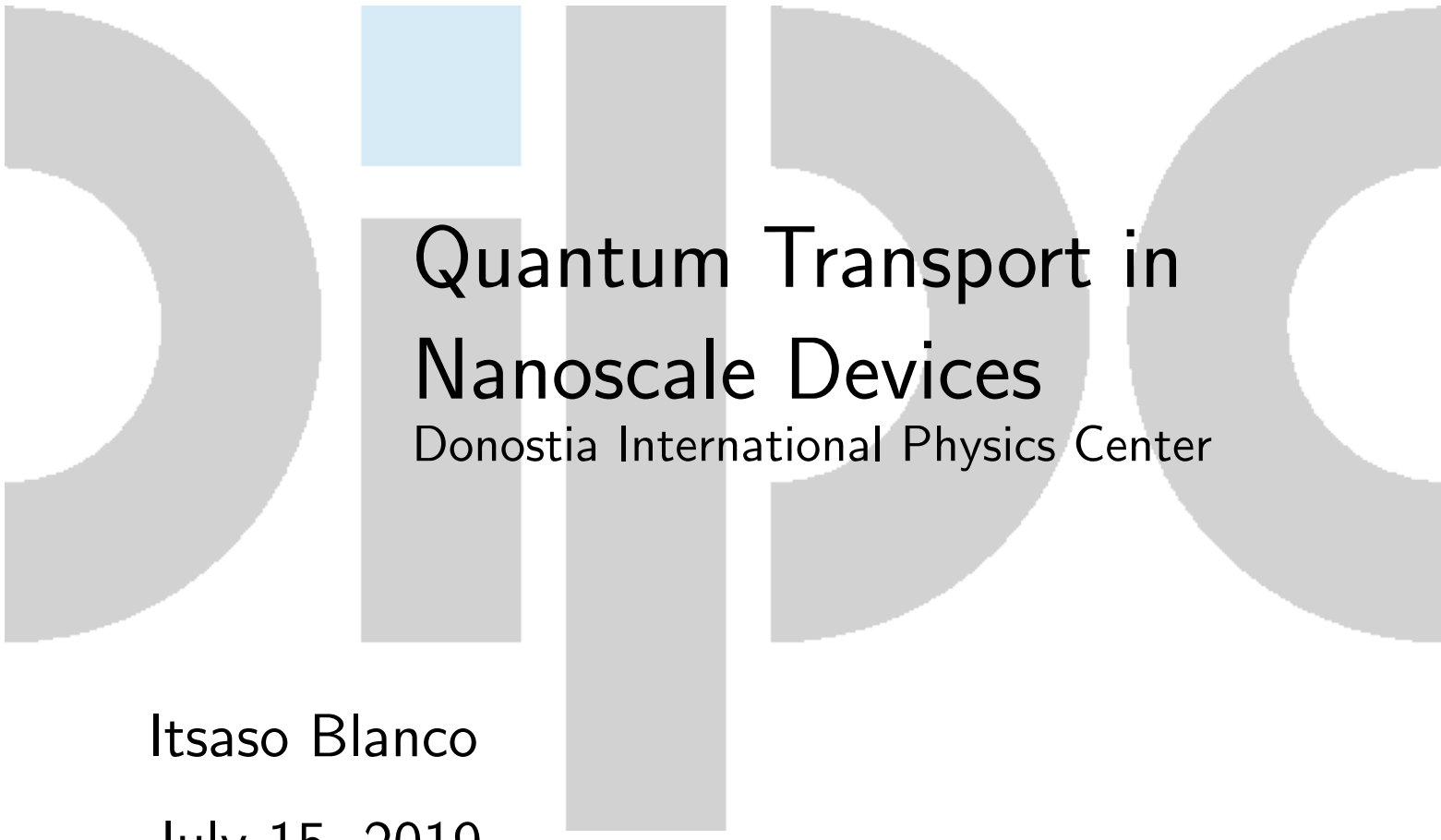

Quantum Transport in Nanoscale Devices

Donostia International Physics Center

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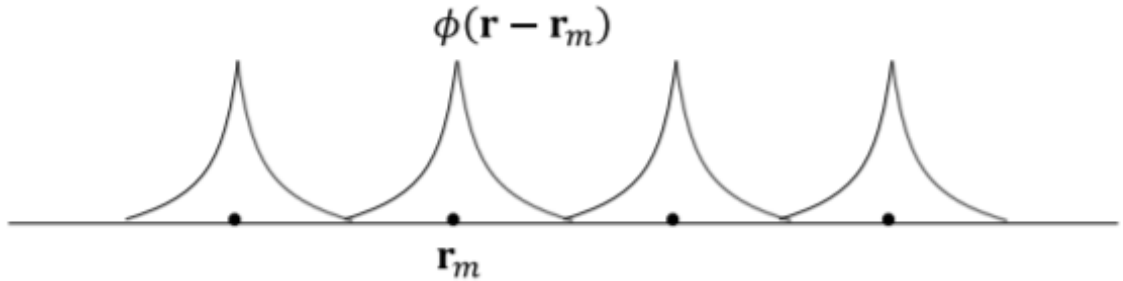
Tight Binding Model

Introduction

- Large potential $\rightarrow$ electrons are tightly bound to ionic cores.
- $H = H_{at} + \Delta U$



Tight Binding Model

Introduction

- The wavefunctions of the crystal to be a linear combination of the atomic orbitals (LCAO).
- $\Psi_k(r) = \sum_m C_{km}\phi(r - r_m)$
- Bloch's Theorem $\rightarrow \Psi(r) = \frac{1}{\sqrt{N}} \sum e^{ikr} u(r)$

Tight Binding Model

1D Chain

- Most basic example $\rightarrow$ atoms only interact with nearest neighbours.
- Atomic TISE $\rightarrow H_{at} |\psi\rangle = E_{at} |\psi\rangle$
- Total TISE $\rightarrow H |\Psi\rangle = E_k |\Psi\rangle$
- Eigenvalues $\rightarrow E_k = E_{at} - t(e^{ika} + e^{-ika}) = E_{at} - t(2coska)$

Tight Binding Model

1D Chain

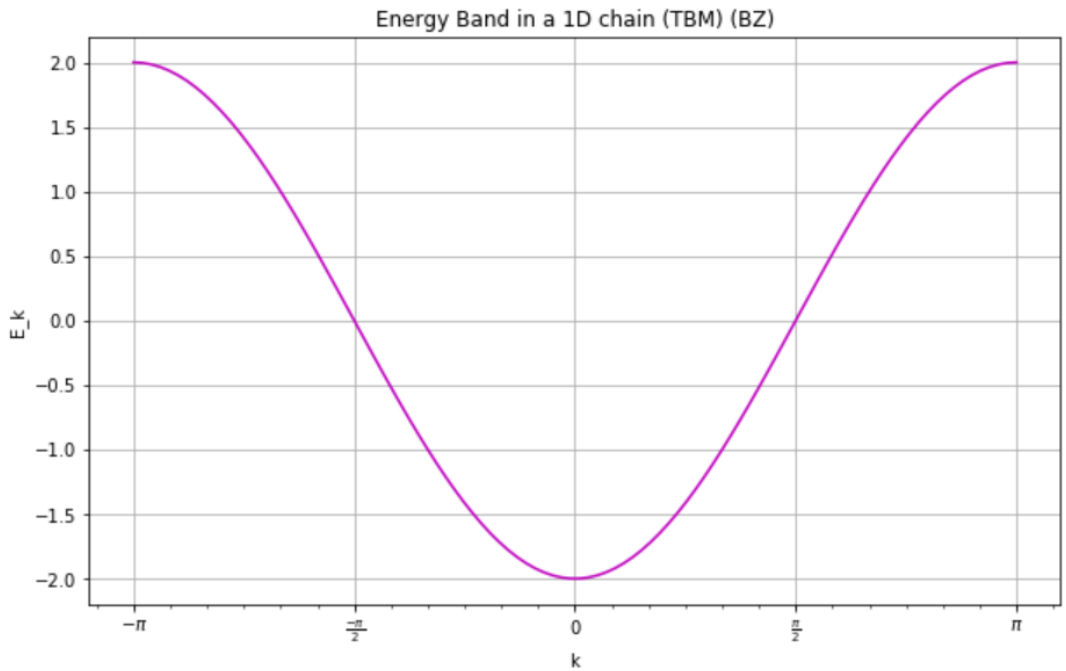
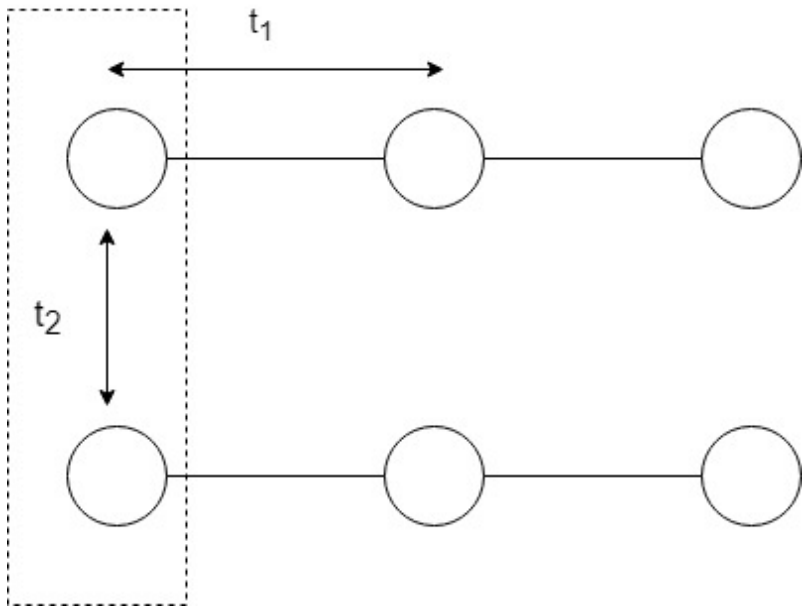


Figure: Diagram showcasing a 1-dimensional atomic chain energy band.

Tight Binding Model

2 Atomic Chains

- Instead of 2 nearest neighbours, each atom has 4.
- $\alpha \rightarrow$ Onsite energies and the interactions within the unit cell
- $\gamma \rightarrow$ Interactions for nearest neighbours.
- $\alpha = \begin{pmatrix} \alpha_1 & t_2 \\ t_2 & \alpha_2 \end{pmatrix}$
- $\gamma = \begin{pmatrix} t_1 & 0 \\ 0 & t_1 \end{pmatrix}$



Tight Binding Model

2 Atomic Chains

- $H = -\alpha - \gamma(e^{ika} + e^{-ika})$

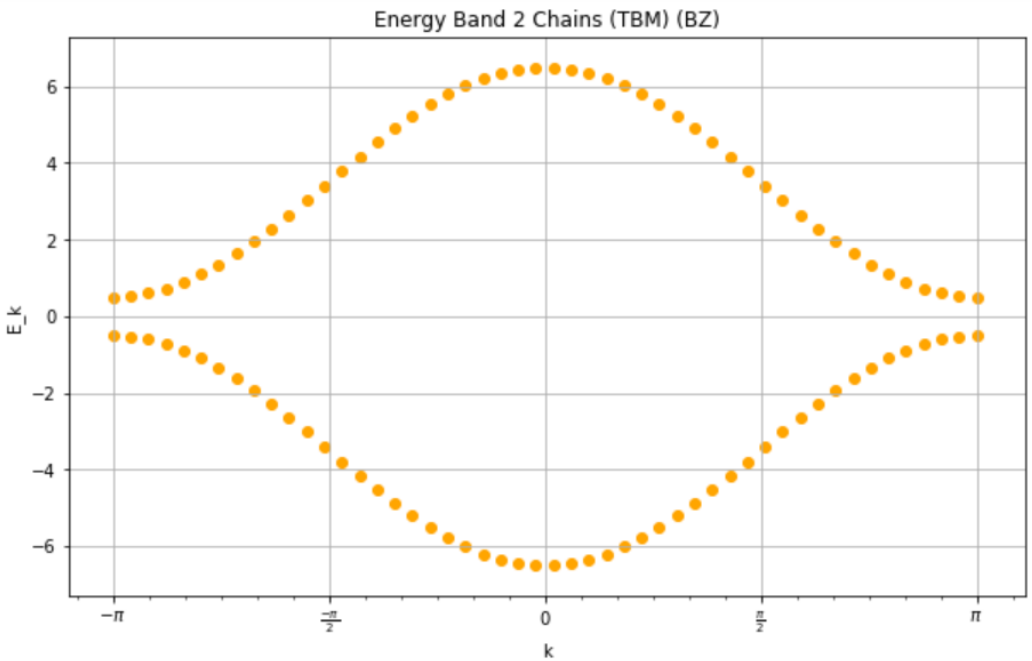


Figure: Diagram showcasing the energy bands of a 2 chain atomic system.

GNRs

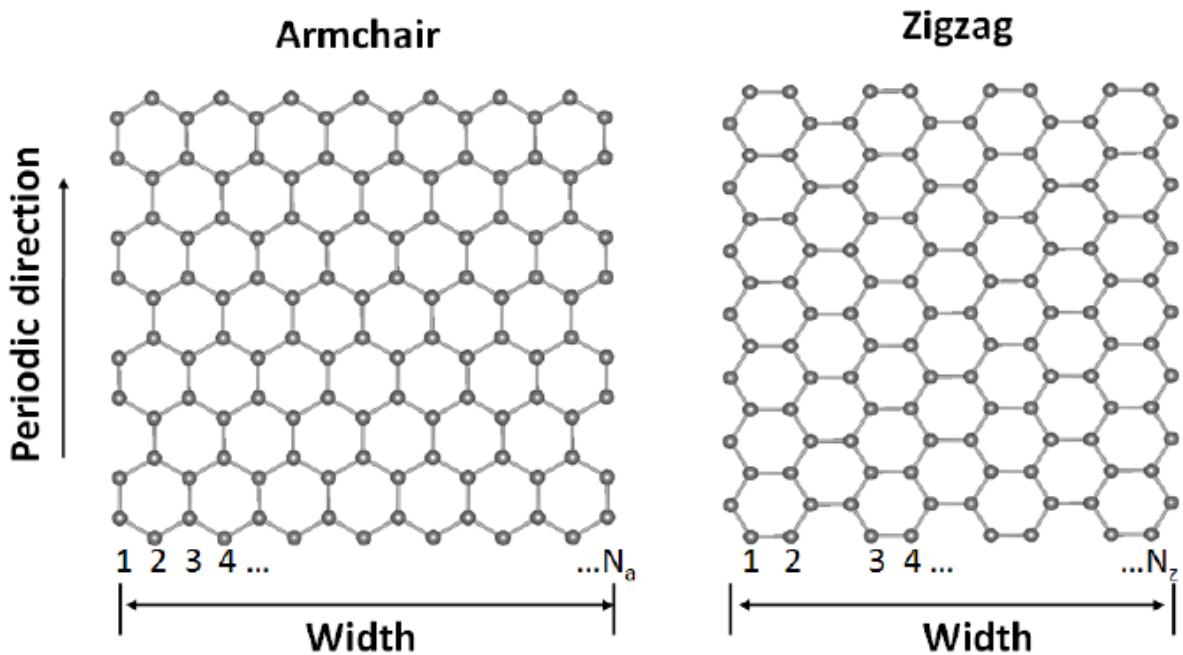


Figure: Diagram showcasing Armchair vs Zigzag GNRs.