Simetrías latentes de grafos y Hamiltonianos efectivos con aplicación al modelo SSH

FMP - GTMC 2023

Estructura de la charla

NOTA: La charla esta basada en un arxiv de 11 de Oct de 2023[1].

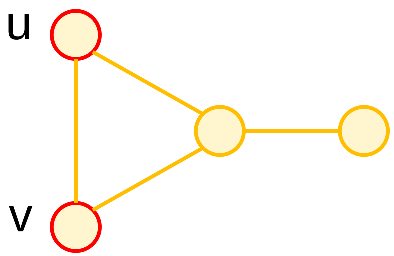
Voy aseguir los trabajos de Malte Rötgen y una presentación online[2].

- Dos ejemplos de motivación.
- Algo de teoría básica de grafos y Reducción Isoespectral.
- Modelo de tight-binding SSH.
- Aplicación de las simetrías latentes.

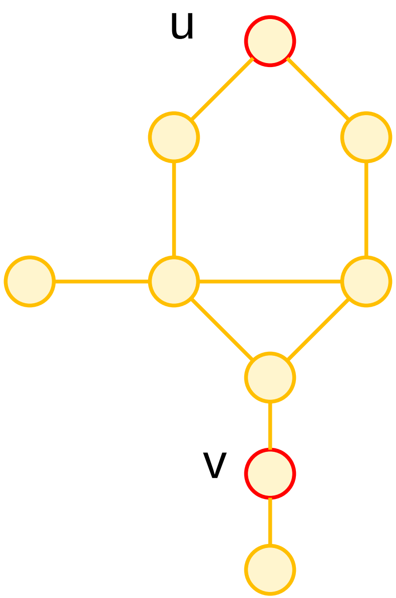
[1] M. Röntgen, X. Chen, W. Gao, M. Pyzh, P. Schmelcher, V. Pagneux, V. Achilleos, and A. Coutant, Latent Su-Schrieffer-Heeger Models, arXiv:2310.07619.https://arxiv.org/abs/2310.07619
[2] M. Röntgen (2022, November 8), Latent symmetries: An introduction. https://doi.org/10.52843/meta-mat.7d7p2h

Simetrías en Modelo de TB...sin simetría[1]

Simetría de reflexión



Simetría Latente



[1] D. Smith and B. Webb, Hidden Symmetries in Real and Theoretical Networks, Physica A: Statistical Mechanics and Its Applications 514, 855 (2019).

¿Como chequearlo?

In[39]:= `MatrixForm[H]`

Out[39]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

In[41]:= `MatrixForm[Transpose[N[Eigenvectors[H]]]]`

Out[41]//MatrixForm=

[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.378618	2.	-0.563154	1.41421	-1.41421	-1.	1.38171	-1.69717	0.
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.143351	-1.	0.317143	-1.	-1.	-1.	1.90912	2.88039	-1.
0.856649	-3.	0.682857	-1.	-1.	0.	-0.909116	-1.88039	1.
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.378618	2.	-0.563154	-1.41421	1.41421	-1.	1.38171	-1.69717	0.
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
1.	4.	1.	0.	0.	1.	1.	1.	0.

In[38]:= `GraphPlot[H, VertexLabels → "Name"]`

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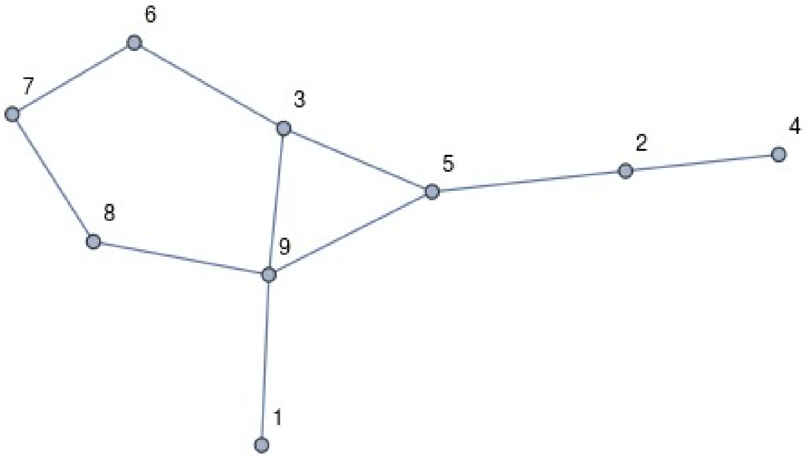


Reducción isoespectral

$$H\Psi = E\Psi$$

$$H\Psi = \begin{pmatrix} H_{SS} & H_{S\overline{S}} \\ H_{\overline{S}S} & H_{\overline{SS}} \end{pmatrix} \begin{pmatrix} \Psi_S \\ \Psi_{\overline{S}} \end{pmatrix} = E \begin{pmatrix} \Psi_S \\ \Psi_{\overline{S}} \end{pmatrix}$$

$$\begin{aligned} H_{SS}\Psi_S + H_{S\overline{S}}\Psi_{\overline{S}} &= E\Psi_S \\ H_{\overline{S}S}\Psi_S + H_{\overline{SS}}\Psi_{\overline{S}} &= E\Psi_{\overline{S}} \end{aligned}$$

Reducción isoespectral

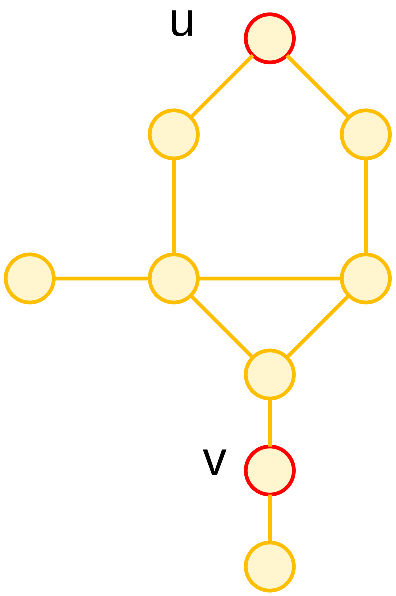
$$H_{SS}\Psi_S + H_{S\overline{S}}\frac{1}{H_{\overline{SS}} - E}H_{\overline{S}S}\Psi_S \quad = \quad E\Psi_S$$

$$\left(H_{SS} + H_{S\overline{S}}\frac{1}{H_{\overline{SS}} - E}H_{\overline{S}S} - E\mathbb{I}\right)\Psi_S = 0$$

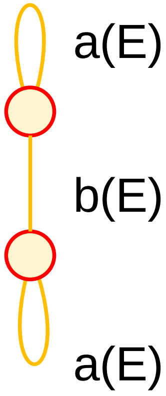
$$(\mathcal{R}_E(H,S) - E\mathbb{I})\Psi_S = 0$$

$\mathcal{R}_E(H,S)$ Es la reducción isoespectral de H en el conjunto S (Teoria de grafos). Es un Hamiltoniano Efectivo.

Simetrías en el Hamiltoniano Effectivo



S={u,v}



$$\Leftrightarrow \begin{pmatrix} a(E) & b(E) \\ b(E) & a(E) \end{pmatrix}$$

Relación entre los autovalores de R y H

El problema de autovalores del Hamiltoniano efectivo es,

$$det(\mathcal{R}_E(H,S) - E\mathbb{I}) = 0$$

Pero es no-lineal! Ya que tiene E, tanto en el autovalor como en la matriz.

Corollary 1.1. *For $M \in \mathbb{C}^{n\times n}$, let S and $\bar{S}$ form a nonempty partition of N. Then*

(i) $\sigma(\mathscr{R}(M;S)) = \sigma(M) - \sigma(M_{\bar{S}\bar{S}})$; *and*
(ii) $\sigma^{-1}(\mathscr{R}(M;S)) = \sigma(M_{\bar{S}\bar{S}}) - \sigma(M)$.

Si H y $H_{\bar{S}\bar{S}}$ no tienen autovalores en común, entonces el espectro de $\mathcal{R}_E(H,S)$ y H son iguales .

[1]L. Bunimovich and B. Webb, Isospectral Transformations: A New Approach to Analyzing Multidimensional Systems and Networks (Springer New York, New York, NY, 2014).

1 Forma de detectar simetrias latentes

Si $\mathbb{H}^{n}_{u,u} = \mathbb{H}^{n}_{v,v}$ Entonces u y v tienen una simetría latente.

En teoría de grafos los elementos $(G^n)_{u,v}$ de las potencias de la matriz de adyacencia G (H en TB para nosotros), indican la cantidad de caminos diferentes en el grafo para ir de u a v en n pasos.

Además, u y v **tienen que tener la misma cantidad de conexiones.**

Ver los trabajos para ver otras formas de detectar las simetrias latentes[1].

[1]D. Smith and B. Webb, Hidden Symmetries in Real and Theoretical Networks, Physica A: Statistical Mechanics and Its Applications 514, 855 (2019).

Test para el grafo ejemplo

/MatrixForm=

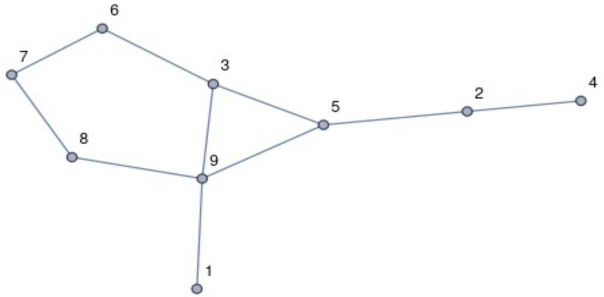
$$\begin{pmatrix} 1&0&1&0&1&0&0&1&0\\ 0&2&1&0&0&0&0&0&1\\ 1&1&3&0&1&0&1&1&1\\ 0&0&0&1&1&0&0&0&0\\ 1&0&1&1&3&1&0&1&1\\ 0&0&0&0&1&2&0&1&1\\ 0&0&1&0&0&0&2&0&1\\ 1&0&1&0&1&1&0&2&0\\ 0&1&1&0&1&1&1&0&4 \end{pmatrix}$$

/MatrixForm=

$$\begin{pmatrix} 0&1&1&0&1&1&1&0&4\\ 1&0&1&2&4&1&0&1&1\\ 1&1&2&1&5&4&1&2&6\\ 0&2&1&0&0&0&0&0&1\\ 1&4&5&0&2&1&2&1&6\\ 1&1&4&0&1&0&3&1&2\\ 1&0&1&0&2&3&0&3&1\\ 0&1&2&0&1&1&3&0&5\\ 4&1&6&1&6&2&1&5&2 \end{pmatrix}$$

In[38]:= `GraphPlot[H, VertexLabels → "Name"]`

Out[38]=



atrixForm=

$$\begin{pmatrix} 4&1&6&1&6&2&1&5&2\\ 1&6&6&0&2&1&2&1&7\\ 6&6&15&1&9&3&6&7&10\\ 1&0&1&2&4&1&0&1&1\\ 6&2&9&4&15&7&2&8&9\\ 2&1&3&1&7&7&1&5&7\\ 1&2&6&0&2&1&6&1&7\\ 5&1&7&1&8&5&1&8&3\\ 2&7&10&1&9&7&7&3&21 \end{pmatrix}$$

atrixForm=

$$\begin{pmatrix} 2&7&10&1&9&7&7&3&21\\ 7&2&10&6&19&8&2&9&10\\ 10&10&22&6&31&21&10&16&37\\ 1&6&6&0&2&1&2&1&7\\ 9&19&31&2&20&11&15&11&38\\ 7&8&21&1&11&4&12&8&17\\ 7&2&10&2&15&12&2&13&10\\ 3&9&16&1&11&8&13&4&28\\ 21&10&37&7&38&17&10&28&24 \end{pmatrix}$$

Modificación de la red sin romper SL

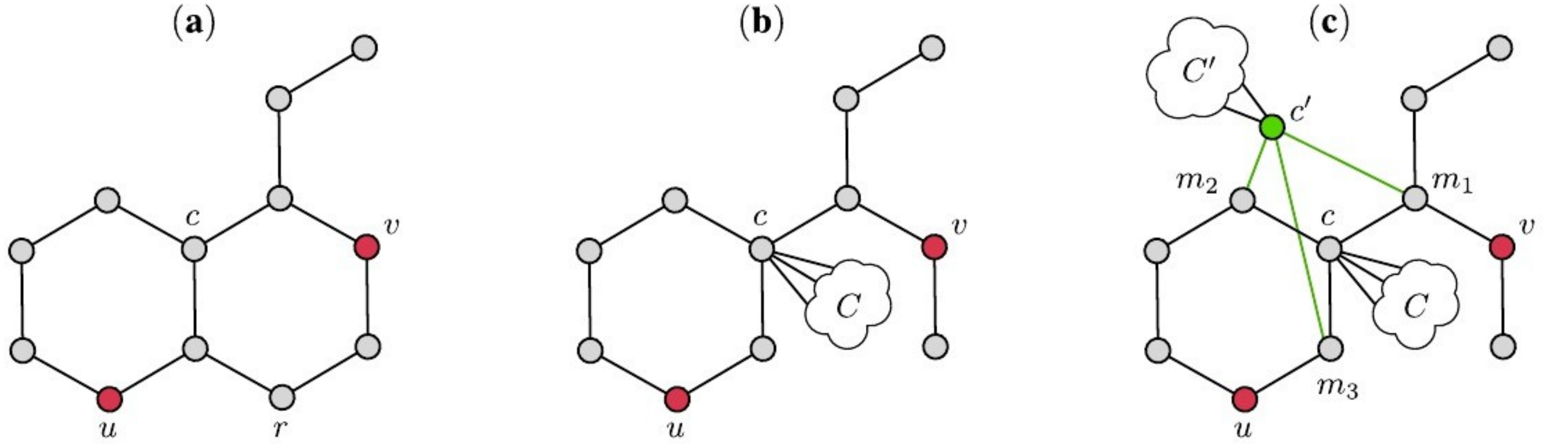
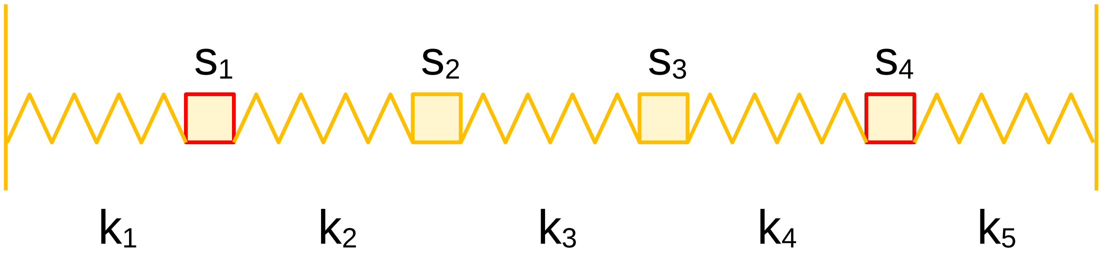


Fig. 2. (a) A molecular graph, taken from Ref. [8], which has two cospectral vertices u, v and two "unrestricted substitution points" (USPs) c, r. **(b)** The USPs are vertices which can be connected to any arbitrary graph C (as done with c) or also removed from the graph (as done with r), without breaking the cospectrality of u, v. **(c)** In the present work we generalize USPs to vertex subsets called "walk multiplets", an example here being the subset $\mathbb{M} = \{m_1, m_2, m_3\}$. We can connect this subset to a new vertex c', which we can in turn connect to an arbitrary graph C', without breaking the cospectrality of u, v. The added vertex c' is a walk "singlet", which is identified as an USP.

[8] C. V. Morfonios, M. Pyzh, M. Röntgen, and P. Schmelcher, Cospectrality Preserving Graph Modifications and Eigenvector Properties via Walk Equivalence of Vertices, Linear Algebra and Its Applications 624, 53 (2021).

Modelo de resortes



$$\mathbb{V}\boldsymbol{s} = m\omega^2\boldsymbol{s}$$

$$\mathbb{V}_{i,j} = \frac{\partial^2 U}{\partial s_i \partial s_j}$$

$$U = \frac{1}{2}\sum_{i=0} k_{i+1}(s_{i+1} - s_i)^2 \quad s_0 = s_5 \equiv 0$$

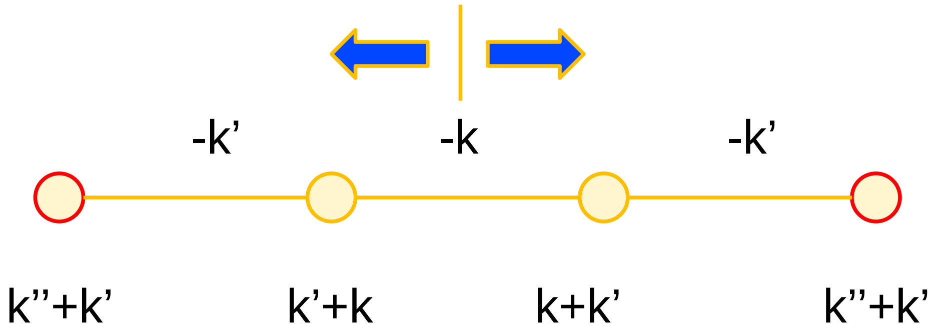
$$k_1 = k_5 = k''$$

$$k_2 = k_4 = k'$$

$$k_3 = k$$

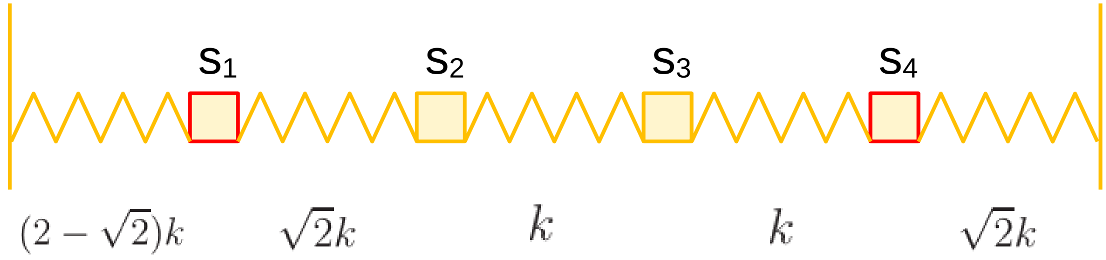
Modelo de resortes

$$\mathbb{V} = \begin{pmatrix} k'' + k' & -k' & 0 & 0 \\ -k' & k' + k & -k & 0 \\ 0 & -k & k + k' & -k' \\ 0 & 0 & -k' & k'' + k' \end{pmatrix}$$



Vemos que hay una simetria en los sitios 1 y 4 que se manifiesta en la matriz y el grafo.
Los autovectores van a ser simétricos o antisimétricos en 1 y 4, y en 2 y 3.

Modelo de resortes



$$\mathbb{V} = \begin{pmatrix} 2k & -\sqrt{2}k & 0 & 0 \\ -\sqrt{2}k & (1+\sqrt{2})k & -k & 0 \\ 0 & -k & 2k & -k \\ 0 & 0 & -k & (1+\sqrt{2})k \end{pmatrix}$$

Modelo de resortes

Si hacemos la reducción isoespectral en 1 y 3, se tiene que,

$$\mathcal{R}_\lambda(H,\{1,3\}) = \begin{pmatrix} 2-\frac{2}{-\lambda+\sqrt{2}+1} & -\frac{\sqrt{2}}{-\lambda+\sqrt{2}+1} \\ -\frac{\sqrt{2}}{-\lambda+\sqrt{2}+1} & 2-\frac{2}{-\lambda+\sqrt{2}+1} \end{pmatrix} \Longrightarrow \begin{pmatrix} a(E) & b(E) \\ b(E) & a(E) \end{pmatrix}$$

Con lo cual se hace evidente la simetría latente.

Modelo SSH

- Es un modelo TB muy estudiado.
- Presenta una transición de fase topológica.
- Es soluble exactamente.

Modelo SSH

$$H\Psi = \begin{array}{c} \begin{array}{cc|cc|cc} A_{n-1} & B_{n-1} & A_n & B_n & A_{n+1} & B_{n+1} \end{array} \\ \left(\begin{array}{cc|cc|cc} 0 & v & 0 & 0 & 0 & 0 \\ v & 0 & w & 0 & 0 & 0 \\ \hline 0 & w & 0 & v & 0 & 0 \\ 0 & 0 & v & 0 & w & 0 \\ \hline 0 & 0 & 0 & w & 0 & v \\ 0 & 0 & 0 & 0 & v & 0 \end{array}\right) \end{array} \left(\begin{array}{c} \Psi_A e^{ika(n-1)} \\ \Psi_B e^{ika(n-1)} \\ \hline \Psi_A e^{ika(n)} \\ \Psi_B e^{ika(n)} \\ \hline \Psi_A e^{ika(n+1)} \\ \Psi_B e^{ika(n+1)} \end{array}\right) = \varepsilon \left(\begin{array}{c} \Psi_A e^{ika(n-1)} \\ \Psi_B e^{ika(n-1)} \\ \hline \Psi_A e^{ika(n)} \\ \Psi_B e^{ika(n)} \\ \hline \Psi_A e^{ika(n+1)} \\ \Psi_B e^{ika(n+1)} \end{array}\right)$$

Modelo SSH

$$\begin{pmatrix} 0 & v + we^{-ika} \\ v + we^{-ika} 0 & \end{pmatrix} \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix} = \varepsilon \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix}$$

$$\varepsilon_{\pm} = \pm\sqrt{v^2 + w^2 + 2vw\cos(ka)}$$

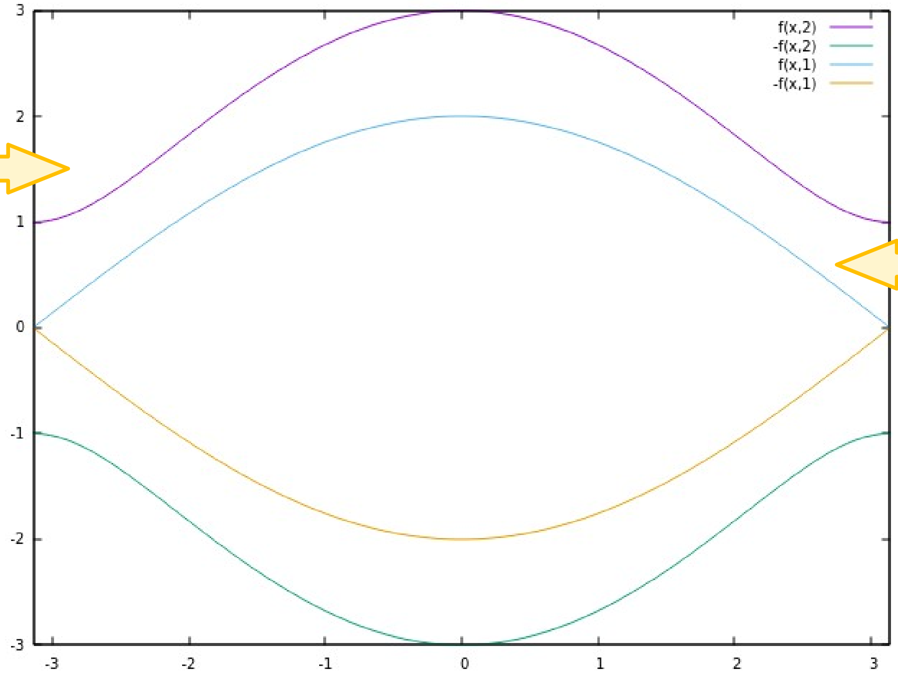
Simetría en v y w.

$$\phi_{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{\phi_k} \\ 1 \end{pmatrix} \qquad \phi_k = \frac{w\sin(ka)}{v + w\cos(ka)}$$

Sin simetría en v y w

Dispersion de SSH

w > v
w < v



w=v

Caracterizando los estados

$$A_-(k) = i\left\langle \phi_- \left| \frac{\mathrm{d}}{\mathrm{d}k} \right| \phi_- \right\rangle = \frac{1}{2}\frac{\mathrm{d}\phi_k}{\mathrm{d}k}$$

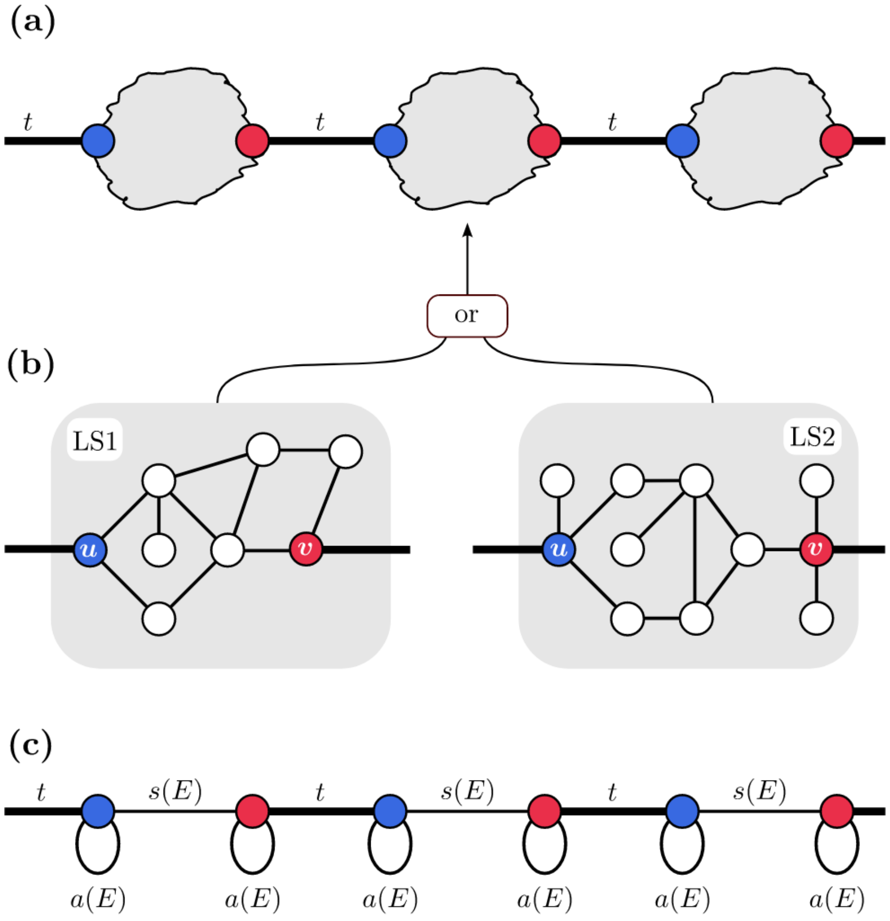
Fase de Berry

$$g = -\frac{1}{\pi}\int_{\mathrm{BZ}} A_-(k)\mathrm{d}k = \begin{cases} 0 & v > w \\ \text{undefined} & v = w \\ 1 & v < w \end{cases},$$

Winding number

Entonces, los estados con v > w y v < w son topológicamente distintos y para pasar de uno a otro debemos pasar por una fase conductora (v=w).

Modelo ssh para una cadena con S. L.



$$\widetilde{H}_S^{(B)}(E,k) = \begin{pmatrix} a(E) & s(E) + t\, e^{ik} \\ s(E) + t\, e^{-ik} & a(E) \end{pmatrix} .$$

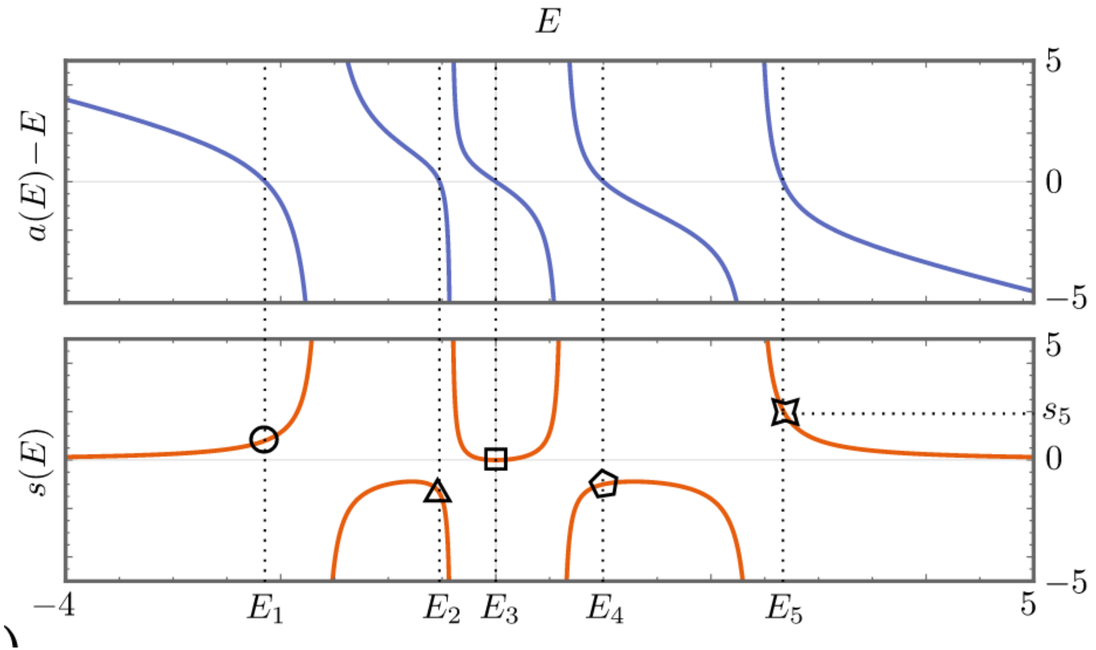
SSH efectivo

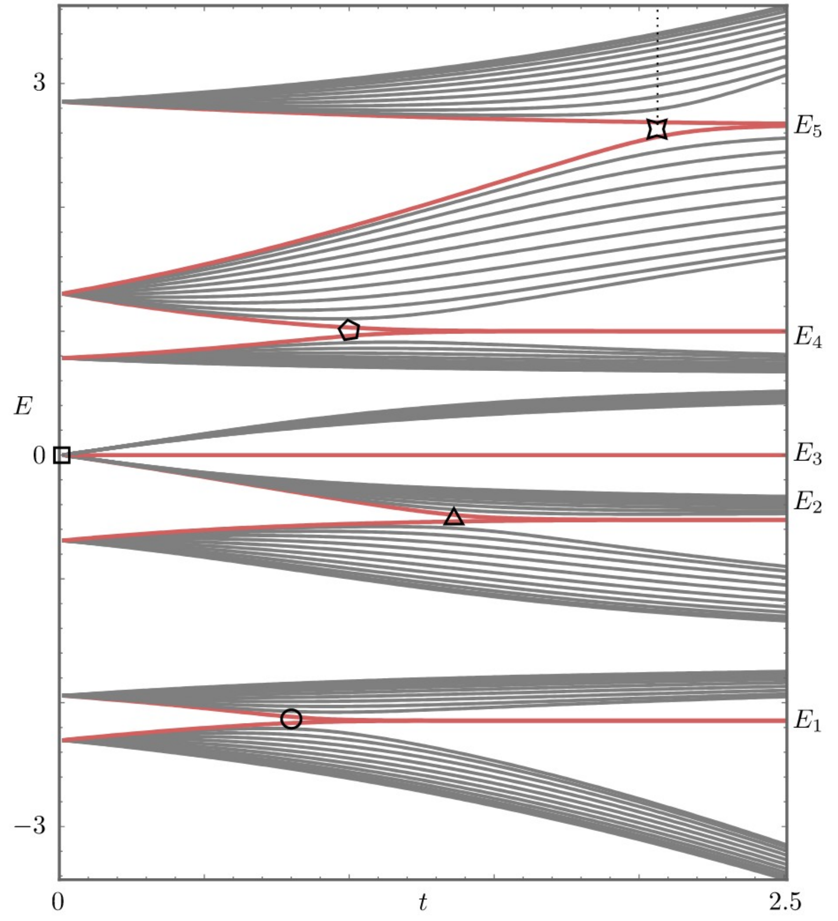
$$\begin{pmatrix} 0 & s(E) + te^{ik} \\ s(E) + te^{-ik} & 0 \end{pmatrix} \Psi_S(k) = \epsilon \, \Psi_S(k) \, , \qquad \epsilon = E - a(E).$$

Ahora, las transiciones topológicas en el SSH se dan en ε=0, valor en que
Debería ser –> s(E)=t (v=w).

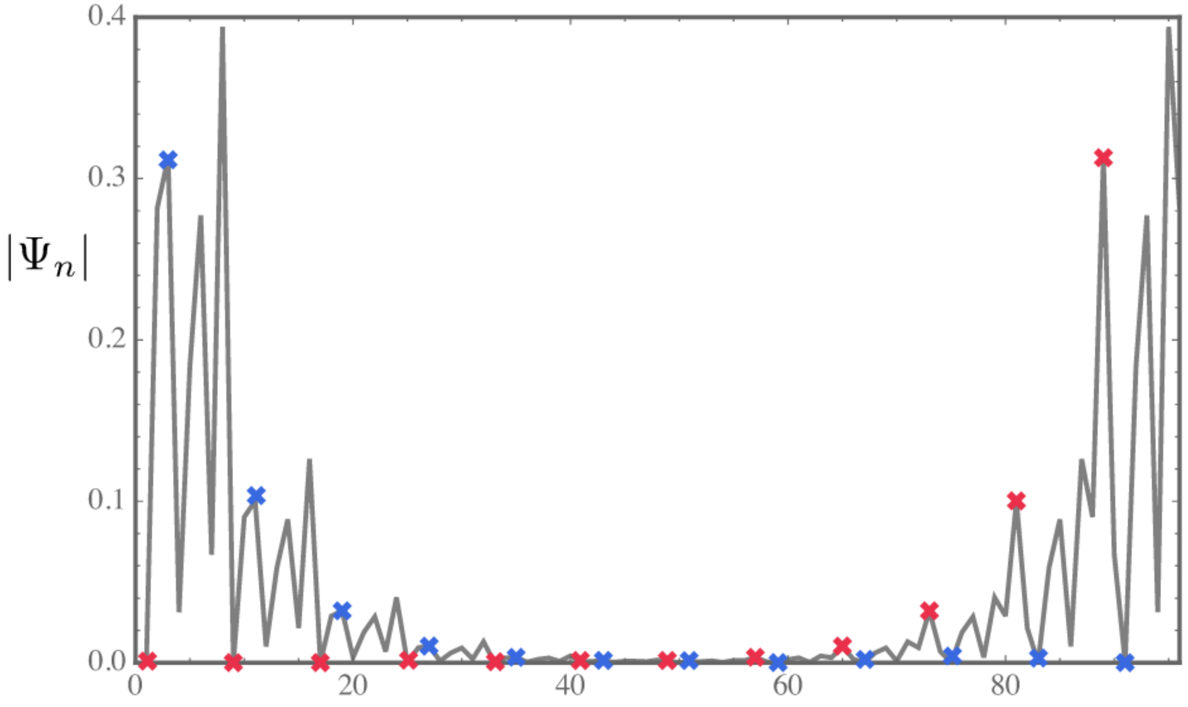
Al final, si lo es, pero no me queda claro por que si lo es!

Estructura de banda del SSH latente





Estados topologicos para E1



Gracias por escuchar!

[1]M. Kempton, J. Sinkovic, D. Smith, and B. Webb, Characterizing Cospectral Vertices via Isospectral Reduction, Linear Algebra and Its Applications 594, 226 (2020).

[2]D. Smith and B. Webb, Hidden Symmetries in Real and Theoretical Networks, Physica A: Statistical Mechanics and Its Applications 514, 855 (2019).

[3]M. Röntgen, Latent Symmetries: An Introduction - Presented by Dr. Malte Röntgen, (seminario grabado).

[4]M. Röntgen, M. Pyzh, C. V. Morfonios, and P. Schmelcher, On Symmetries of a Matrix and Its Isospectral Reduction, arXiv:2105.12579.

[5]M. Röntgen, M. Pyzh, C. V. Morfonios, N. E. Palaiodimopoulos, F. K. Diakonos, and P. Schmelcher, Latent Symmetry Induced Degeneracies, Phys. Rev. Lett. 126, 180601 (2021).

[6]L. Bunimovich and B. Webb, Isospectral Transformations: A New Approach to Analyzing Multidimensional Systems and Networks (Springer New York, New York, NY, 2014).
[7]M. Röntgen, X. Chen, W. Gao, M. Pyzh, P. Schmelcher, V. Pagneux, V. Achilleos, and A. Coutant, Latent Su-Schrieffer-Heeger Models, arXiv:2310.07619.

[8] C. V. Morfonios, M. Pyzh, M. Röntgen, and P. Schmelcher, Cospectrality Preserving Graph Modifications and Eigenvector Properties via Walk Equivalence of Vertices, Linear Algebra and Its Applications 624, 53 (2021).