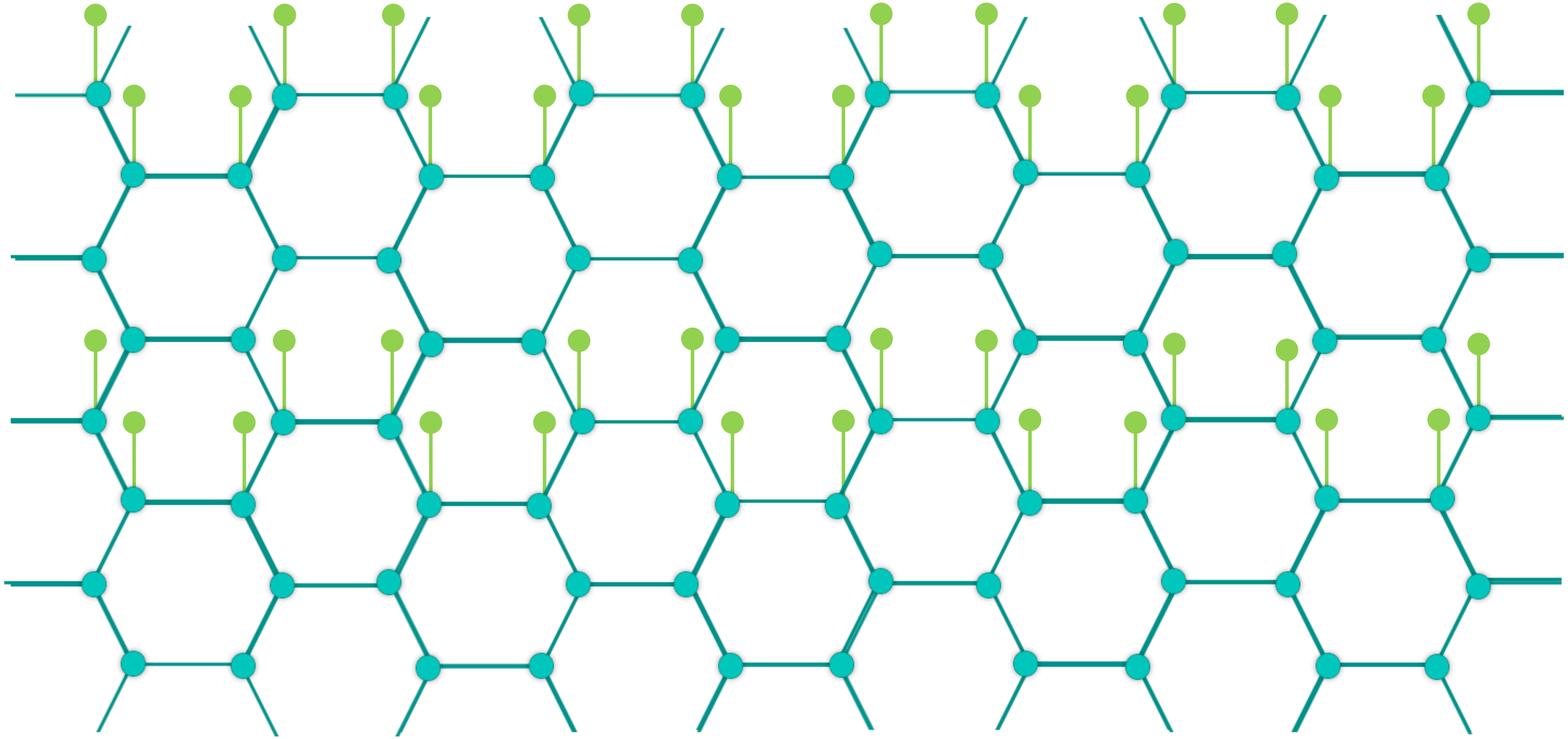
# Graphone: Half hydrogenated graphene (rectangle type)



● : A carbon atom corresponds to a vertex with a degree of 3 or 4.

● : A hydrogen atom corresponds to a pendant vertex.

# Graphone: Half hydrogenated graphene (another type)



: A carbon atom corresponds to a vertex with a degree of 3 or 4.

: A hydrogen atom corresponds to a pendant vertex.

## Spectra of graphs

Let $G=(V(G),E(G))$ be a graph, where $V(G)$ and $E(G)$ are the sets of vertices and edges.

The Laplacian $L_G$ is defined as follows:

$$(L_G\psi)(x)=\frac{1}{\deg x}\sum_{y\sim x}\psi(y), \quad x\in V(G),$$

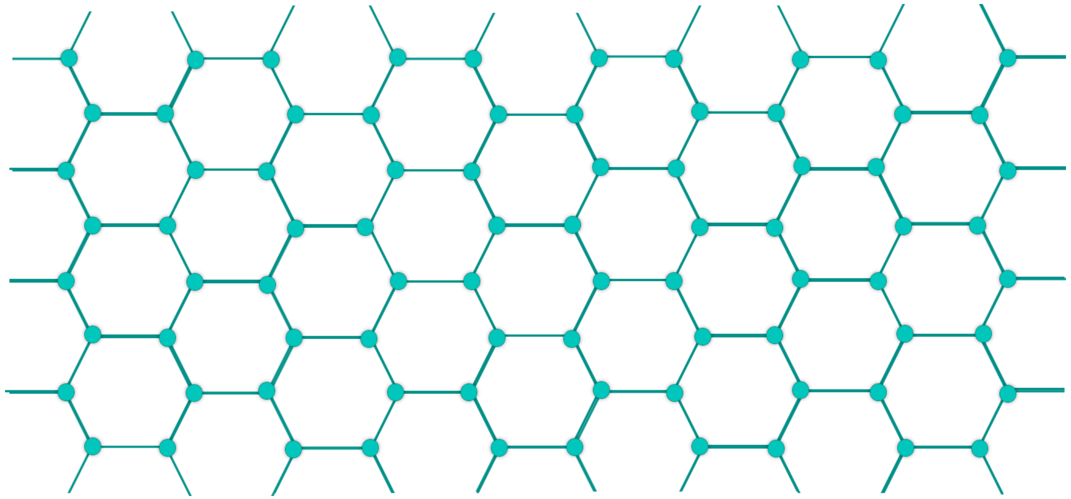
where $\psi$ is in the Hilbert space

$$\ell^2_{\mathrm{w}}(V(G))=\left\{\psi:V(G)\to\mathbb{C}\mid \sum_{x\in V(G)}|\psi(x)|^2\deg x<\infty\right\}.$$

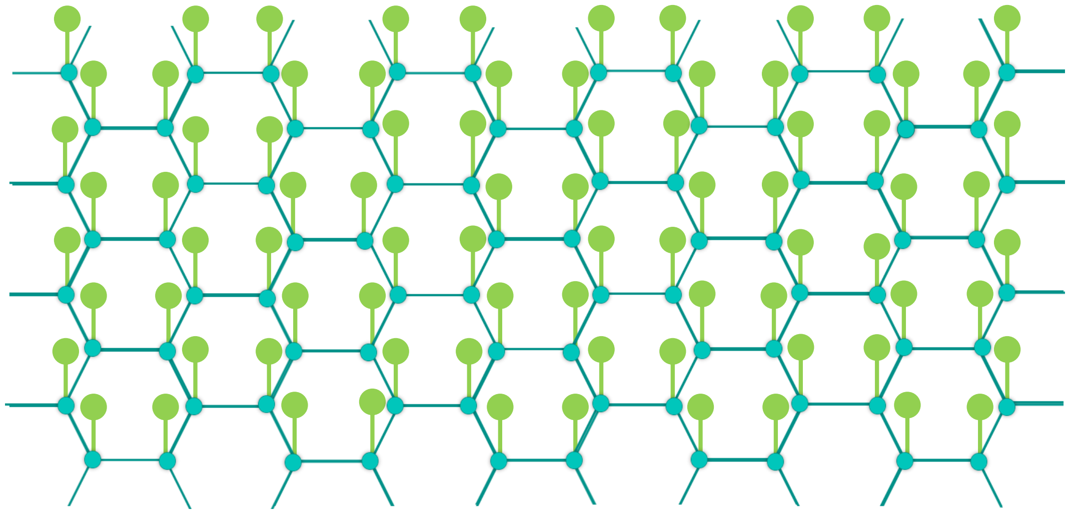
It is well known that $L_G$ is bounded, self-adjoint and

$$\mathrm{Spec}(L_G)\subset[-1,1].$$

Graphene



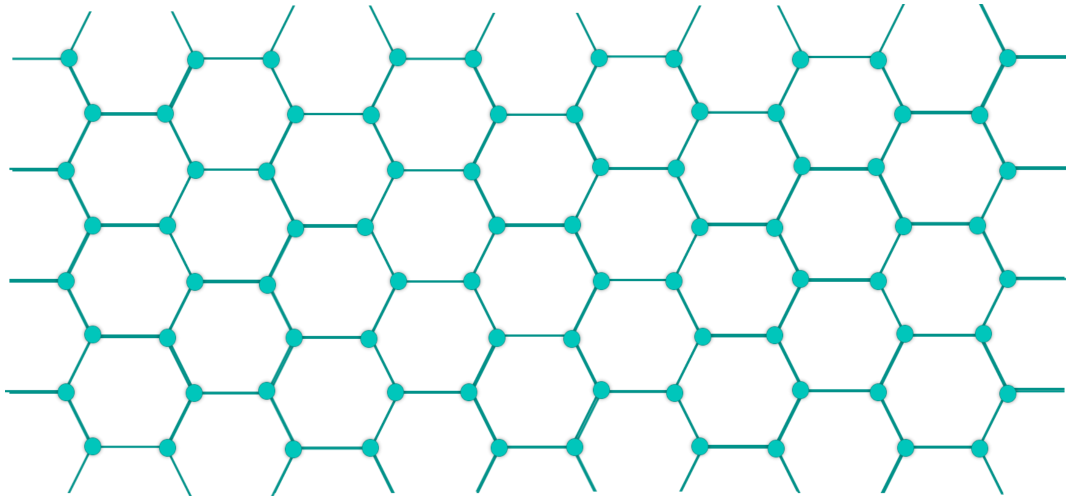
Graphane



**The spectrum of the Laplacian on the graph that corresponds to graphene is**

$$\mathrm{Spec}(L_G) = [-1, 1].$$

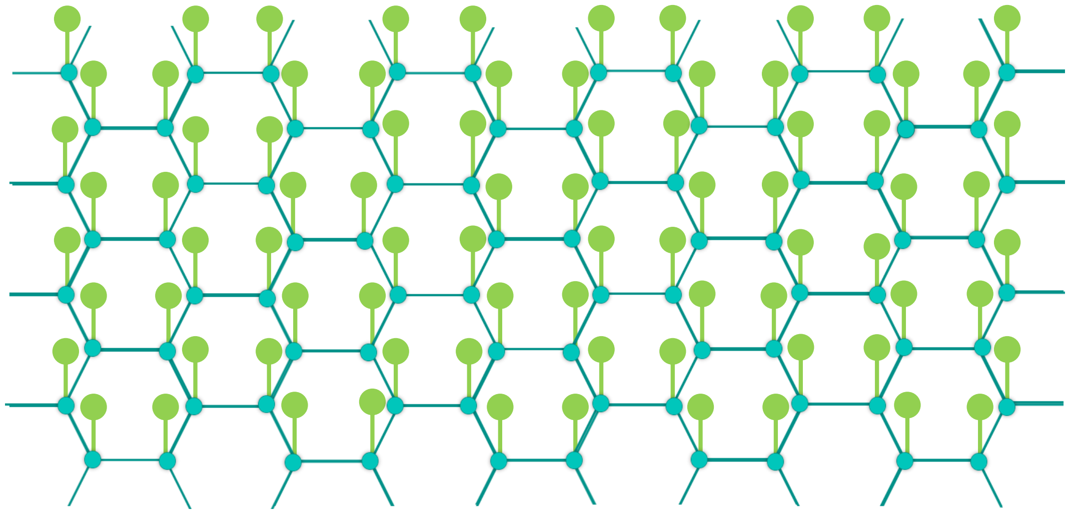
**Graphene**



The spectrum of the Laplacian on the graph $G_0$ that corresponds to graphene is

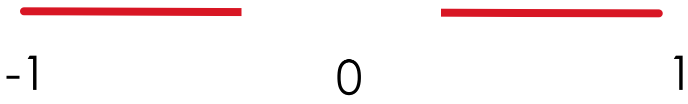
$$\mathrm{Spec}(L_G) = [-1, 1].$$


**Graphane**



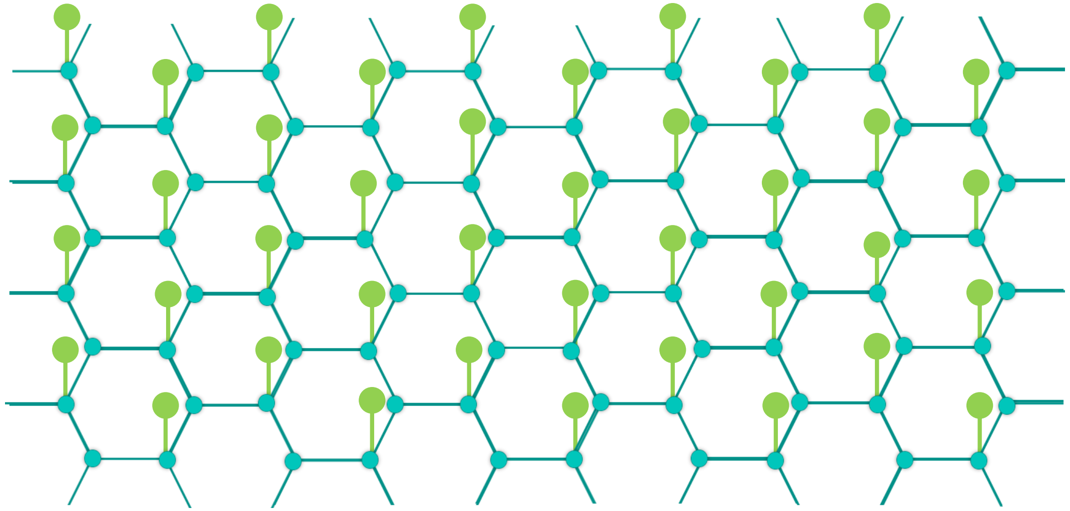
The spectrum of the Laplacian on the graph that corresponds to graphane is

$$\mathrm{Spec}(L_G) = \left[-1, -\frac{1}{4}\right] \cup \left[\frac{1}{4}, 1\right]$$

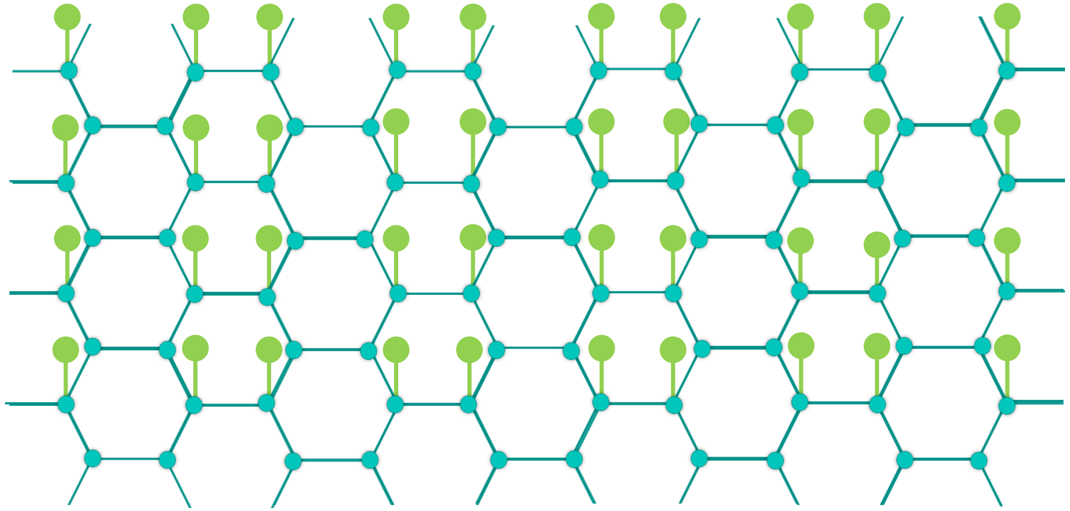




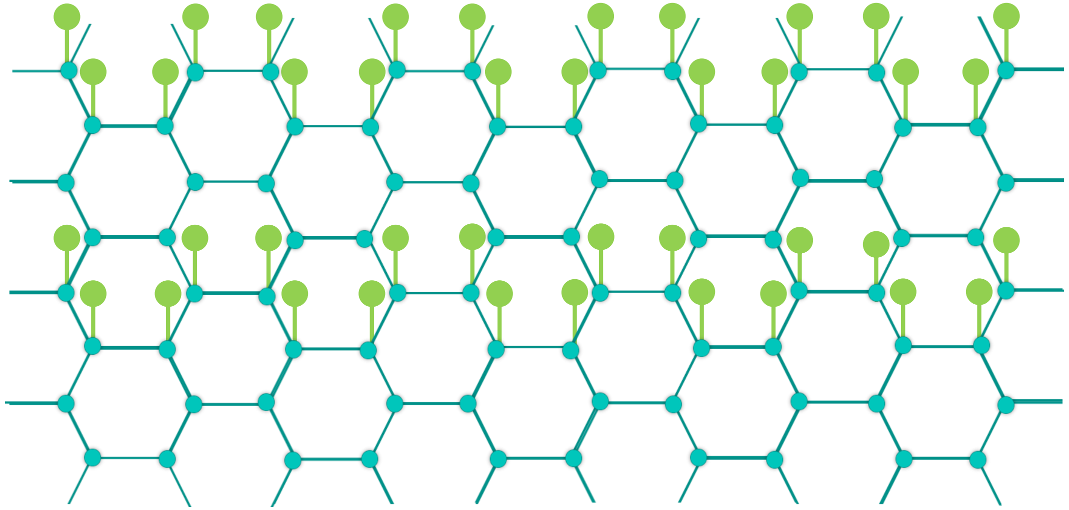

**A spectral gap opens!**



Triangle type



Rectangle type



Another type

**What do you think the spectra of graphones are?**

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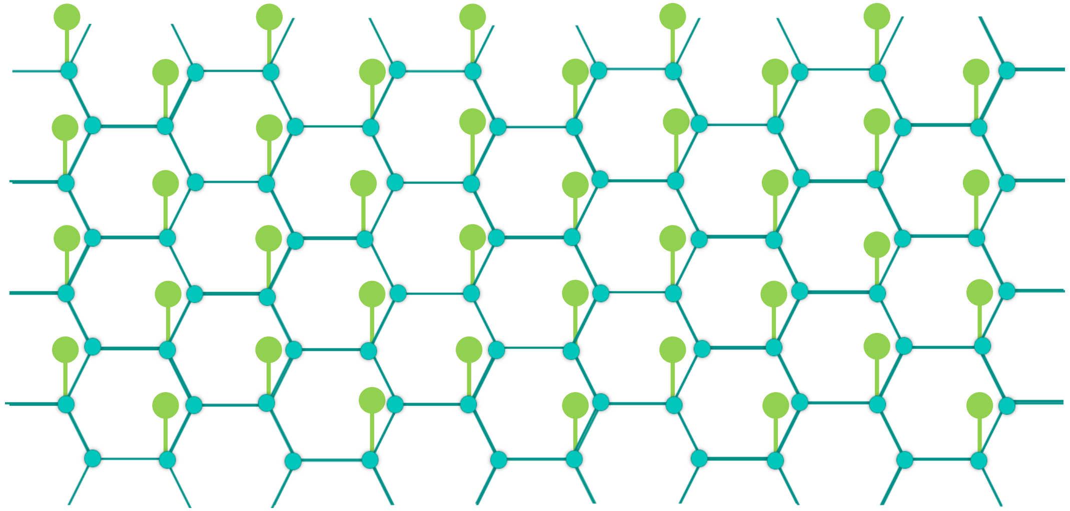
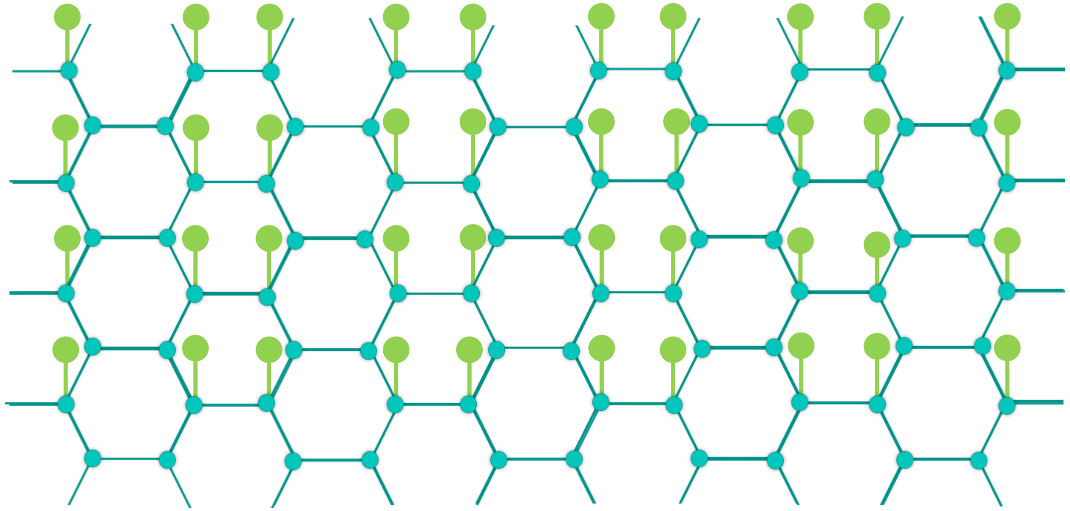
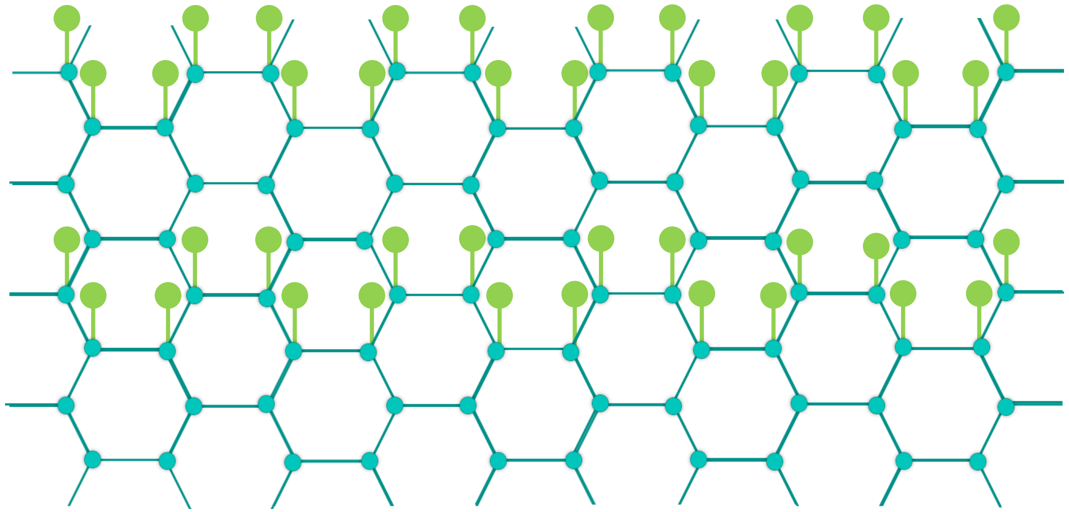




**Triangle type**

**Spectral gap near 0 and zero eigenvalue exist**

-1 -1/2 0 1/2 1



**Another type**

**No spectral gap exists**

-1 1

**Rectangle type**

**Spectral gap near 0**

-1 0 1

In this talk, we focus on the following problem:

**What arrangement of pendants makes a spectral gap near zero and zero eigenvalue?**

**Definition:** We say that an operator $A$ has a spectral gap near zero if

$$m(A) := \left(\inf \mathrm{Spec}(A^2) \setminus \{0\}\right)^{1/2} > 0$$

$A$ has a spectral gap near zero

$$\Longrightarrow \quad \mathrm{Spec}(A) \cap ((-m(A), 0) \cup (0, m(A))) = \emptyset$$

$A$ has no spectral gap near zero

$$\Longrightarrow \quad \mathrm{Spec}(A) \cap [-\epsilon, \epsilon] \neq \emptyset \quad \text{with some } \epsilon > 0.$$

# 2. Preliminary

# Adjacency operator and Laplacian

**The adjacency operator $A_G$ of a graph $G = (V(G), E(G))$ is**

$$(A_G\psi)(x) = \sum_{y\sim x} \psi(y), \quad x \in V(G),$$

**where $\psi$ is a vector in the Hilbert space**

$$\ell^2(V(G)) = \left\{ \psi : V(G) \to \mathbb{C} \mid \sum_{x\in V(G)} |\psi(x)|^2 < \infty \right\}.$$

**Lemma**

**(1)** $\dim\ker L_G = \dim\ker A_G$

**(2)** $m(L_G) > 0 \iff m(A_G) > 0$

**From this lemma,
it suffices to know the
spectrum of $A_G$.**

## Proof of Lemma

**(1) is proven as follows. Note that**

$$U^* L_G U = D^{-1/2} A_G D^{-1/2}$$

**where** $U : \ell^2(V(G)) \to \ell^2_{\mathrm{w}}(V(G))$ **is a unitary defined by**

$$U = D^{-1/2}\psi, \quad \psi \in \ell^2(V(G))$$

**with**

$$(D\psi)(x) = (\deg x)\psi(x), \quad x \in V(G).$$

**We know that**

$$\ker(U^* L_G U) = \{D^{1/2}\psi \mid \psi \in \ker A_G\}$$

**which implies** $\dim\ker L_G = \dim\ker A_G$ .

## Proof of Lemma

**(2) is also proven by**

$$U^* L_G U = D^{-1/2} A_G D^{-1/2} \, ,$$

**which implies**

$$\left( \sup_{x \in V(G)} \deg x \right) m(L_G) \geq m(A_G) \text{ **provided** } m(A_G) > 0 \, ,$$

**and**

$$m(A_G) \geq \left( \inf_{x \in V(G)} \deg x \right) m(L_G) \text{ **provided** } m(L_G) > 0 \, .$$

**Therefore**

$$m(L_G) > 0 \Longleftrightarrow m(A_G) > 0.$$

**Assume that $G$ have pendant vertices:**

$$\Lambda_G := \{x \in V(G) \mid \deg x = 1\} \neq \emptyset$$

**Let $V_2 (\neq \emptyset) \subset \Lambda_G$ be an arbitrary set and**

$$V_1 := \{x \in V(G) \mid x \sim y, y \in V_2\}.$$

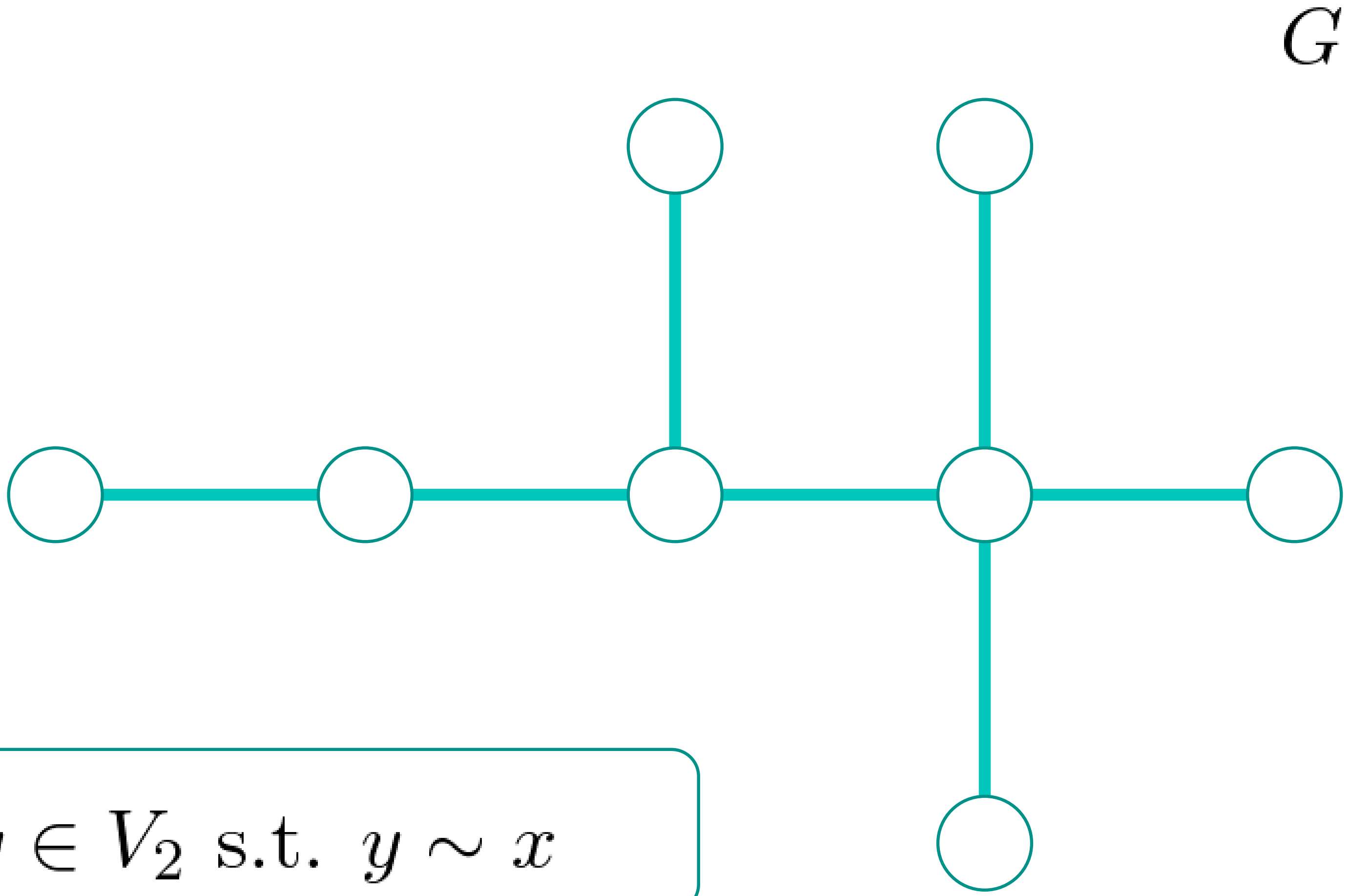
**Suppose that**

**(H0)** $\forall x \in V_1, \exists_1 y \in V_2 \text{ s.t. } y \sim x$

**Put**

$$V_0 := V(G) \cap V_1^c \cap V_2^c$$

# Example of a graph satisfying (H0):

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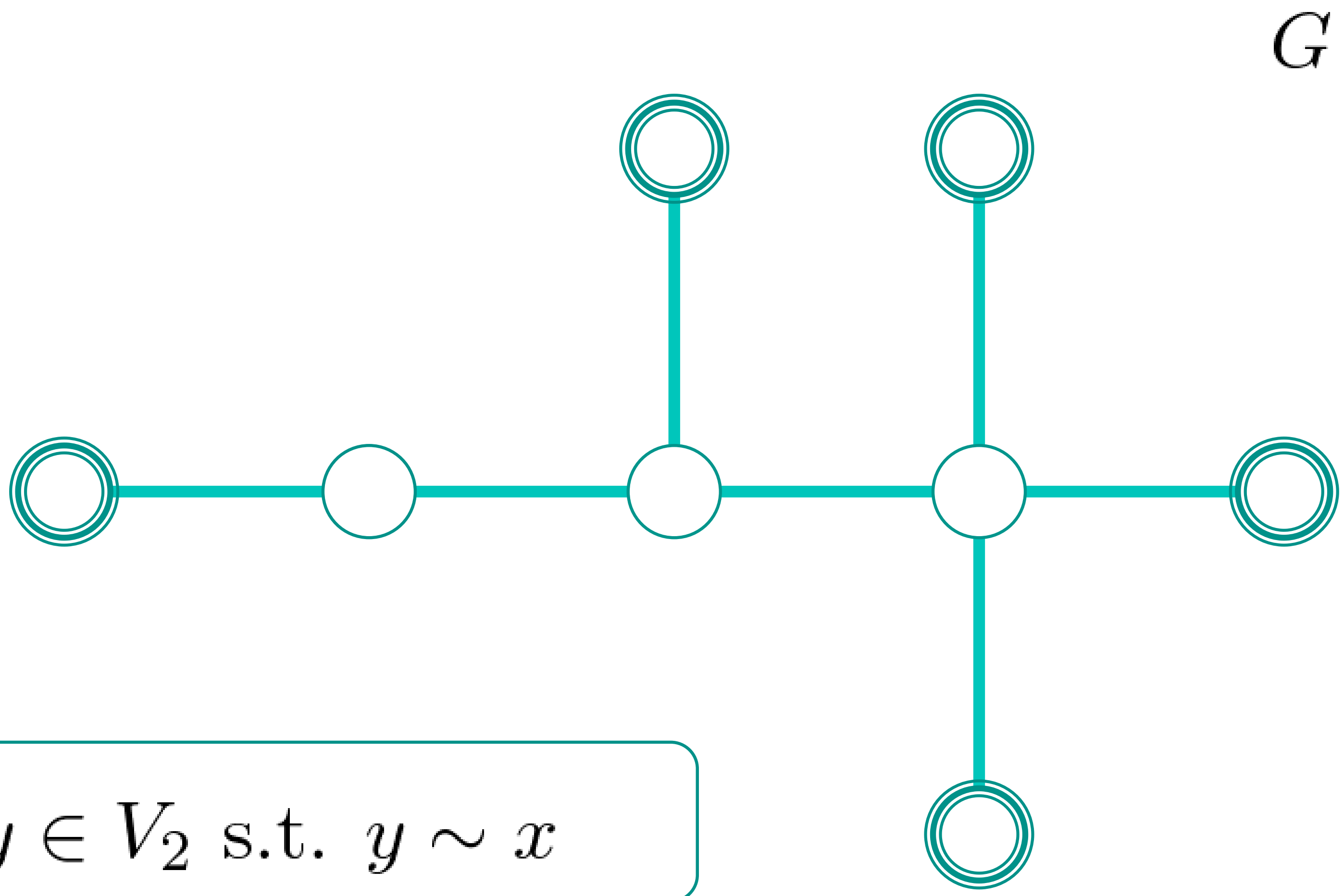


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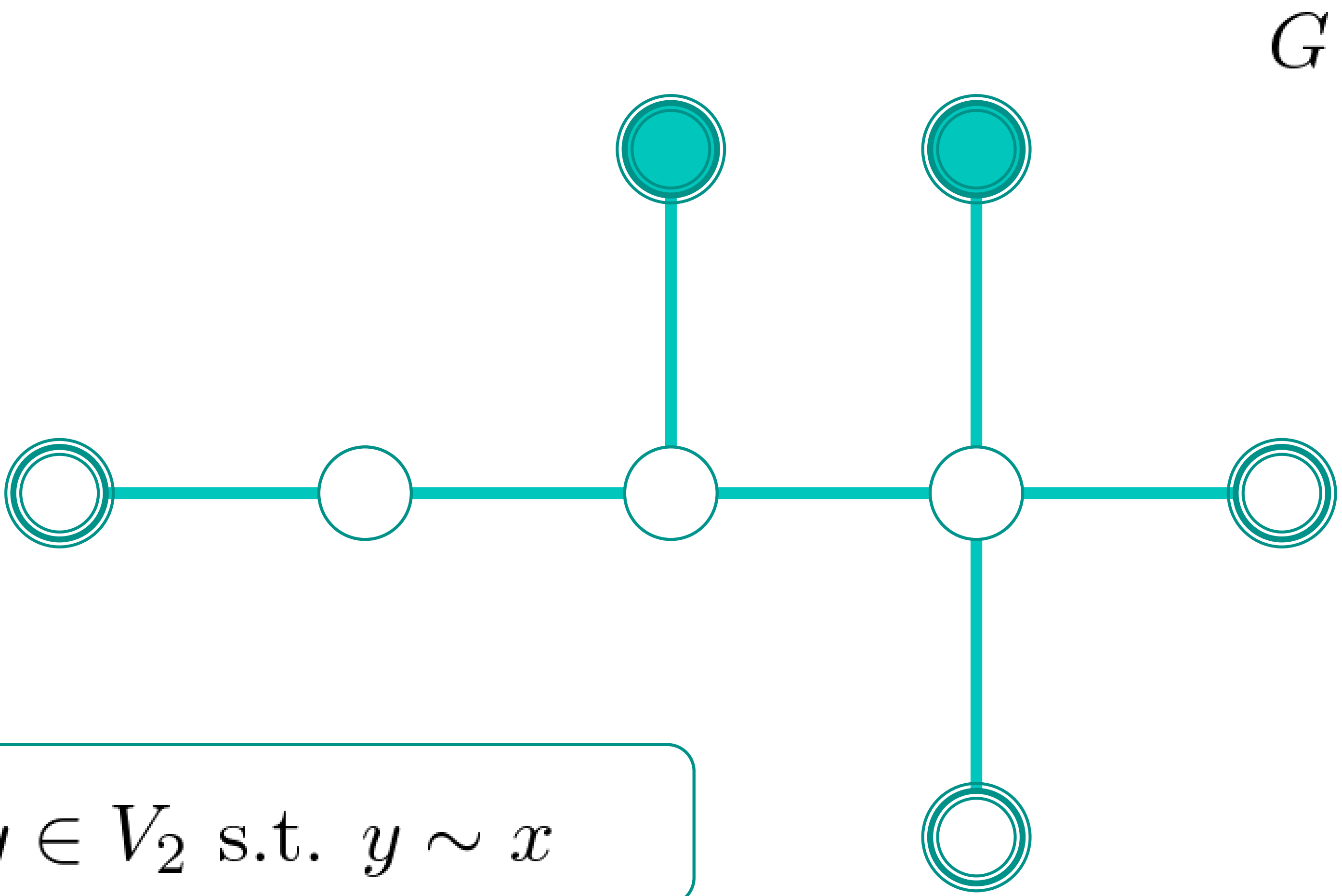
# Example of a graph satisfying (H0):

$\in \Lambda_G$

$\in V_2$

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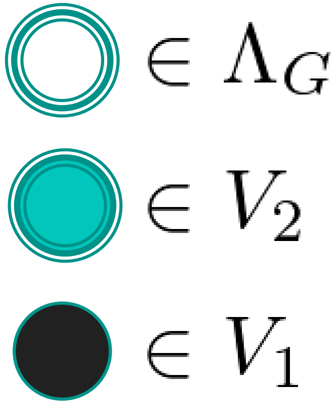


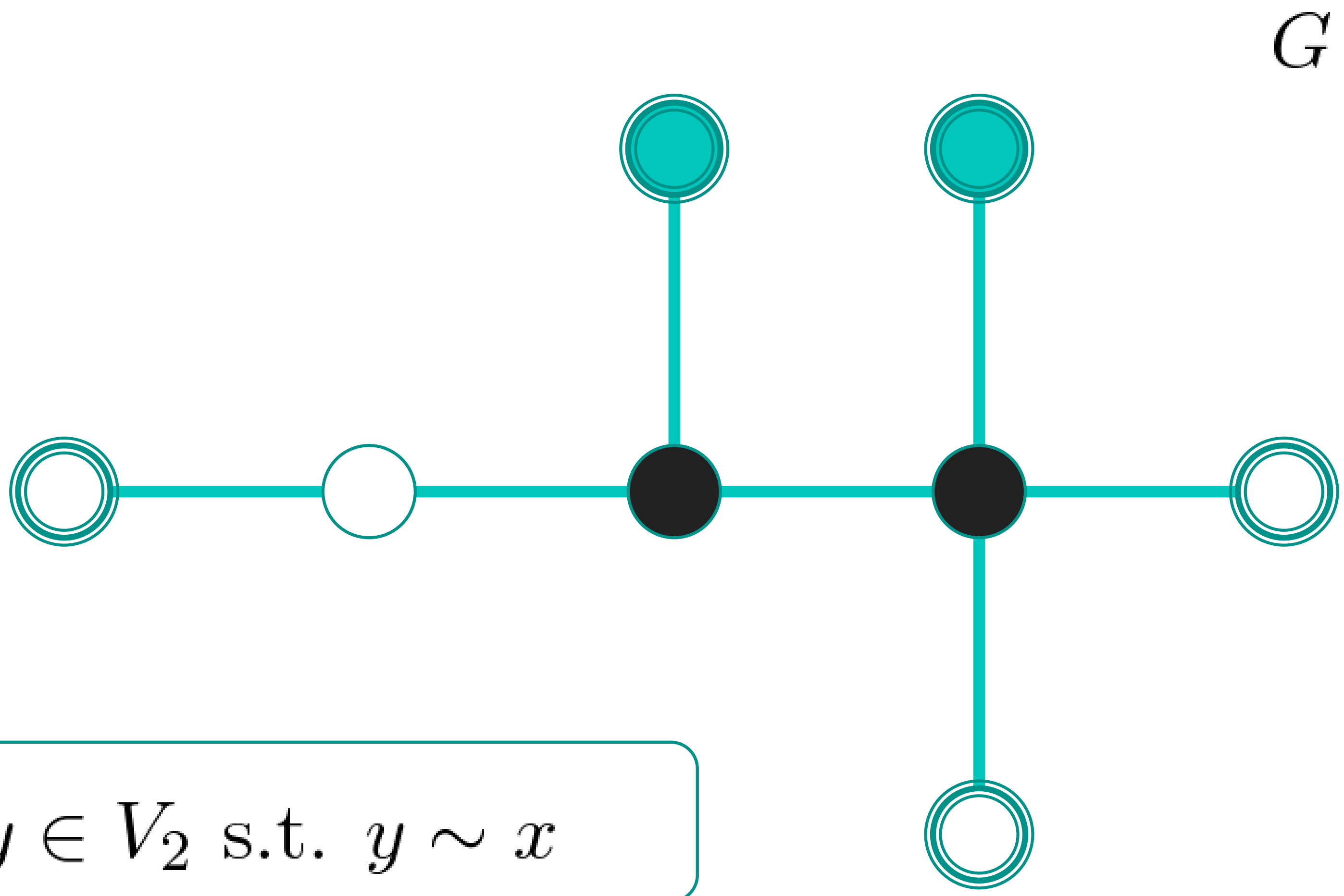


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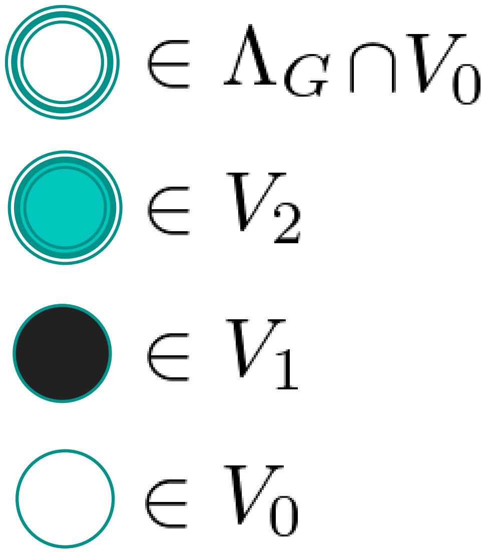
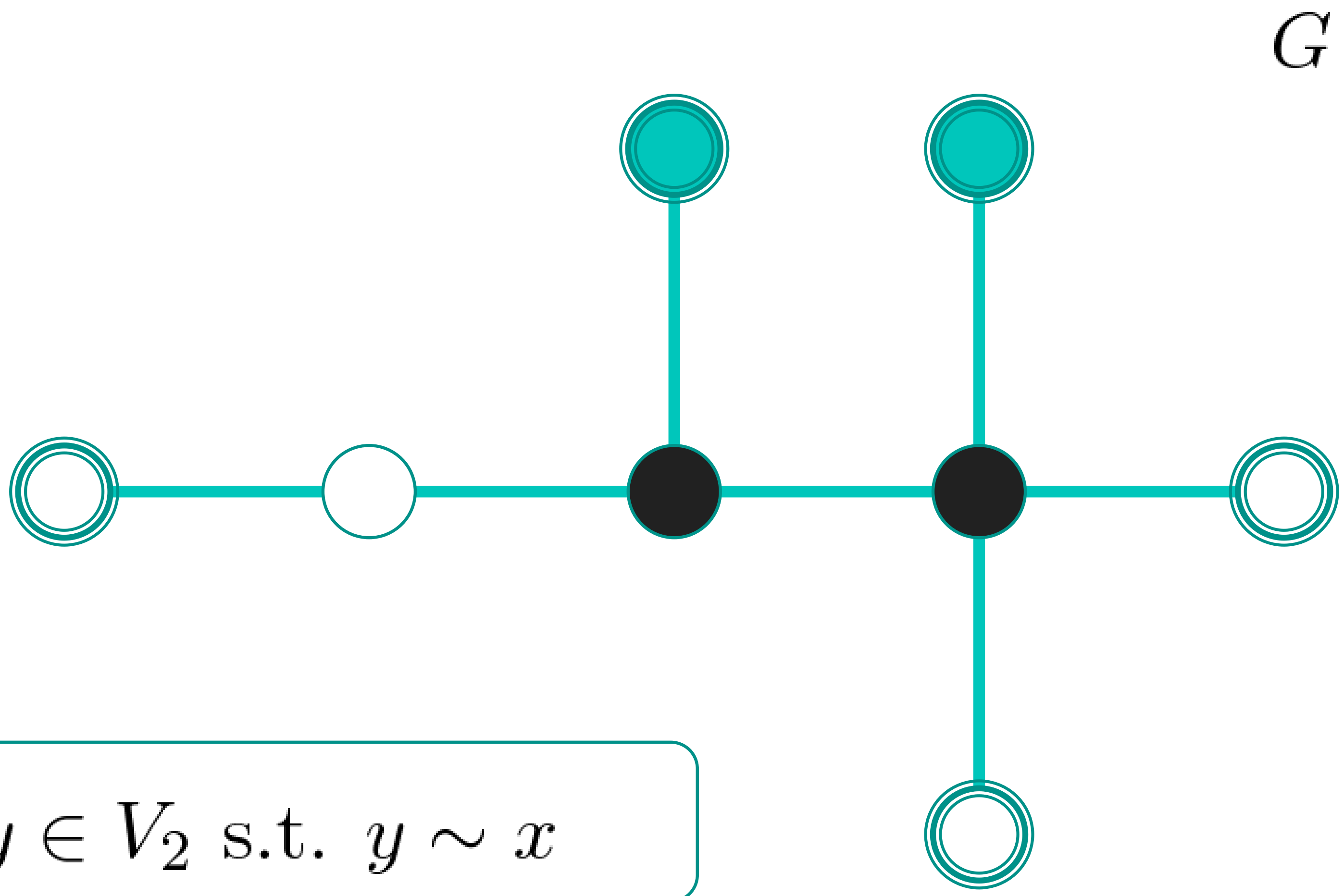
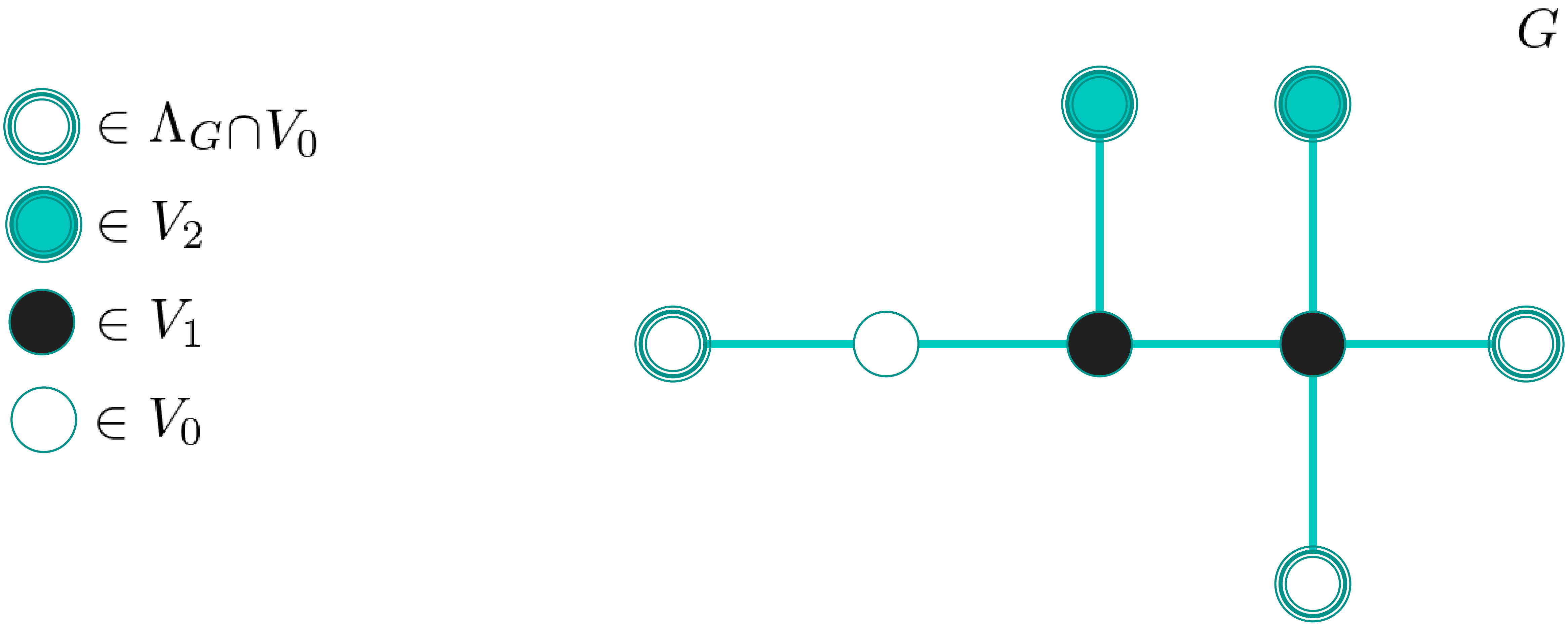



**(H0)** $\forall x \in V_1, \exists_1 y \in V_2 \text{ s.t. } y \sim x$

**For a graph $G$ satisfying (H0),**
**we define a graph $G_1$ by removing vertices of $V_2$ from $G$ ,**



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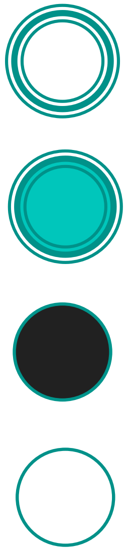


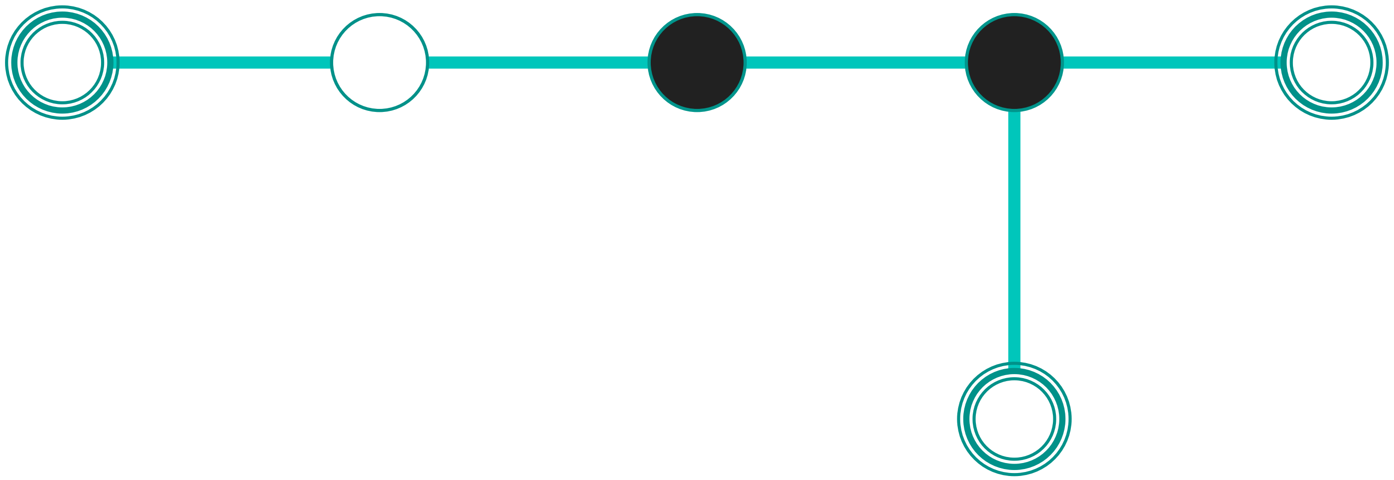
$\in \Lambda_G \cap V_0$

$\in V_2$

$\in V_1$

$\in V_0$

$G_1$



**For a graph $G$ satisfying (H0),**
**we define a graph $G_1$ by removing vertices of $V_2$ from $G$,**
**and $G_0$ by removing vertices of $V_1$ from $G_1$.**

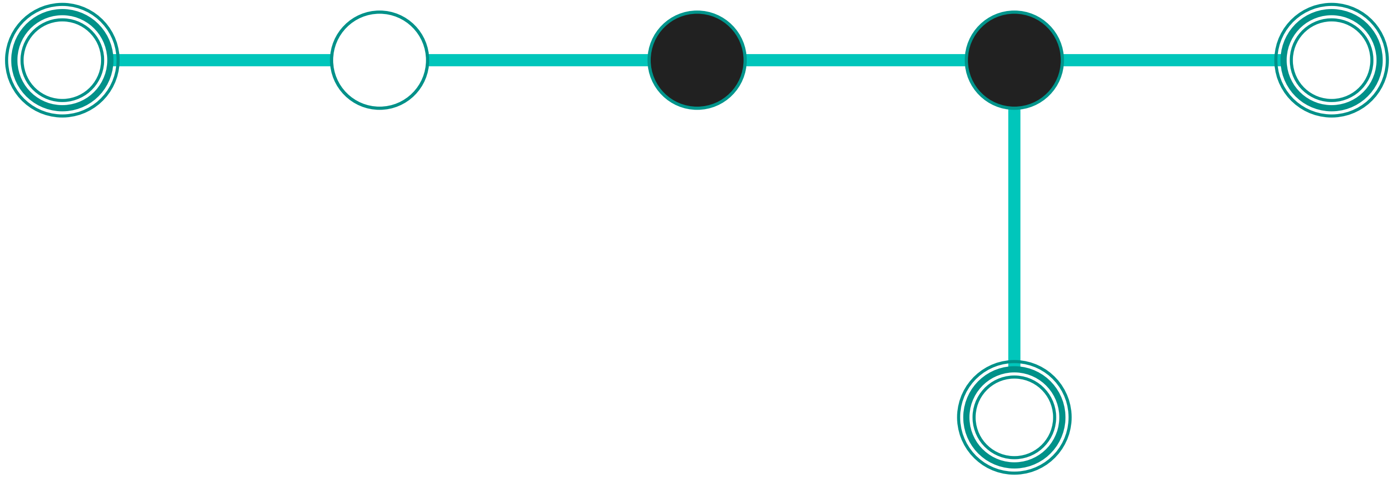
$G_1$

$\in \Lambda_G \cap V_0$

$\in V_2$

$\in V_1$

$\in V_0$



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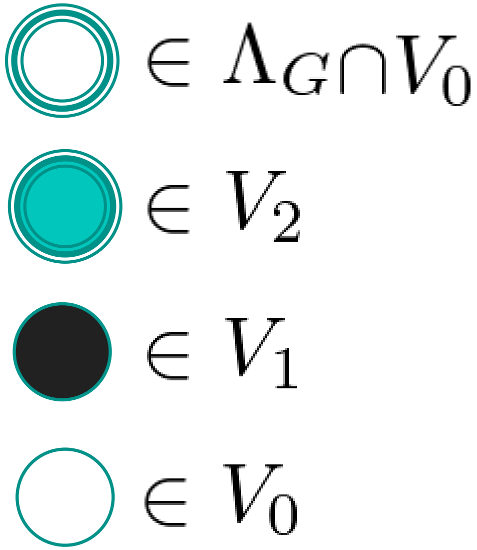



$G_0$

**Let $G$ satisfy (H0). Then $\ell^2(V(G))$ can be decomposed into**

$$\ell^2(V(G)) = \ell^2(V_0) \oplus \ell^2(V_1) \oplus \ell^2(V_2)$$

**and $A_G$ can be written as**

$$A_G = \begin{pmatrix} A_{00} & A_{01} & A_{02} \\ A_{10} & A_{11} & A_{12} \\ A_{20} & A_{21} & A_{22} \end{pmatrix},$$

**where $A_{ij} : \ell^2(V_j) \to \ell^2(V_i)$ is defined as**

$$(A_{ij}\psi_j)(x) = \begin{cases} \sum_{y \sim x; y \in V_j} \psi_j(y), & x \in V_i \\ 0, & x \notin V_i \end{cases}.$$

The following hold:

$$A_{00} = A_{G_0}, \quad \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix} = A_{G_1}$$

$$A_{22} = A_{20} = A_{02} = 0, \quad A_{ij}^* = A_{ji}.$$

We have

$$A_G = \begin{pmatrix} A_{G_1} & T^* \\ T & 0 \end{pmatrix},$$

where

$$A_{G_1} = \begin{pmatrix} A_{G_0} & A_{01} \\ A_{10} & A_{11} \end{pmatrix}, \quad T = (0, A_{21}), \quad T^* = \begin{pmatrix} 0 \\ A_{12} \end{pmatrix}.$$

# 3. Main Results

## Existence of a zero eigenvalue

**Let $G$ satisfy (H0) and $G_0$ be as above.**

**Theorem 1. (S.)** $$\dim\ker A_G = \dim\ker A_{G_0}$$

**In particular, $A_G$ has zero eigenvalue iff. $A_{G_0}$ has zero eigenvalue.**

**Remark:**
**For bipartite finite graphs, the same statement is found in the book entitled "Spectra of graphs'' by Cvetković, Doob and Sachs.**
**Theorem 1 means that the same statement holds true for infinite graphs that are not bipartite.**

## Sketch of proof.

**Let** $\psi_0 \in \ker A_{G_0}$. **Then**

$$\psi := \begin{pmatrix} \psi_0 \\ 0 \\ -A_{21}A_{10}\psi_0 \end{pmatrix} \in \ker A_G .$$

**Indeed, we have**

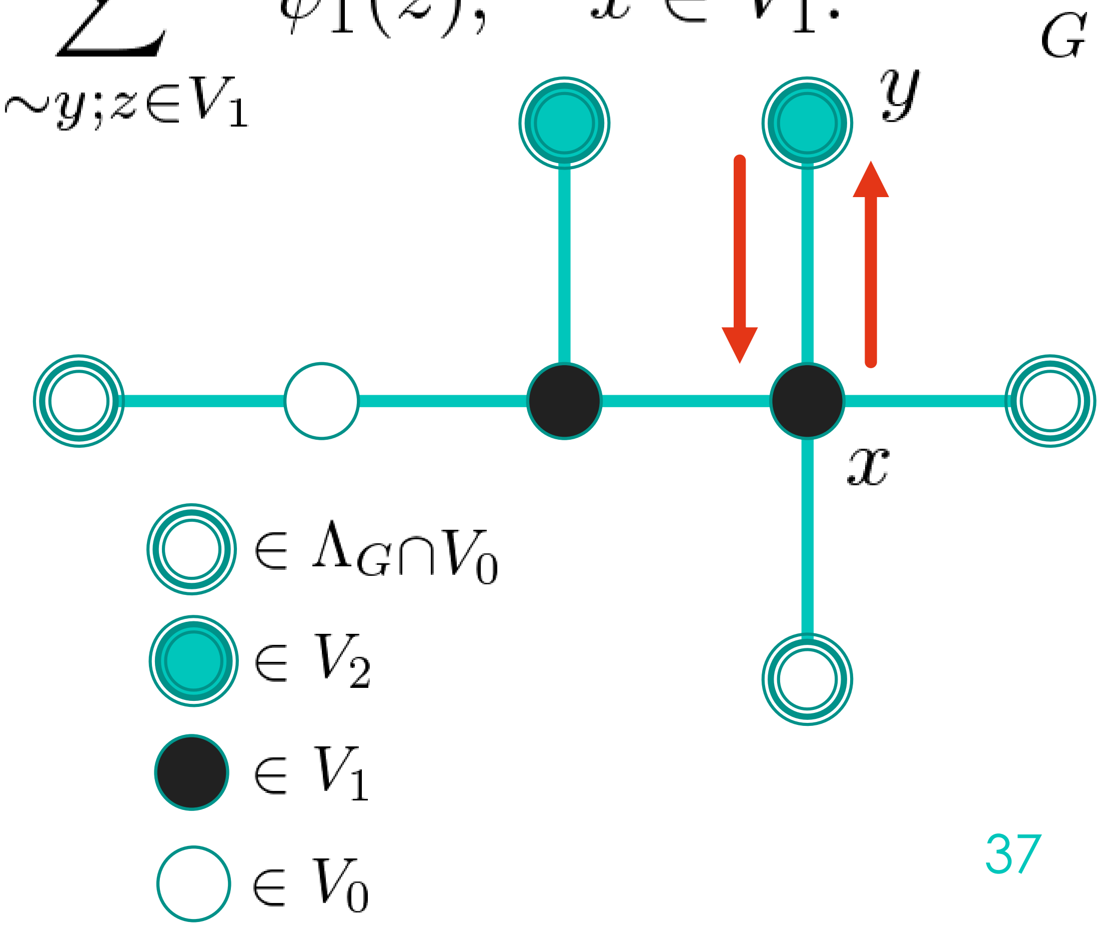
$$A_G\psi = \begin{pmatrix} A_{G_0} & A_{01} & 0 \\ A_{10} & A_{11} & A_{12} \\ 0 & A_{21} & 0 \end{pmatrix} \begin{pmatrix} \psi_0 \\ 0 \\ -A_{21}A_{10}\psi_0 \end{pmatrix}$$

$$= \begin{pmatrix} A_{G_0}\psi_0 \\ A_{10}\psi_0 - \boxed{A_{12}A_{21}}A_{10}\psi_0 \\ 0 \end{pmatrix}$$

**We have**

$$(A_{12}A_{21}\psi_1)(x) = \sum_{y\sim x; y\in V_2} (A_{21}\psi_1)(y)$$

$$= \sum_{y\sim x; y\in V_2} \sum_{z\sim y; z\in V_1} \psi_1(z), \quad x \in V_1.$$




**From (H0):**

$$\forall x \in V_1,\ \exists_1 y \in V_2 \text{ s.t. } y \sim x$$

**we have** $z = x$ .

**Hence**

$$(A_{12}A_{21}\psi_1)(x) = \psi_1(x)$$

**and**

$$\boxed{A_{12}A_{21} = \mathrm{id}_{\ell^2(V_1)}\ .}$$

**Hence we have**

$$A_G\psi = \begin{pmatrix} A_{G_0}\psi_0 \\ A_{10}\psi_0 - A_{12}A_{21}A_{10}\psi_0 \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 \\ A_{10}\psi_0 - \mathrm{id}_{\ell^2(V_1)}A_{10}\psi_0 \\ 0 \end{pmatrix} = 0.$$

**We can prove that**

$$\ker A_G = \left\{ \begin{pmatrix} \psi_0 \\ 0 \\ -A_{21}A_{10}\psi_0 \end{pmatrix} \middle| \psi_0 \in \ker A_{G_0} \right\},$$

**which implies that** $\dim\ker A_G = \dim\ker A_{G_0}$.

## Isospectral transformation

**Let $G$ be a graph (possibly not satisfying (H0)) and $G_1$ be as above.**
**Let $H_\lambda$ be the discrete Schrödinger operator on $G_1$ defined by**

$$H_\lambda = A_{G_1} + \lambda^{-1} V, \quad \lambda \neq 0,$$

**where**

$$V(x) = \begin{cases} n_x, & x \in V_1 \\ 0, & x \in V_0 \end{cases}$$

**with**

$$n_x = \#\{y \in V_2 \mid y \sim x\}.$$

**Theorem 2. (S.)** $\lambda \in \mathrm{Spec}(A_G) \iff \lambda \in \mathrm{Spec}(H_\lambda)$
**and**

$$\dim \ker(A_G - \lambda) = \dim \ker(H_\lambda - \lambda).$$

## Proof of Theorem 2

We use the following well-known lemma.

**Lemma.** Let

$$B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

be a bounded self-adjoint operator on $\mathcal{H}_1 \oplus \mathcal{H}_2$ with

$$B_{ij} : \mathcal{H}_j \to \mathcal{H}_i .$$

If $(B_{22} - \lambda)^{-1}$ is bounded, then

$$F(\lambda) := B_{11} - B_{12}(B_22 - \lambda)^{-1} B_{21} - \lambda$$

is bounded self-adjoint on $\mathcal{H}_1$,

$$\lambda \in \mathrm{Spec}(B) \Longleftrightarrow 0 \in \mathrm{Spec}(F(\lambda))$$

and

$$\dim\ker(B - \lambda) = \dim\ker(F(\lambda))$$



We call $F(\lambda)$ the Feshbach map of $B$.

## Proof of Theorem 2

**Applying the above lemma to** $A_G = \begin{pmatrix} A_{G_1} & T^* \\ T & 0 \end{pmatrix}$ **as**

$$B_{11} = A_{G_1}, \quad B_{12} = T^*, \quad B_{21} = T, \quad B_{22} = 0,$$

**the Feshbach map of** $A_G$ **is**

$$F(\lambda) = A_{G_1} + \lambda^{-1}\boxed{T^*T} - \lambda$$

**since** $(B_{22} - \lambda)^{-1} = -\lambda^{-1}$ **is bounded provided** $\lambda \neq 0$.

**Here we get**

$$T^*T = \begin{pmatrix} 0 \\ A_{12} \end{pmatrix} (0, A_{21})$$

$$= \begin{pmatrix} 0 & 0 \\ 0 & A_{12}A_{21} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & n_x \end{pmatrix} = V(x).$$

**Hence we have** $F(\lambda) = H_\lambda - \lambda$.

## Corollary of Theorem 2 (absence of a gap)

**Let $G_1 = \mathbb{Z}$ and $G$ be a graph obtained by adding pendant vertices to $G_1$.**

**Corollary 1. Suppose that**

$$\exists\{x_n\} \in \mathbb{Z} \text{ s.t. } ([x_n - n, x_n + n] \cap \mathbb{Z}) \subset V_0 .$$

**Then**

$$[-2, 2] \subset \mathrm{Spec}(A_G) .$$

**In particular, there is no spectral gap near zero:** $m(A_G) = 0$ **.**

**Proof of Corollary 1: It suffices to show the spectrum of $H_\lambda = A_\mathbb{Z} + \lambda^{-1}V$ includes $\mathrm{Spec}(A_\mathbb{Z}) = [-2, 2]$, which comes from $([x_n - n, x_n + n] \cap \mathbb{Z}) \cap \mathrm{supp}V = \emptyset$.**

**Remark: This corollary can be generalized to $G_1 = \mathbb{Z}^d$ and hexagonal lattice.**

## Corollary of Theorem 2 (existence of a gap)

**Let $G$ be a graph obtained by adding pendant vertices to each vertex of a graph $G_1$.**

**Corollary 2.** $A_G$ **has a spectral gap near zero:** $m(A_G) > 0$.

**Proof of Corollary 2:** **By assumption,** $V(x) \equiv 1$.

**Let** $\lambda_0^{-1} := \sup_{x \in V(G_1)} \deg_{G_1} x$. **Then, for** $\lambda > 0$ **sufficiently small,**

$$\begin{aligned} H_\lambda - \lambda &= A_{G_1} + \lambda^{-1} - \lambda \\ &= \left(A_{G_1} + \lambda_0^{-1}\right) + \left(\lambda^{-1} - \lambda_0^{-1} - \lambda\right) \\ &\geq \lambda^{-1} - \lambda_0^{-1} - \lambda > \epsilon \end{aligned}$$

**with some** $\epsilon > 0$.

## Criteria for existence of a gap.

**Let $G$ be a graph obtained by adding pendant vertices to $G_1$.**

**Theorem 3.** $m(A_{G_0}) > 0 \Longrightarrow m(A_G) > 0$.

## Sketch of proof:

**Since $n_x \geq 1 \quad (x \in V_1)$, we know that $(A_{11} + \lambda^{-1} n_x - \lambda)^{-1}$ is bounded if $|\lambda|$ is sufficiently small.**

**Hence the Feshbach map of**

$$H_\lambda - \lambda = \begin{pmatrix} A_{G_0} - \lambda & A_{01} \\ A_{10} & A_{11} + \lambda^{-1} n_x - \lambda \end{pmatrix}$$

**can be defined by**

$$F_0(\lambda) = A_{G_0} - \lambda - A_{01}(A_{11} + \lambda^{-1} n_x - \lambda)^{-1} A_{10}$$

**provided $0 < |\lambda| << 1$.**

We can show that

$$F_0(\lambda)^2 \geq A_{G_0}^2 - C|\lambda|$$

with some $C > 0$ independent of $0 < |\lambda| << 1$.

By assumption, $m(A_{G_0}) > 0$.
If $A_{G_0}$ has no zero eigenvalue, then we know that

$$F_0(\lambda)^2 \geq m(A_{G_0})^2 - C|\lambda| > 0 \quad (0 < |\lambda| << 1),$$

which implies that

$$m(A_G) > 0.$$

It the case where $A_{G_0}$ has a zero eigenvalue, it can be proven by employing the Feshbach map of $F_0(\lambda)$.

## Remark.

For a periodic graph $G$, we can show that

**Theorem 4.** Suppose that $A_G$ has no zero eigenvalue. Then:

$$m(A_{G_0}) = 0 \Longrightarrow m(A_G) = 0\,.$$

This is equivalent to the reverse statement of Theorem 3:

$$m(A_G) > 0 \Longrightarrow m(A_{G_0}) > 0$$

We omit the proof.

**Thank you for your kind attention!**