One dimensional tight-binding chain

In this basic tutorial we will address how to compute the band structure of a one dimensional tight binding model.

The Hamiltonian of a one dimensional tight binding chain takes the form

$$H = \sum_n c_n^\dagger c_{n+1} + h.c.$$

This model can be diagonalized analytically, giving rise to a diagonal Hamiltonian of the form

$$H = \sum_k \epsilon_k \Psi_k^\dagger \Psi_k$$

where energy momentum dispersion takes the form

$$\epsilon_k = 2\cos k$$

With the pyqula library, the previous band structure can be computed as

```
from pyqula import geometry
g = geometry.chain() # geometry of the 1D chain
h = g.get_hamiltonian() # generate the Hamiltonian
(k,e) = h.get_bands() # compute band structure
```

Including second and third neighbor hopping

By default, the Hamiltonian generated includes only first neighbor hopping $t_1 = 1$. However, we may want to consider a generalized Hamiltonian of the form

$$H = \sum_n c_n^\dagger c_{n+1} + t_2 \sum_n c_n^\dagger c_{n+2} + t_3 \sum_n c_n^\dagger c_{n+3} + h.c.$$

To compute the eigenvalues in this generalized model taking $t_2 = 0.2$ and $t_3 = 0.3$, we write

```
from pyqula import geometry
g = geometry.chain() # geometry of the 1D chain
h = g.get_hamiltonian() # generate the Hamiltonian
(k,e) = h.get_bands(tij=[1.0,0.2,0.3]) # compute band structure
```

Including an external Zeeman field

In the following we will consider that we want to add an external Zeeman field to the electronic system. We now include the existence of a spin degree of freedom, considering the Hamiltonian

$$H = H_0 + H_Z$$

where H_0 is the original tight binding Hamiltonian

$$H_0 = \sum_{n,s} c^\dagger_{n,s} c_{n+1,s} + h.c.$$

and

$$H_Z = \sum_{n,s,s'} \vec{B} \cdot \vec{\sigma}^{s,s'} c^\dagger_{n,s} c_{n,s'}$$

with n running over the sites and s, s' running over the spin degree of freedom. The magnetic field takes the form $\vec{B} = (B_x, B_y, B_z)$, and σ_α are the spin Pauli matrices. To add a magnetic field of the form $\vec{B} = (0.1, 0.2, 0.3)$ to our chain we write

```
from pyqula import geometry
g = geometry.chain() # geometry of the 1D chain
h = g.get_hamiltonian() # generate the Hamiltonian
h = g.add_zeeman([0.1,0.2,0.3]) # add the Zeeman field
(k,e) = h.get_bands() # compute band structure
```

Two dimensional band structures

In the following we move on to consider a two dimensional mutliorbital model, in particular a honeycomb lattice. The Hamiltonian takes the form

$$H = \sum_{\langle ij \rangle} c^\dagger_i c_j + h.c.$$

where $\langle ij \rangle$ denotes first neighbors of the honeycomb lattice. This model can be diagonalized analytically, giving rise to a diagonal Hamiltonian of the form

$$H = \sum_{k,\alpha} \epsilon_{k,\alpha} \Psi^\dagger_{k,\alpha} \Psi_{k,\alpha}$$

where α is the band index.

The previous calculation can be performed as

```
from pyqula import geometry
g = geometry.honeycomb_lattice() # geometry of the 2D model
h = g.get_hamiltonian() # generate the Hamiltonian
(k,e) = h.get_bands() # compute band structure
```

Superconductivity

Up to now we have focused on Hamiltonians that contain only normal terms, namely that the full Hamiltonian can be written as

$$H_0 = \sum_{ijss'} t_{ijss'} c^\dagger_{i,s} c_{j,s'}$$

where ij runs onver sites and ss' over spins.

In the presence of superconductivity, an anomalous term appears in the Hamiltonian taking the form

$$H_{SC} = \sum_{ijss'} \Delta^{ss'}_{ij} c_{i,s} c_{j,s'} + h.c.$$

To solve the Hamiltonian

$$H = H_0 + H_{SC}$$

we define a Nambu spinor that takes the form

$$\Psi_n = \begin{pmatrix} c_{n,\uparrow} \\ c_{n,\downarrow} \\ c^\dagger_{n,\downarrow} \\ -c^\dagger_{n,\uparrow} \end{pmatrix}$$

and rewrite the Hamiltonian as

$$H = \Psi^\dagger \mathcal{H} \Psi$$

where $\mathcal{H}$ is the nambu Hamiltonian. In this new basis, the Hamiltonian can be written in a diagonal form as

$$H = \sum_\alpha \epsilon_\alpha \Psi^\dagger_\alpha \Psi_\alpha$$

where ϵ_α are the Nambu eigenvalues.

s-wave superconductivity

The simplest form of superconductivity is spin-singlet s-wave superconductivity. A minimal superconducting term of this form can be written as

$$H_{SC} = \Delta_0 \sum_n c_{n,\uparrow} c_{n,\downarrow} + h.c.$$

In the following, we address the electronic structure of a triangular lattice with s-wave superconductivity, whose Hamiltonian takes the form

$$H = H_0 + H_{SC}$$

with

$$H_0 = \sum_{\langle ij \rangle} c_i^\dagger c_j + h.c.$$

The previous Hamiltonian can be computed for $\Delta_0 = 0.2$ as

```
from pyqula import geometry
g = geometry.triangular_lattice() # geometry of the 2D model
h = g.get_hamiltonian() # generate the Hamiltonian
h.add_swave(0.2) # add s-wave superconductivity
(k,e) = h.get_bands() # compute band structure
```

Note that due to the BdG nature of the Hamiltonian, the bandstructure shows both the electron and hole states