Instituto de Ciencia de Materiales de Madrid

MathQ

a **Mathematica** *simulator for quantum systems*

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Code **rewrite** vs. code **reuse**

- New project $\longrightarrow$ new code
- Inheriting past code is often problematic
  - *Documentation*
  - *Implementation*
  - *Debugging*

Code **rewrite** vs. code **reuse**

- Domain specific language *(DSL)*
  - *Ab-initio: Siesta, VASP, QuantumEspresso, Gaussian, etc…*
  - *Equivalent for tight-binding problems?*

kwant (Python)

pybinding (Python)

QBox (Julia)

NEMO5 (custom)

EQuUs (Matlab)

MathQ (Mathematica)

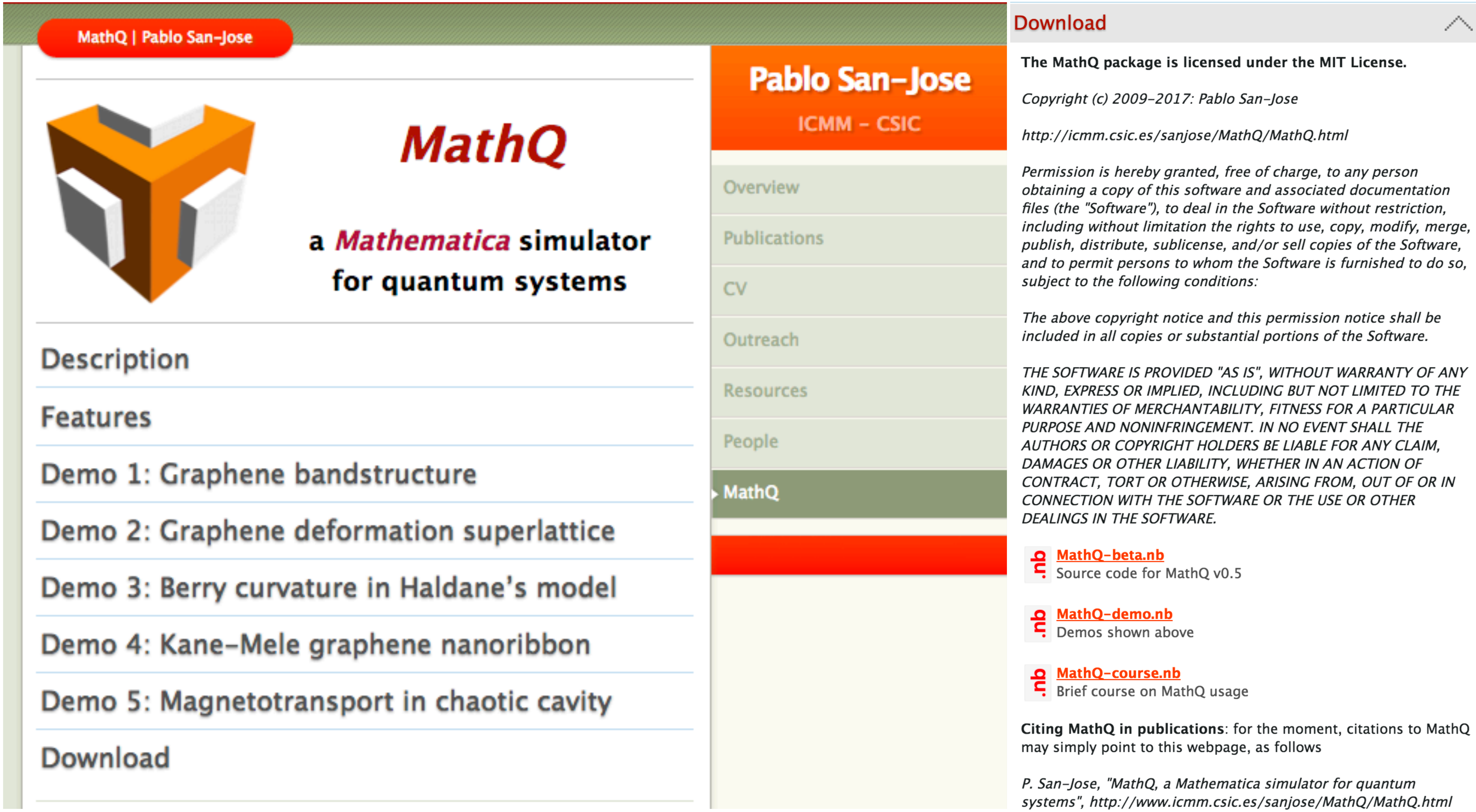
The *Mathematica* language

- Some advantages of ***Mathematica***
  - *Vast technology stack*
  - *Everything is built-in*
  - *Unique documentation/example system*
  - *Very optimised high-level numerical algorithms*
  - *Strong symbolic side*
  - *High-quality visualisations*
  - *Very nice notebook environment*

The *Mathematica* language

- Some disadvantages of ***Mathematica***
  - ***Proprietary***
  - *Expensive licenses (unless you are a student)*
  - *Expensive parallelisation in clusters (licenses!)*
  - *Non-trivial interoperability with other languages*
  - *Substantial memory overhead for numerics*
  - *Syntax can be made very obscure (too compact)*

MathQ, a *Mathematica* package



MathQ | Pablo San-Jose

MathQ

a *Mathematica* simulator for quantum systems

Description

Features

Demo 1: Graphene bandstructure

Demo 2: Graphene deformation superlattice

Demo 3: Berry curvature in Haldane's model

Demo 4: Kane-Mele graphene nanoribbon

Demo 5: Magnetotransport in chaotic cavity

Download

Pablo San-Jose

ICMM - CSIC

Overview

Publications

CV

Outreach

Resources

People

MathQ

Download

The MathQ package is licensed under the MIT License.

.nb MathQ-beta.nb
Source code for MathQ v0.5

.nb MathQ-demo.nb
Demos shown above

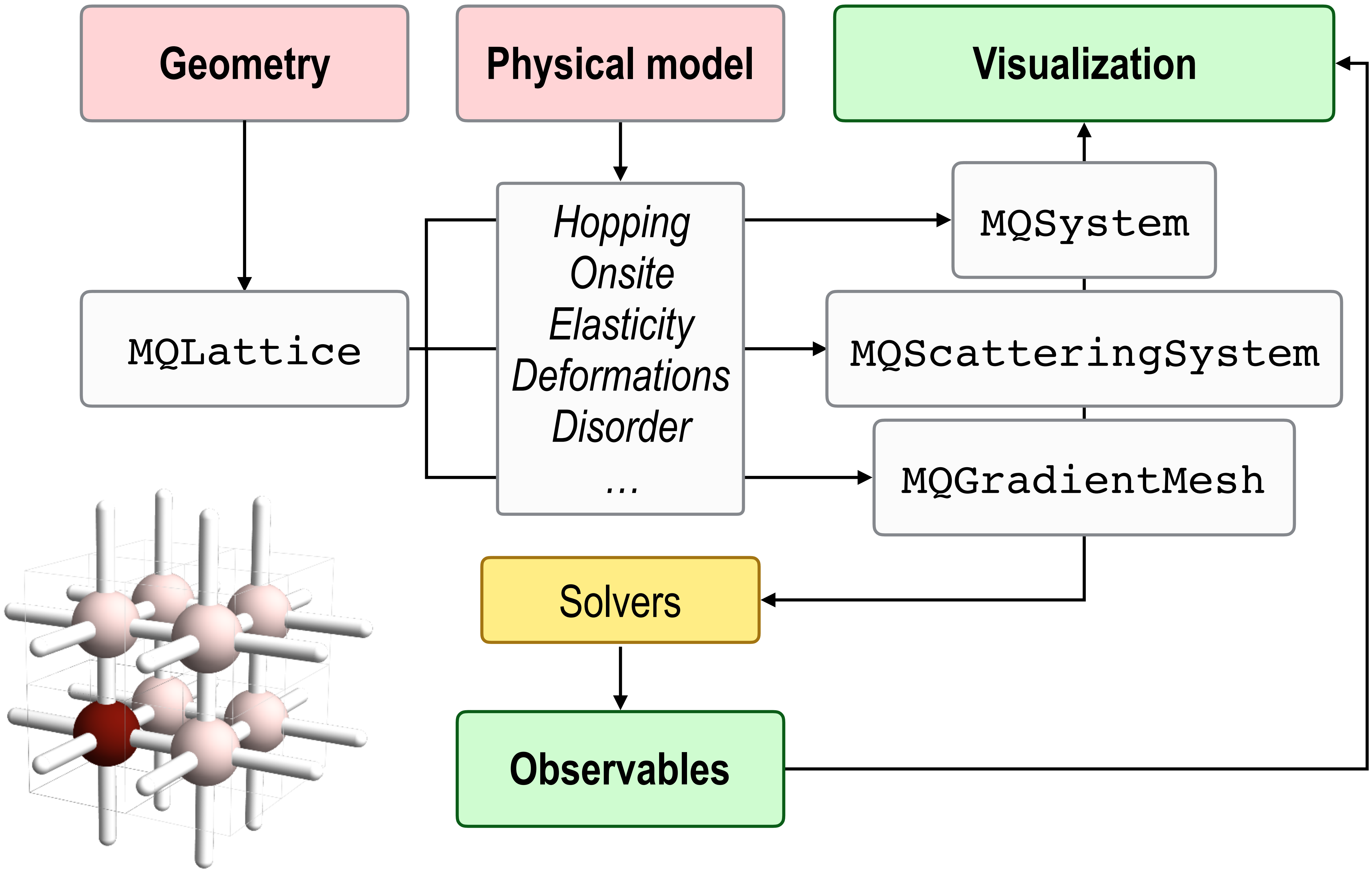
.nb MathQ-course.nb
Brief course on MathQ usage

Citing MathQ in publications: for the moment, citations to MathQ may simply point to this webpage, as follows

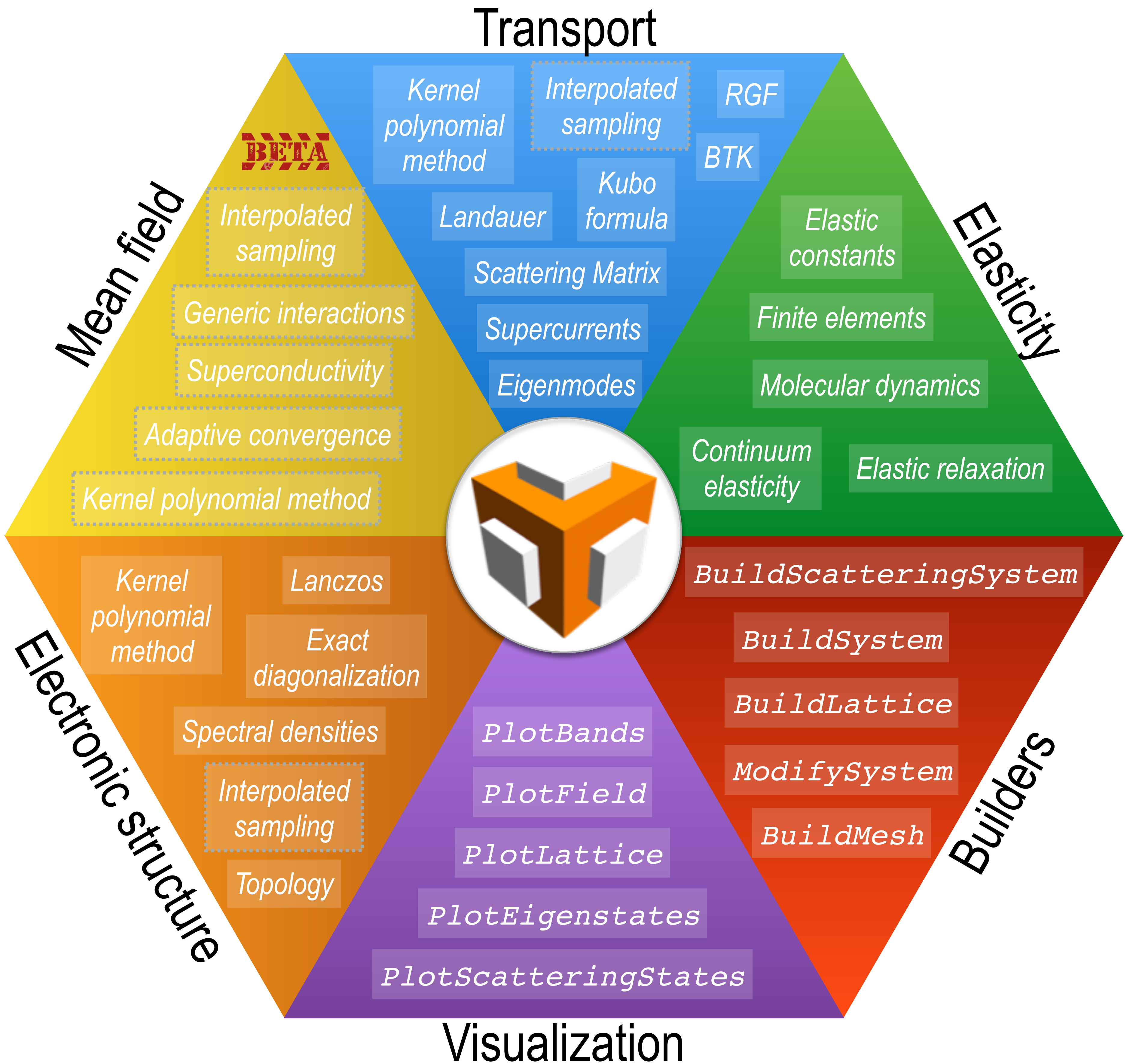
P. San-Jose, "MathQ, a Mathematica simulator for quantum systems", http://www.icmm.csic.es/sanjose/MathQ/MathQ.html

http://www.icmm.csic.es/sanjose/MathQ/MathQ.html

MathQ structure



MathQ structure (v0.5)



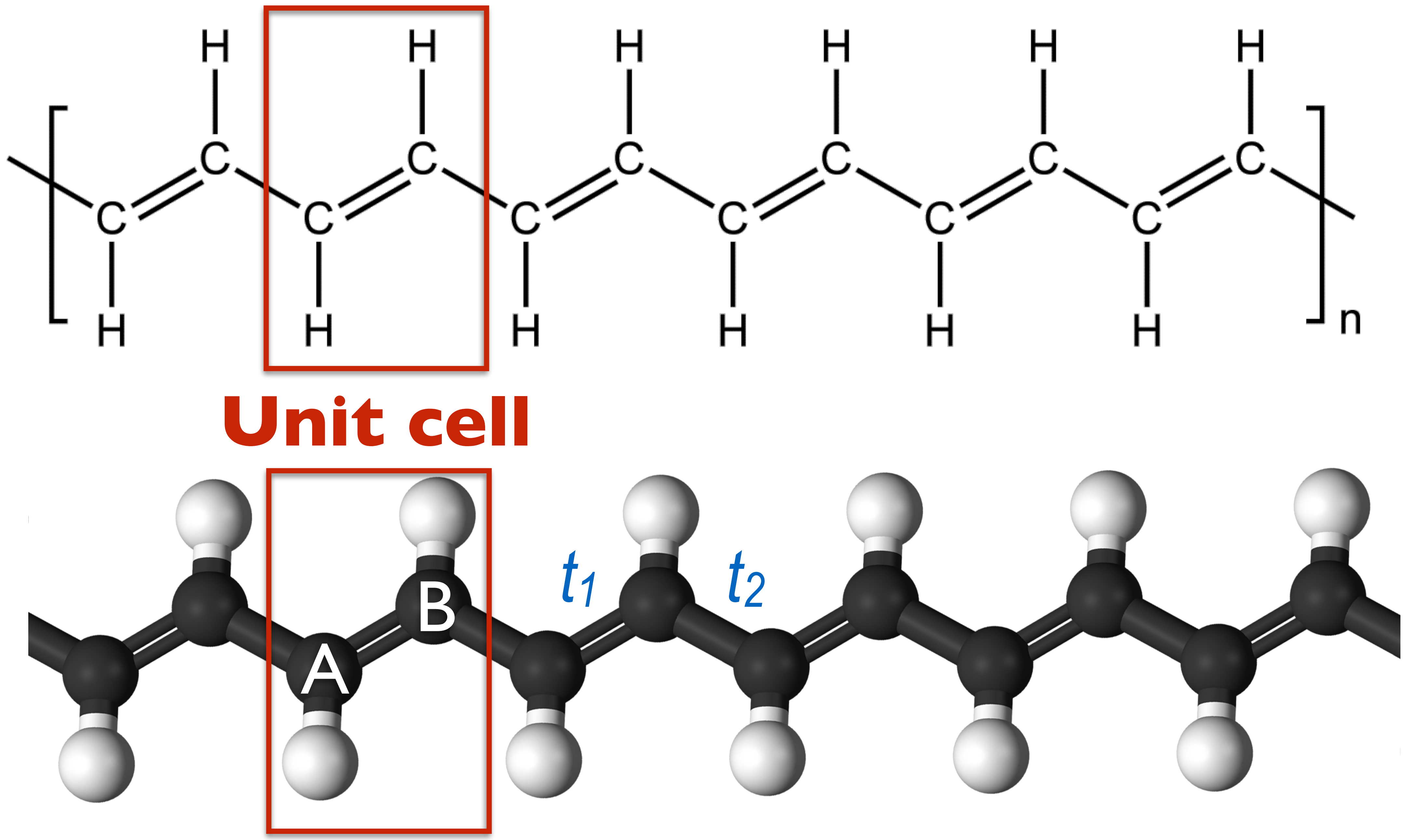
Demo time!

Su–Schrieffer–Heeger model

Bulk-boundary correspondence

Polyacetylene

- 1D carbon chain with alternating bonds



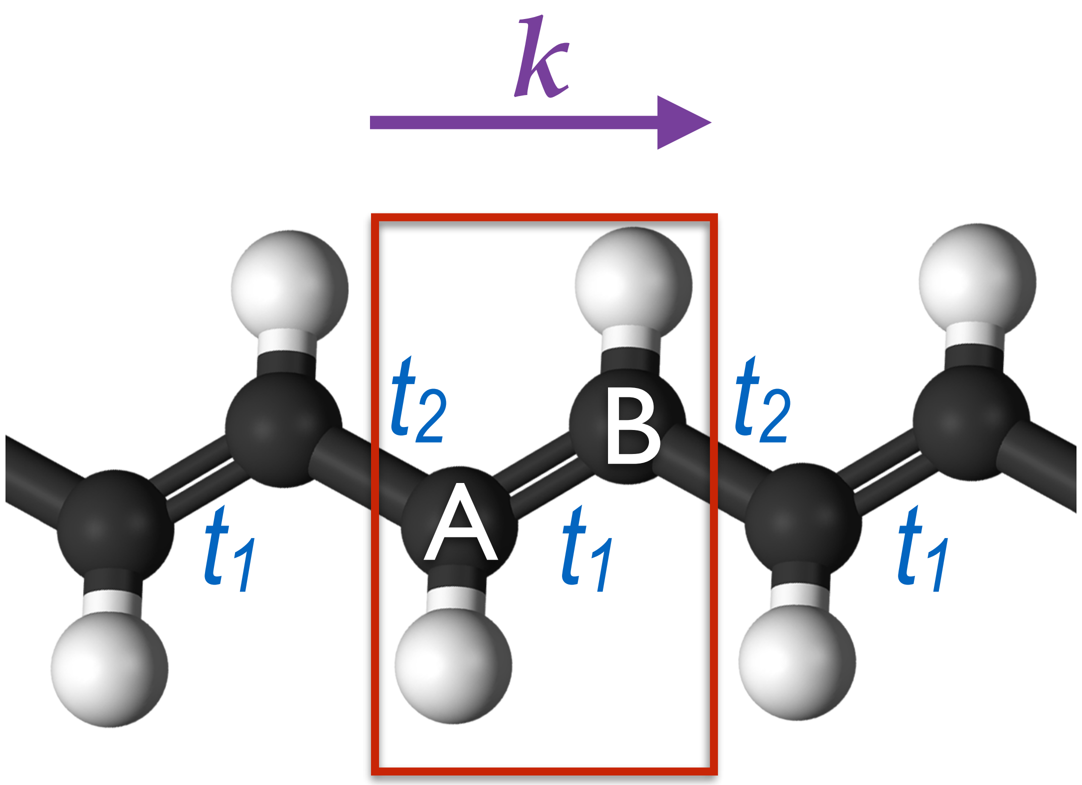
SSH model

- 1D carbon chain with alternating bonds

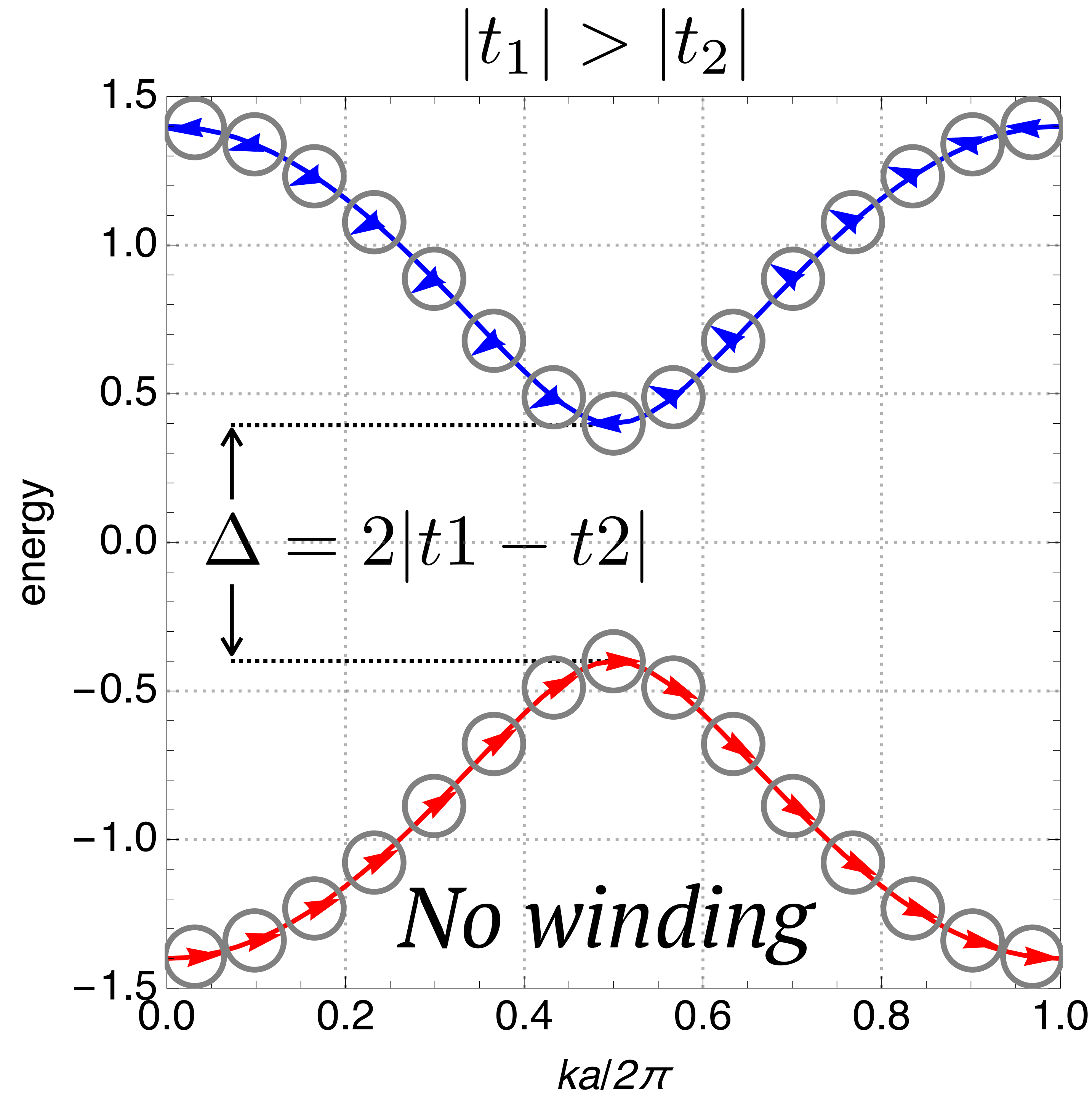
$$H_{SSH} = \begin{pmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & 0 & t_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & t_1 & 0 & t_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & t_2 & 0 & t_1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & t_1 & 0 & t_2 & 0 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & t_2 & 0 & t_1 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & t_1 & 0 & t_2 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 0 & t_2 & 0 & t_1 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 0 & 0 & t_1 & 0 & t_2 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t_2 & 0 & t_1 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t_1 & 0 & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots
\end{pmatrix}$$

SSH bandstructure

- The two sublattices define a pseudospin

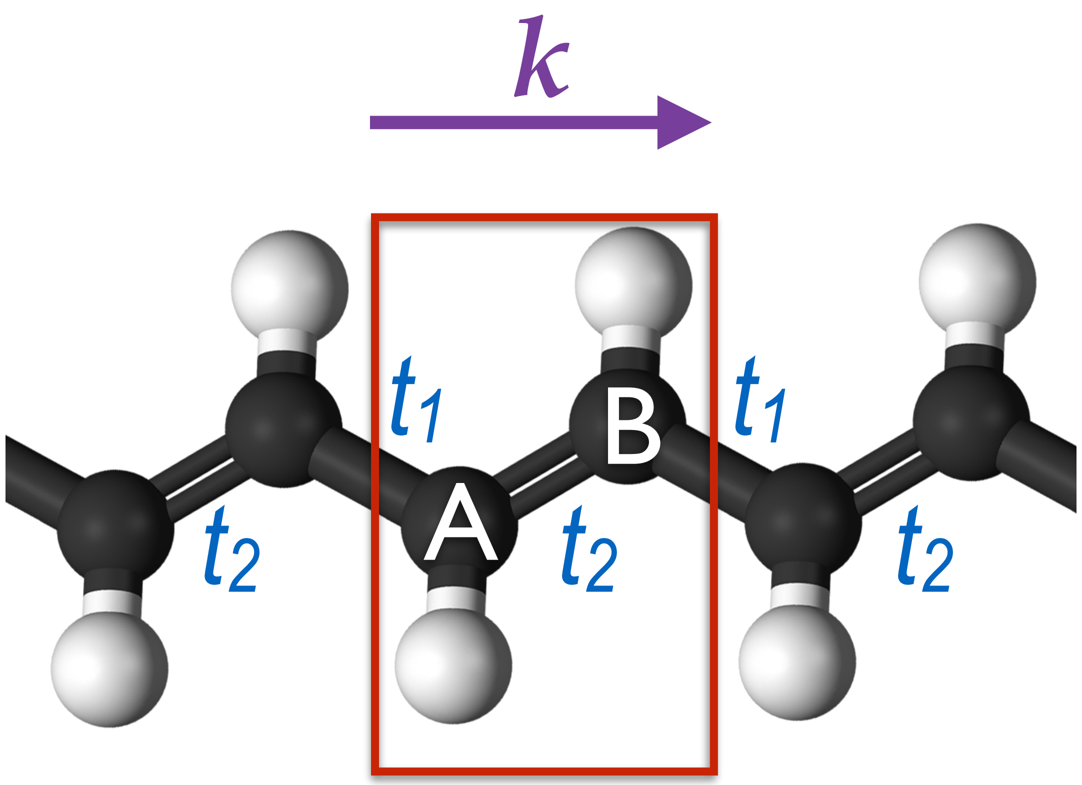


$$\langle x_n|\Psi_k\rangle = \begin{pmatrix} \psi_k^A \\ \psi_k^B \end{pmatrix} e^{ikx_n}$$

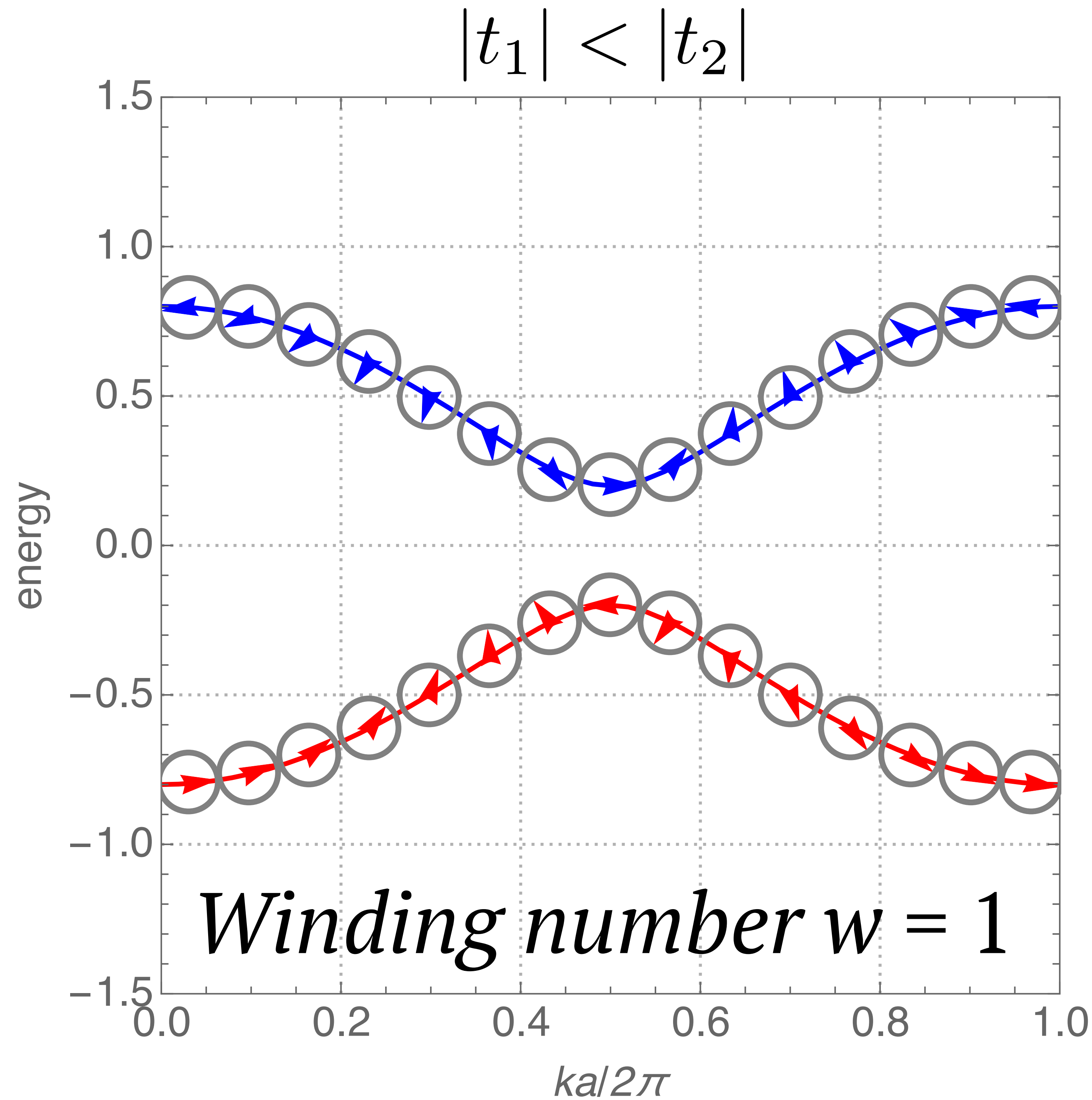


SSH bandstructure

- The two sublattices define a pseudospin



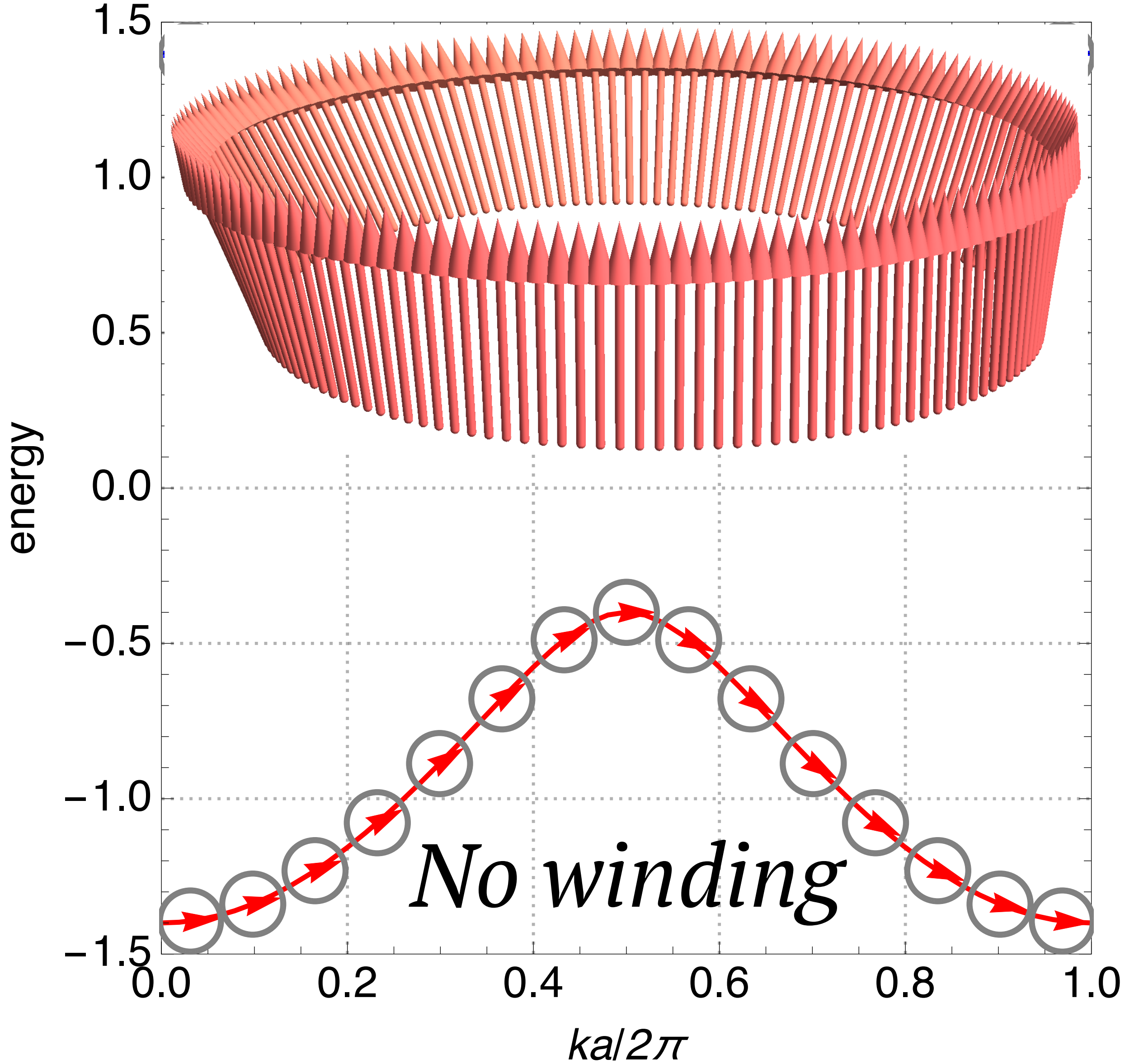
$$\langle x_n | \Psi_k \rangle = \begin{pmatrix} \psi_k^A \\ \psi_k^B \end{pmatrix} e^{ikx_n}$$



SSH bandstructure

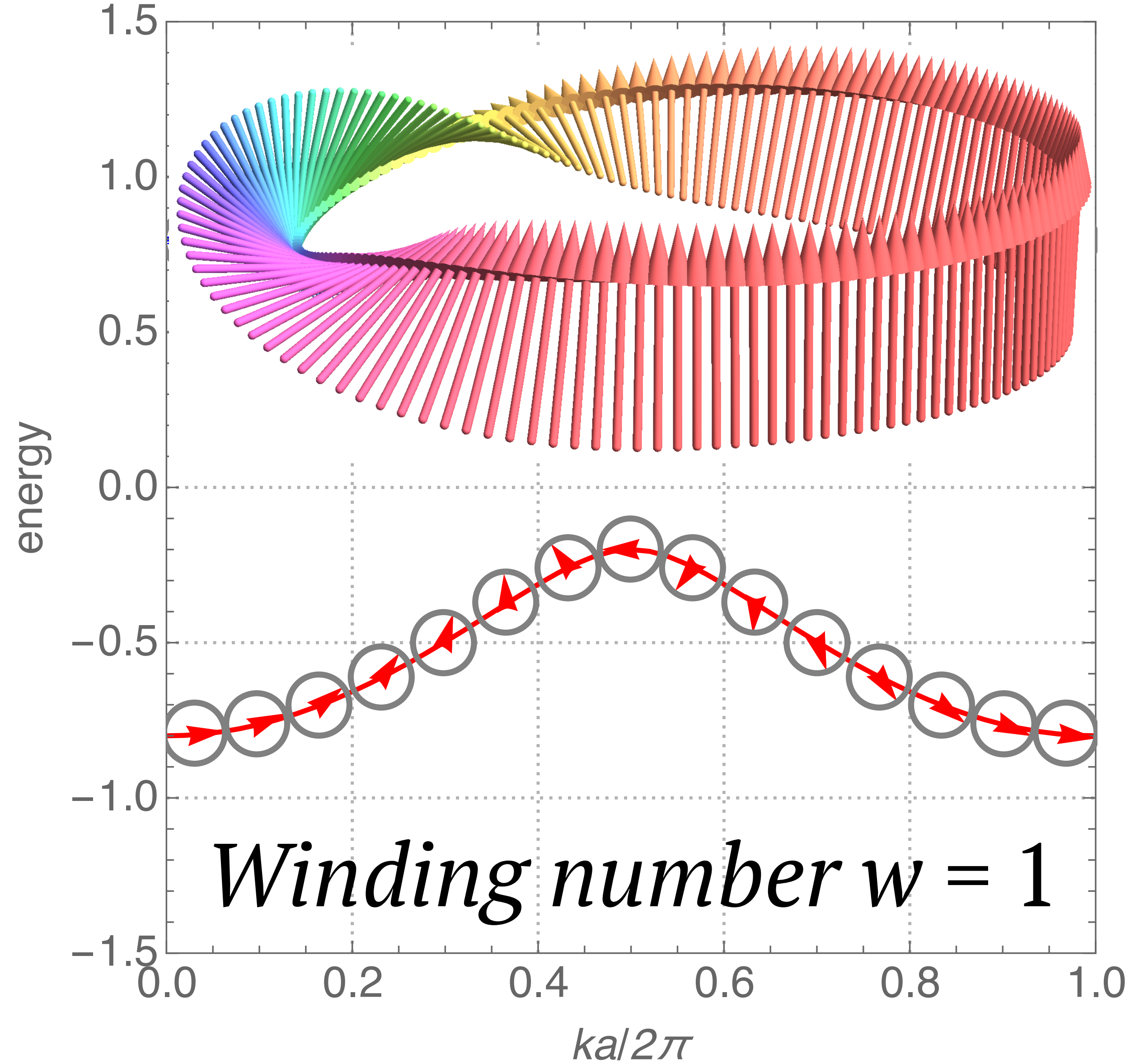
- The two sublattices define a pseudospin

$|t_1| > |t_2|$



Topologically trivial

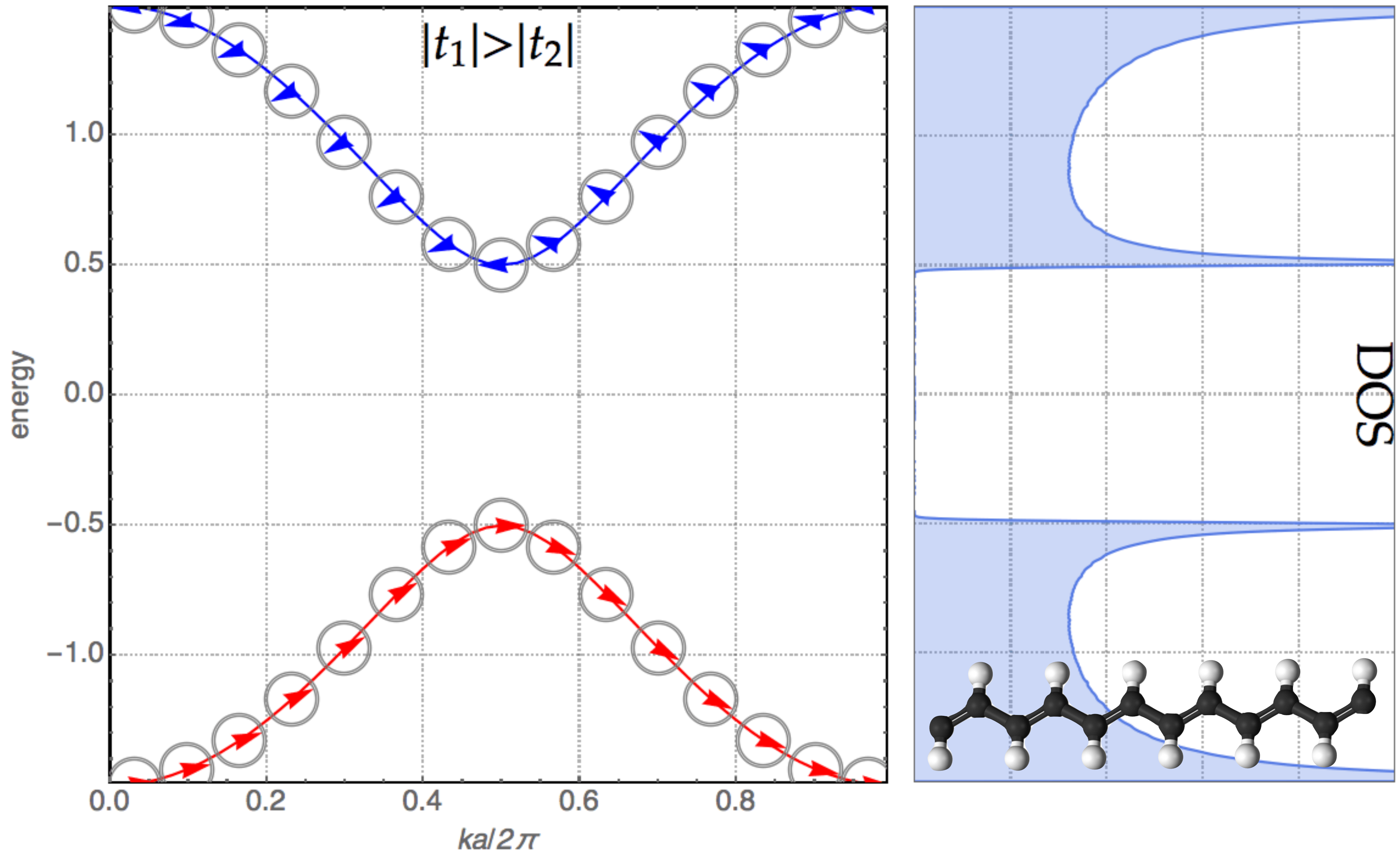
$|t_1| < |t_2|$



Topologically non-trivial

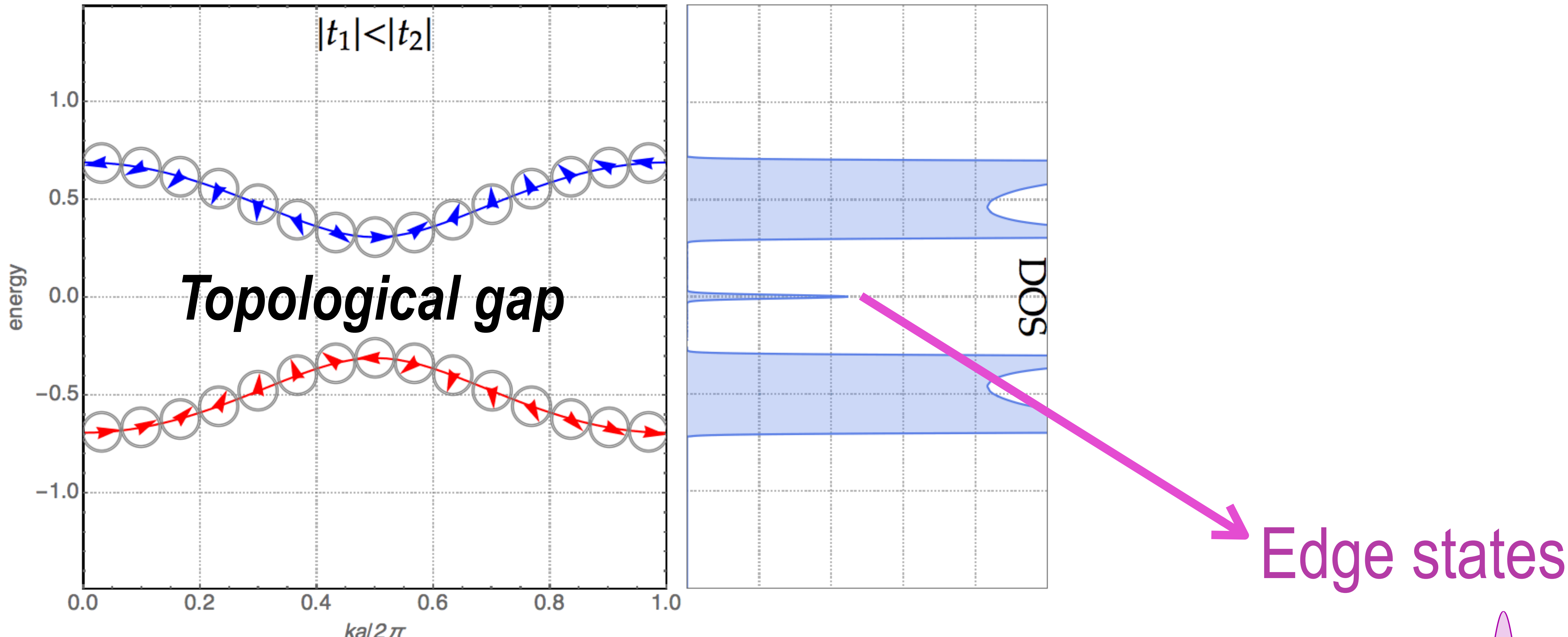
SSH bandstructure

- Topological transition at $|t_1| = |t_2|$ *(gap inversion)*

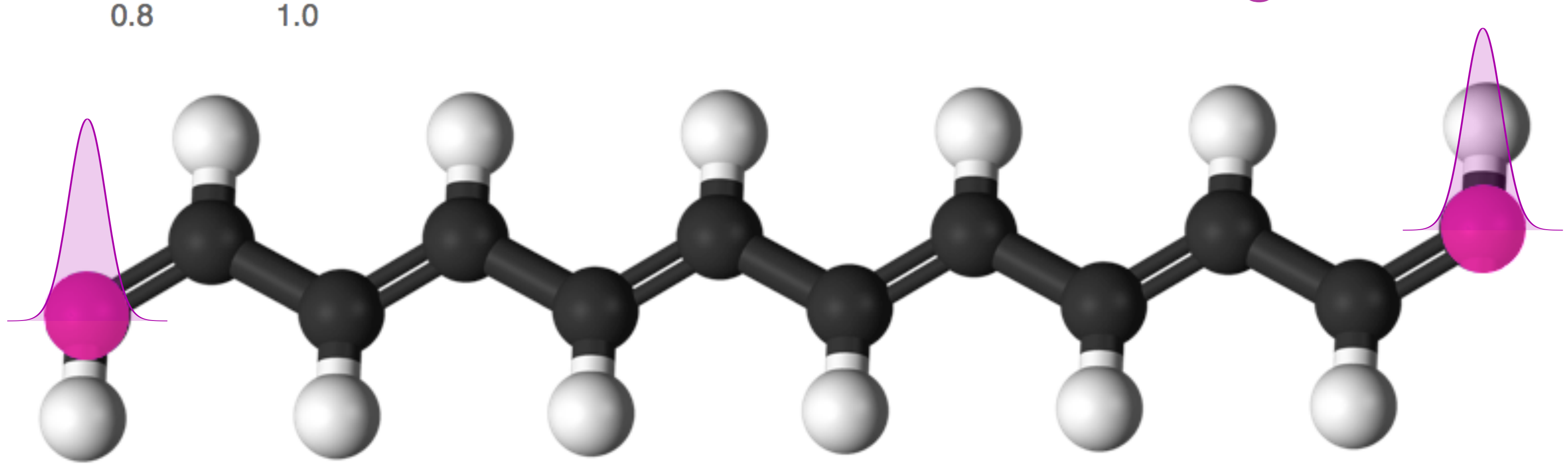


Topological insulator

- Topological transition at $|t_1| = |t_2|$ *(gap inversion)*



Bulk-boundary correspondence



Kitaev model

Majorana zero modes

The Kitaev model

Unpaired Majorana fermions in quantum wires

A Yu Kitaev

Physics-Uspekhi, Volume 44, Supplement

Consider a chain consisting of $L \gg 1$ sites. Each site can be either empty or occupied by an electron (with a fixed spin direction). The Hamiltonian is

$$H_1 = \sum_j \Big[-w(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) - \mu\left(a_j^\dagger a_j - \frac{1}{2}\right) + \Delta a_j a_{j+1} + \Delta^* a_{j+1}^\dagger a_j^\dagger \Big]. \quad (4)$$

Here w is a hopping amplitude, μ a chemical potential, and $\Delta = |\Delta| e^{i\theta}$ the induced superconducting gap. It is convenient

We may conjecture that the phases (a) and (b) extend to connected domains in the parameter space where the spectrum has a gap. The signs of μ and w seem not to be important, so we actually expect that the phase (a) occurs at $2|w| < |\mu|$ while the phase (b) occupies the domain $2|w| > |\mu|$, $\Delta \neq 0$. (The phase boundary is given by the equation $2|w| = |\mu|$ while $\Delta = 0$, $2|w| > |\mu|$ is a line of normal metal phase inside the domain (b).)

$$|\mu| < 2|w| \Rightarrow \text{Topological}$$
$$|\mu| > 2|w| \Rightarrow \text{Non-topological}$$

$$\hat{H} = \frac{1}{2}\sum_{\alpha,\beta} \left(c_\alpha^\dagger, c_\alpha\right) H_{\alpha,\beta} \begin{pmatrix} c_\beta^\dagger \\ c_\beta \end{pmatrix}$$

SSH - Kitaev mapping

A/B = particle/hole

Haldane model

Berry curvature

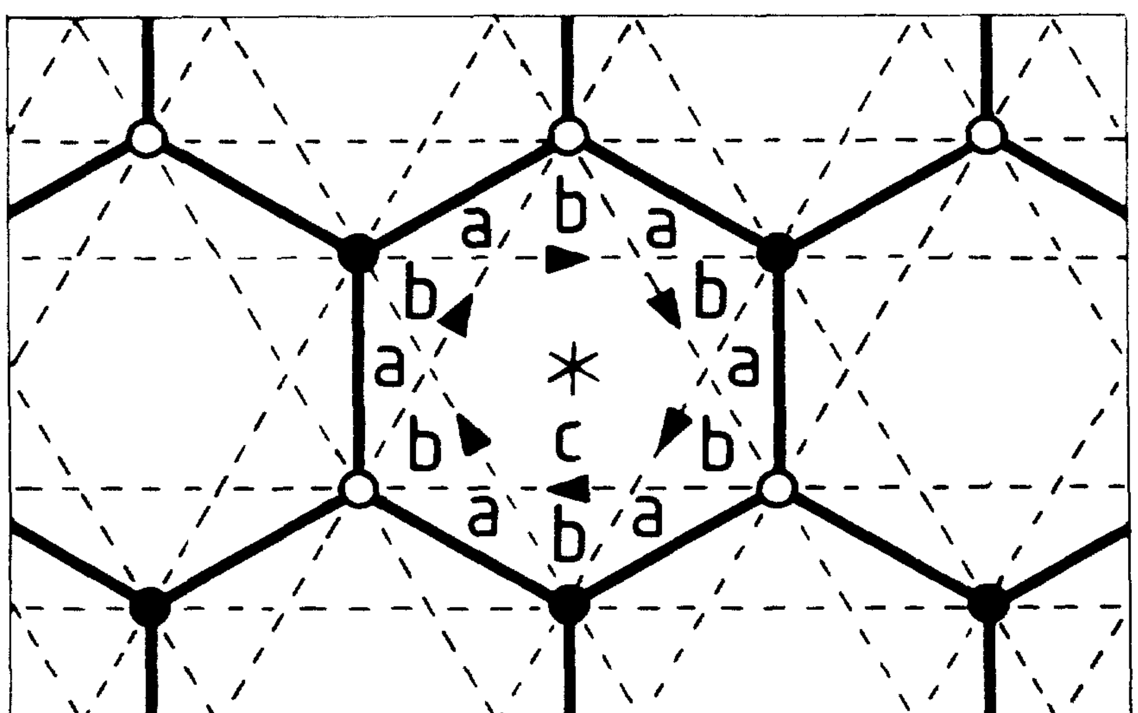
The Haldane model

VOLUME 61, NUMBER 18 PHYSICAL REVIEW LETTERS 31 OCTOBER 1988

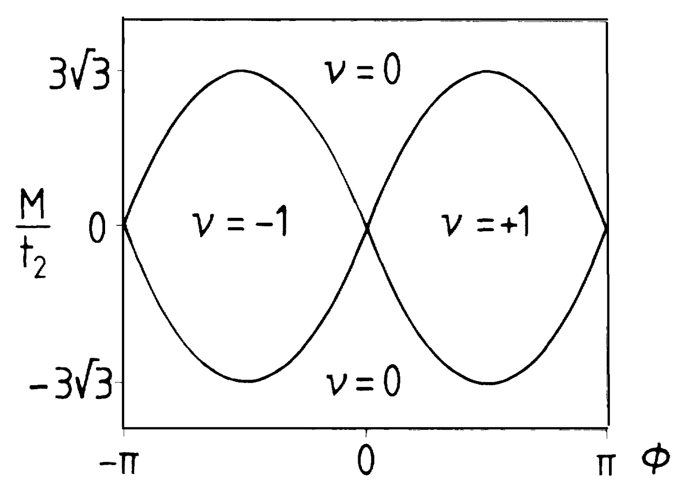
**Model for a Quantum Hall Effect without Landau Levels:
Condensed-Matter Realization of the "Parity Anomaly"**

F. D. M. Haldane
Department of Physics, University of California, San Diego, La Jolla, California 92093
(Received 16 September 1987)

A two-dimensional condensed-matter lattice model is presented which exhibits a nonzero quantization of the Hall conductance σ^{xy} in the *absence* of an external magnetic field. Massless fermions *without spectral doubling* occur at critical values of the model parameters, and exhibit the so-called "parity anomaly" of (2+1)-dimensional field theories.



Spinless graphene
+ valley-dependent mass



Kane - Mele model

Quantum Spin Hall

The Kane-Mele model

PRL **95,** 226801 (2005) PHYSICAL REVIEW LETTERS week ending 25 NOVEMBER 2005

Quantum Spin Hall Effect in Graphene

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(Received 29 November 2004; published 23 November 2005)

We study the effects of spin orbit interactions on the low energy electronic structure of a single plane of graphene. We find that in an experimentally accessible low temperature regime the symmetry allowed spin orbit potential converts graphene from an ideal two-dimensional semimetallic state to a quantum spin Hall insulator. This novel electronic state of matter is gapped in the bulk and supports the transport of spin and charge in gapless edge states that propagate at the sample boundaries. The edge states are nonchiral, but they are insensitive to disorder because their directionality is correlated with spin. The spin and charge conductances in these edge states are calculated and the effects of temperature, chemical potential, Rashba coupling, disorder, and symmetry breaking fields are discussed.

DOI: 10.1103/PhysRevLett.95.226801 PACS numbers: 73.43.−f, 72.25.Hg, 73.61.Wp, 85.75.−d

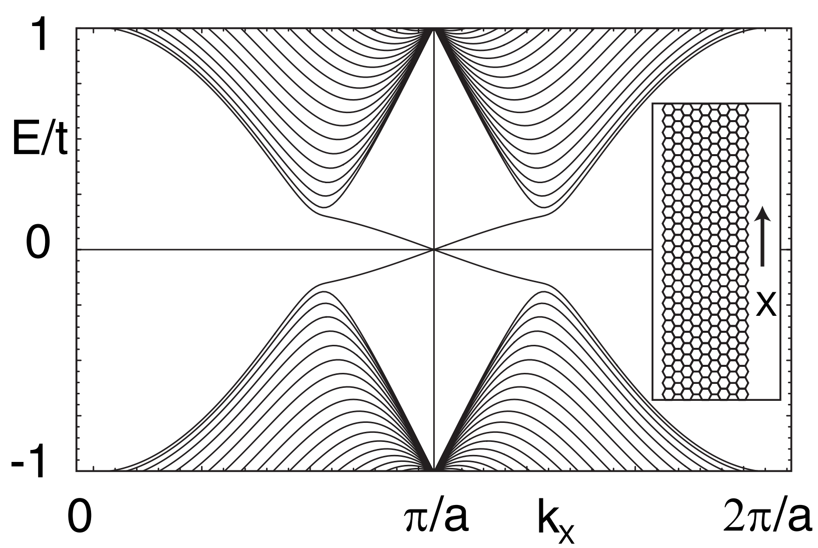
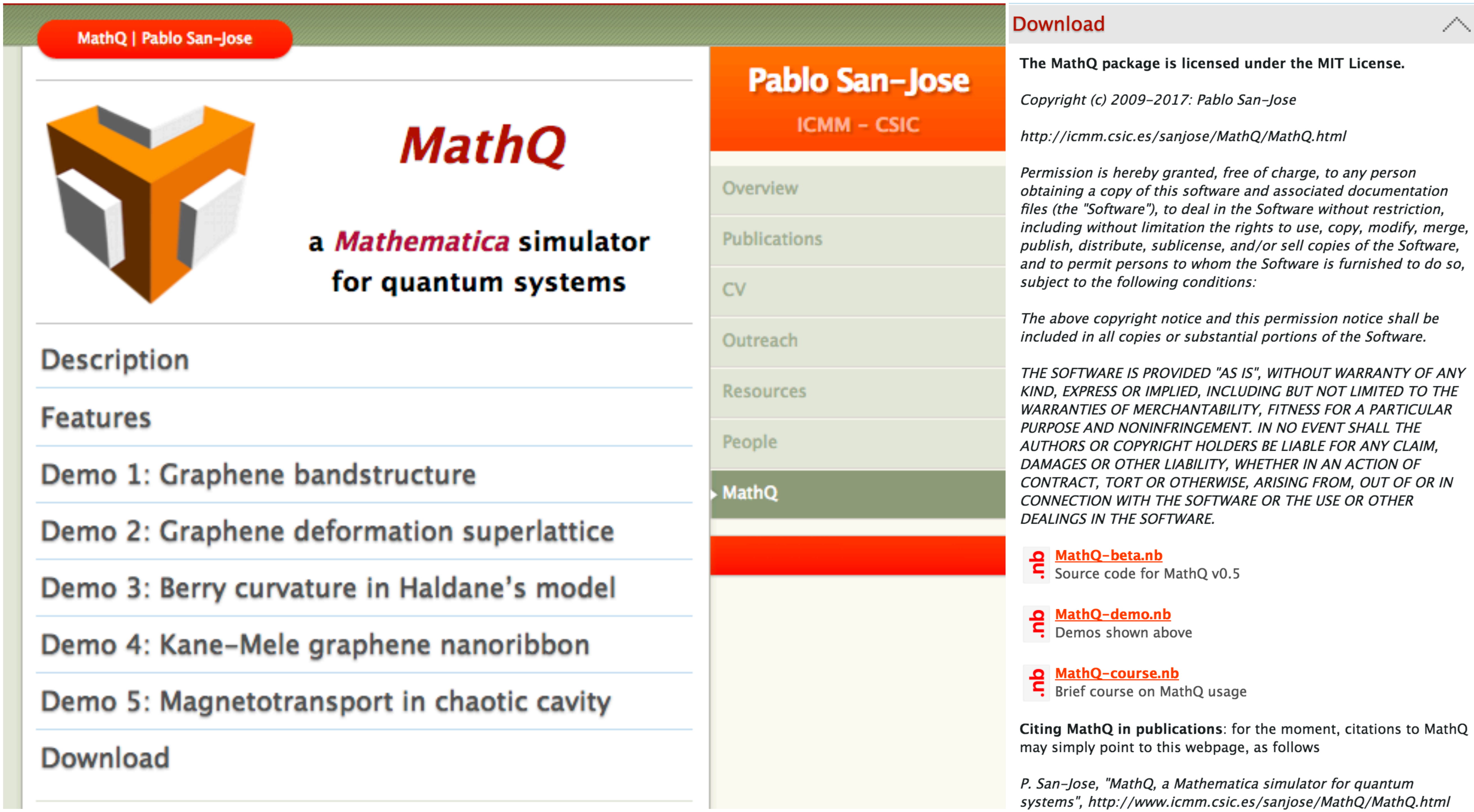


FIG. 1. (a) One-dimensional energy bands for a strip of graphene (shown in inset) modeled by (7) with $t_2/t = 0.03$. The bands crossing the gap are spin filtered edge states.

One Haldane per spin

MathQ, a ***Mathematica*** *package*



http://www.icmm.csic.es/sanjose/MathQ/MathQ.html