

Square lattice toy models for topological analysis

R. A. Montalvo and P. H. Rivera¹

Lab2D4

Research Group on Mesoscopic Physics

Departamento Académico de Física del Estado Sólido
Facultad de Ciencias Físicas
Universidad Nacional Mayor de San Marcos
Lima – Perú

¹priverar@unmsm.edu.pe



Hamiltonian with s orbitals

Finite square lattice

$$\hat{H} = \sum_{i,j} |i,j\rangle E_0 \langle i,j| - \sum_{i,j} (|i,j\rangle t_x \langle i-1,j| - |i,j\rangle t_x \langle i+1,j|) - \sum_{i,j} (|i,j\rangle t_y \langle i,j-1| - |i,j\rangle t_y \langle i,j+1|)$$

where E_0 are s orbitals energy in each atomic site, $t_x < 0$ and $t_y < 0$ are coupling energy between first near neighbors in x and y directions, respectively. For a square lattice $t_x \approx t_y$.

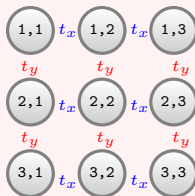


Tight binding

Matrix Hamiltonian

Finite square lattice

$$H = \begin{pmatrix} E_0 & t_x & 0 & t_y & 0 & 0 & 0 & 0 & 0 \\ t_x & E_0 & t_x & 0 & t_y & 0 & 0 & 0 & 0 \\ 0 & t_x & E_0 & 0 & 0 & t_y & 0 & 0 & 0 \\ t_y & 0 & 0 & E_0 & t_x & 0 & t_y & 0 & 0 \\ 0 & t_y & 0 & t_x & E_0 & t_x & 0 & t_y & 0 \\ 0 & 0 & t_y & 0 & t_x & E_0 & 0 & 0 & t_y \\ 0 & 0 & 0 & t_y & 0 & 0 & E_0 & t_x & 0 \\ 0 & 0 & 0 & 0 & t_y & 0 & t_x & E_0 & t_x \\ 0 & 0 & 0 & 0 & 0 & t_y & 0 & t_x & E_0 \end{pmatrix}$$



Magnetic Field

Magnetic phase

Peierls approximation

$$\mathbf{k} \rightarrow \mathbf{k} + \frac{e}{\hbar} \mathbf{A} \rightarrow (k_x, k_y) + \frac{2\pi}{\frac{h}{e}} (0, xB, 0)$$

$$\begin{aligned} \mathbf{k} \cdot \mathbf{r} &\rightarrow \mathbf{k} \cdot \mathbf{r} + \frac{e}{\hbar} \mathbf{A} \cdot \mathbf{r} \rightarrow k_x x + k_y y + \frac{2\pi}{\phi_e} x B y \\ &\rightarrow k_x x + k_y y + 2\pi \frac{\phi}{\phi_e} \rightarrow k_x x + k_y y + 2\pi \frac{p}{q}, \end{aligned}$$

where,

$$\phi = xyB, \quad \text{magnetic flux} \quad \wedge \quad \phi_e = \frac{h}{e}, \quad \text{quantum magnetic flux}$$



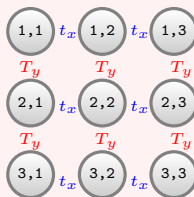
Magnetic Field

Matrix Hamiltonian with magnetic phase

Finite square lattice

$$H = \begin{pmatrix} E_0 & t_x & 0 & T_y & 0 & 0 & 0 & 0 & 0 \\ t_x & E_0 & t_x & 0 & T_y & 0 & 0 & 0 & 0 \\ 0 & t_x & E_0 & 0 & 0 & T_y & 0 & 0 & 0 \\ T_y & 0 & 0 & E_0 & t_x & 0 & T_y & 0 & 0 \\ 0 & T_y & 0 & t_x & E_0 & t_x & 0 & T_y & 0 \\ 0 & 0 & T_y & 0 & t_x & E_0 & 0 & 0 & T_y \\ 0 & 0 & 0 & T_y & 0 & 0 & E_0 & t_x & 0 \\ 0 & 0 & 0 & 0 & T_y & 0 & t_x & E_0 & t_x \\ 0 & 0 & 0 & 0 & 0 & T_y & 0 & t_x & E_0 \end{pmatrix}$$

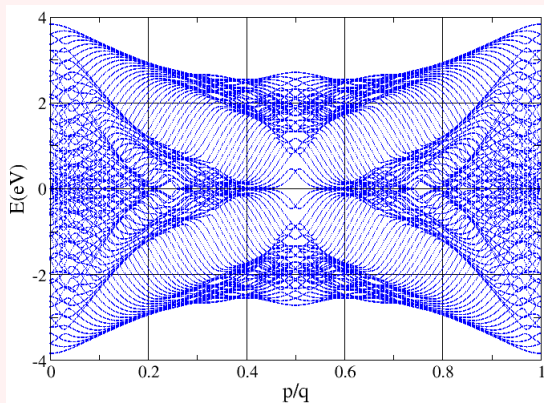
$$T_y = t_y e^{i2\pi(p/q)}$$



Magnetic Field

Hofstadter butterfly

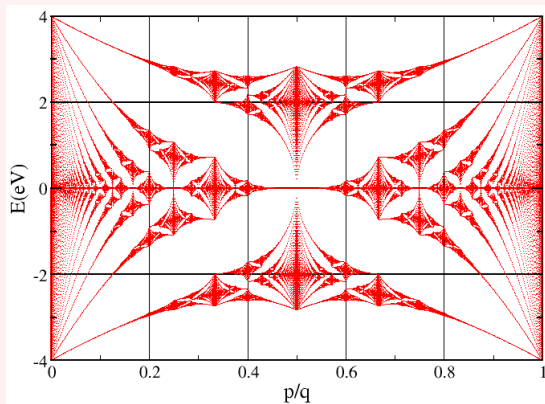
Finite square lattice



Magnetic Field

Hofstadter butterfly: D. R. Hofstadter, Phys. Rev. B **14**, 2239 (1976)

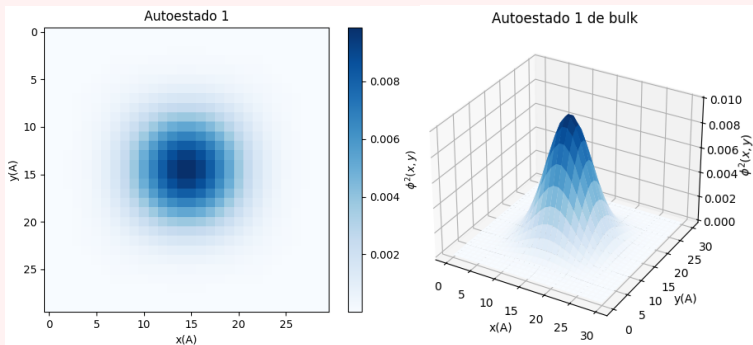
Infinite square lattice



Magnetic Field

Bulk and edge eigenstates

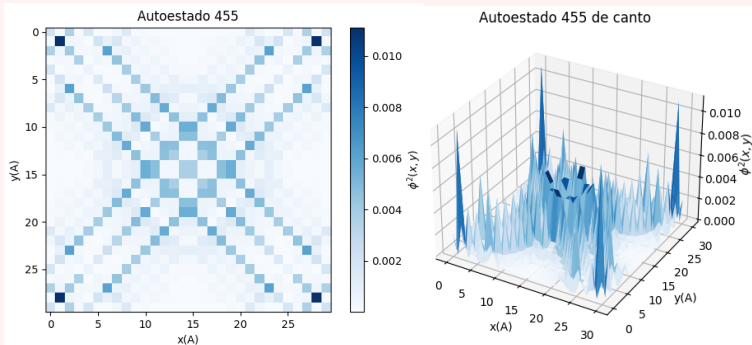
Bulk eigenstates



Magnetic Field

Bulk and edge eigenstates

Edge eigenstates



Hamiltonian with s and p orbitals

Spin orbit coupling

Hamiltonian orbital

$$H_{\text{orb}}(\mathbf{k}) = \begin{pmatrix} \varepsilon_s + 2t_s(C_x + C_y) & -2it_{sp}S_x & -2it_{sp}S_y \\ +2it_{sp}S_x & \varepsilon_p + 2t_{pp\sigma}C_x + 2t_{pp\pi}C_y & 0 \\ +2it_{sp}S_y & 0 & \varepsilon_p + 2t_{pp\pi}C_x + 2t_{pp\sigma}C_y \end{pmatrix},$$

where $C_x = \cos k_x a$, $C_y = \cos k_y a$, $S_x = \sin k_x a$ and $S_y = \sin k_y a$. And on the other hand, t_s , t_{sp} , $t_{pp\sigma}$, $t_{pp\pi}$ are the coupling energy between s , sp , $pp\sigma$ and $pp\pi$ orbitals, and, finally, ε_s and ε_p are s and p orbitals energy, respectively.



Hamiltonian with s and p orbitals

Spin orbit coupling

Intrinsic SOC Hamiltonian

The L_z operator is

$$L_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\Rightarrow L_z^{(3)} = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},$$

where the transformation matrix is

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -1 \\ i & 0 & i \\ 0 & \sqrt{2} & 0 \end{pmatrix}.$$

The intrinsic SOC Hamiltoniano is

$$H_{\text{SOC}}^{(\uparrow)}(\mathbf{k}) = +\frac{\lambda_I}{2} L_z^{(3)}$$

$$H_{\text{SOC}}^{(\downarrow)}(\mathbf{k}) = -\frac{\lambda_I}{2} L_z^{(3)},$$

where λ_I is the intrinsic SOC constant.

$$H_{\uparrow\uparrow}(\mathbf{k}) = H_{\text{orb}}(\mathbf{k}) + \frac{\lambda_I}{2} L_z^{(3)},$$

$$H_{\downarrow\downarrow}(\mathbf{k}) = H_{\text{orb}}(\mathbf{k}) - \frac{\lambda_I}{2} L_z^{(3)}.$$

* C. L. Kane y E. J. Mele; Phys. Rev. Lett. **95**, 226801 (2005).



Hamiltonian with s and p orbitals

Spin orbit coupling

Rashba SOC Hamiltonian

$$H_R(\mathbf{k}) = \frac{\hbar^2}{2m_e^2 c^2} (\nabla V \times \mathbf{p}) \cdot \boldsymbol{\sigma} = \lambda_R \begin{pmatrix} 0 & -2 \sin k_y a & +2 \sin k_x a \\ +2 \sin k_y a & 0 & 0 \\ -2 \sin k_x a & 0 & 0 \end{pmatrix},$$

finally,

$$H(\mathbf{k}) = \begin{pmatrix} H_{\uparrow\uparrow}(\mathbf{k}) & H_{\uparrow\downarrow}(\mathbf{k}) \\ H_{\downarrow\uparrow}(\mathbf{k}) & H_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix},$$

where

$$H_{\uparrow\downarrow}(\mathbf{k}) = H_R(\mathbf{k}), \quad H_{\downarrow\uparrow}(\mathbf{k}) = H_R^\dagger(\mathbf{k}).$$

* E. Rashba, Sov. Phys. Solid State **2**, 1109 (1960).

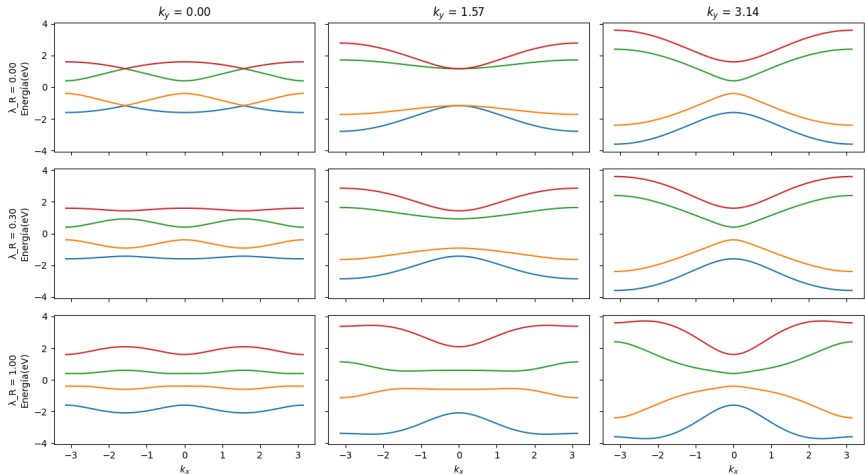
* Y. A. Bychkov and E. Rashba, P. Zh. Eksp. Teor. Fiz. **39**, 66 (1984).



Hamiltonian with s and p orbitals

Spin orbit coupling

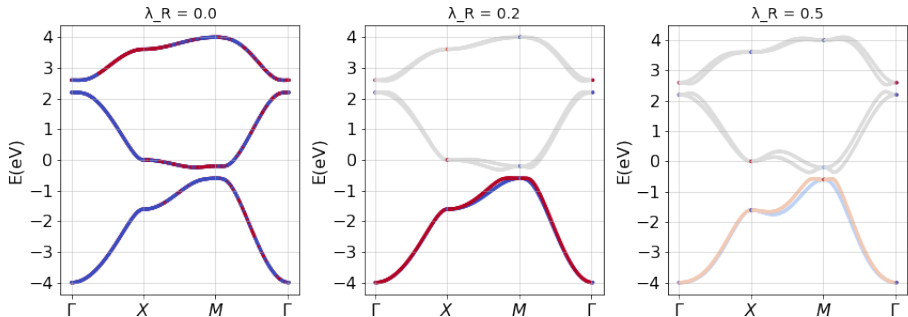
Bandas de bulk (acotado con k_y fijo) para diferentes intensidades del SOC de Rashba



Hamiltonian with s and p orbitals

Spin orbit coupling

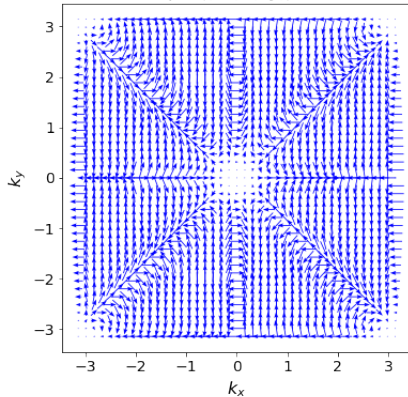
Estructura de bandas coloreado por la polarización de espín (σ_z)



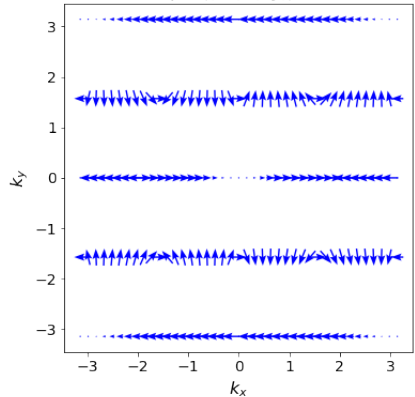
Hamiltonian with s and p orbitals

Spin orbit coupling

Textura de espín ($\langle \sigma_x \rangle$, $\langle \sigma_y \rangle$) en $E_F \approx 1.0$ eV



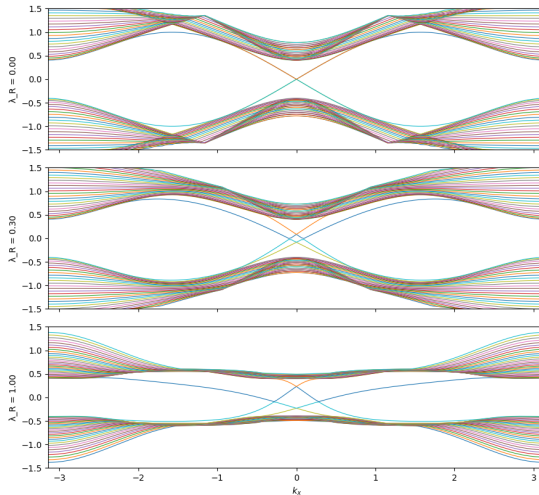
Textura de espín ($\langle \sigma_x \rangle$, $\langle \sigma_y \rangle$) en $E_F \approx 1.0$ eV



Hamiltonian with s and p orbitals

Spin orbit coupling

Estructura de banda de una cinta (finita en y) — estados de borde visibles en la mitad del gap



Topology

Chern number

DVR

Topology

Position space

- Gauss-Bonnet

$$\int d^2r \left(\text{Gauss curvature} \right) = 4\pi(1 - \# \text{holes})$$



Illustration: © Johan Larsson/The Royal Swedish Academy of Sciences

Momentum space

- Chern

$$\int d^2k \left(\text{Berry curvature} \right) = 2\pi \times \# \text{Chern}$$

- Related to the number of topological edges in the corresponding finite system (bulk-boundary correspondence)



APS
physics
MARCH
MEETING2021

MARCH 15-19
ONLINE



Topology

Chern number

Conductancia

$$C = \frac{1}{2\pi} \int_{BZ} d^2\mathbf{k} F$$

BZ : Brillouin zone.

$$\sigma_{xy} = -\frac{e^2}{h} C$$

★ D. Thouless, M. Kohmoto, M. Nightingale, y M. den-Nijs; *Quantized Hall conductance in a two-dimensional periodic potential*, Phys. Rev. Lett. **49**(6), 405 (1982).



Deep learning

Neural networks

QWZ Hamiltonian

$$H(k_x, k_y) = \sin(k_x a)\sigma_x + \sin(k_y a)\sigma_y + (e_s + \cos(k_x a) + \cos(k_y a))\sigma_z$$

$$\sigma_{xy} = \begin{cases} 1/2\pi & 0 < e_s < 2, \\ -1/2\pi & 2 < e_s < 4, \\ 0 & e_s < 0 \quad \vee \quad e_s > 4. \end{cases}$$

* Xiao-Liang Qi, Yong-Shi Wu, and Shou-Cheng Zhang; *Topological quantization of the spin Hall effect in two-dimensional paramagnetic semiconductors*, Phys. Rev. B **74**, 085308 (2006).



Deep learning

Neural networks

Convolutional neural networks

- A Convolutional Neural Network (CNN) is a specialized deep learning model for processing grid-like data, primarily images, mimicking the human visual cortex to automatically learn hierarchical features (edges, shapes, objects) through convolutional layers with filters (kernels) and pooling, making it highly effective for computer vision tasks like image classification, object detection, and facial recognition.
- CNNs use learnable weights in convolutional layers to detect patterns, followed by pooling to reduce dimensionality, and fully connected layers for final classification, enabling end-to-end learning without manual feature engineering.



Deep learning

Neural networks

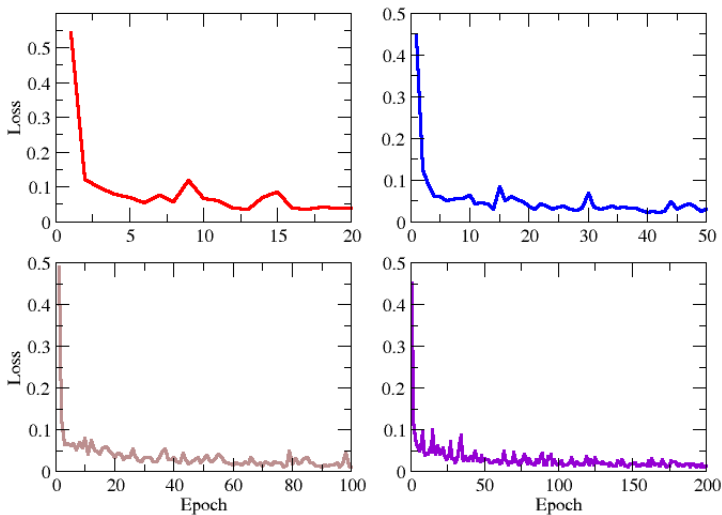
Convolutional Neural Networks and Others

- ① Wenqian Lian, Sheng-Tao Wang, Sirui Lu, Yuanyuan Huang, Fei Wang, Xinxing Yuan, Wengang Zhang, Xiaolong Ouyang, Xin Wang, Xianzhi Huang, Li He, Xiuying Chang, Dong-Ling Deng, and Luming Duan; *Machine Learning Topological Phases with a Solid-State Quantum Simulator*, *Phys. Rev. Lett.* **122**, 210503 (2019).
- ② Huili Zhang, Si Jiang, Xin Wang, Wengang Zhang, Xianzhi Huang, Xiaolong Ouyang, Yefei Yu, Yanqing Liu, Dong-Ling Deng, and L.-M. Duan; *Experimental demonstration of adversarial examples in learning topological phases*, *Nature Communications* **13**, 4993 (2022).



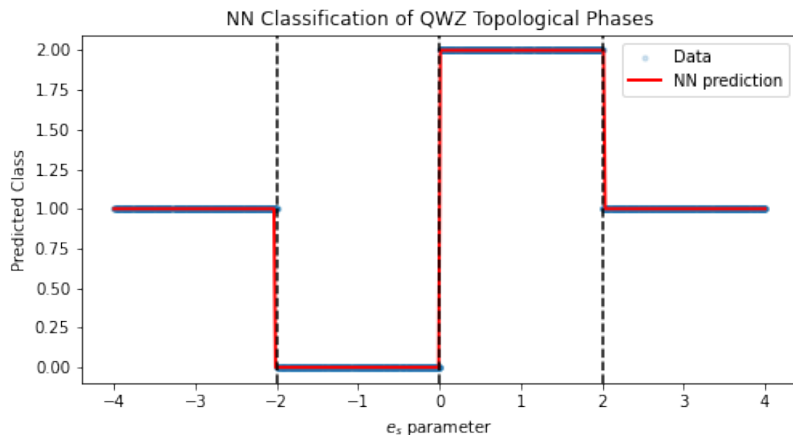
Deep learning

Neural networks: Training results



Deep learning

Neural networks: Data and predictions



Conclusion

Square lattice as toy model even we use to learn fundamental physics.

¡Hay, hermanos, muchísimo que hacer!

- Los procesadores cuánticos de Google, IBM y Rigetti usan junturas Josephson.
- Microsoft tiene procesadores cuánticos basados en los fermiones de Majorana y comparten su uso por el precio módico de US\$135,000/mes.
- Google, Amazon, Apple han declarado que tienen Tensor Neural Processing Units.
- Qant produce NPU fotónicos.

