Aalto-yliopisto
Perustieteiden korkeakoulu

Machine learning for unconventional superconductivity (topic presentation)

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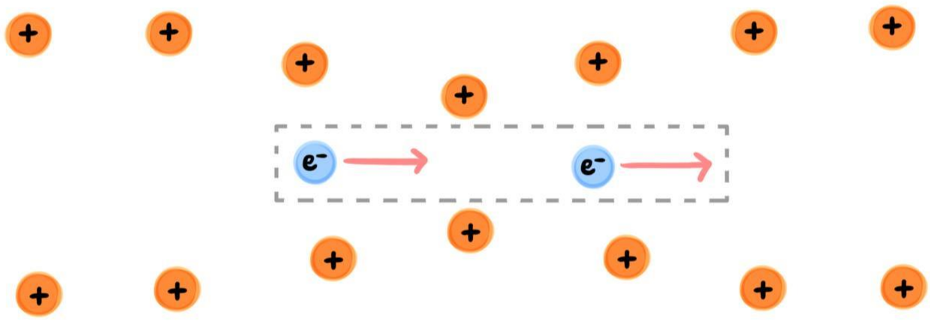
Systeemianalyysin laboratorio

Background: Superconductivity

- Superconducting can happen when electrons pass through the lattice of a metal
  - The vibrations of ions in a lattice cause an **attractive interaction** between electrons
  - Vibrations are waves, and quanta of these vibrations are quasi-particles
    - Conventional superconducting: phonons
    - **Unconventional superconducting**: phonons or other quasi-particles

- A superconducting state is described through **Cooper pairs**
  - The attractive interaction between electrons causes a paired state of electrons to have energy lower than the Fermi energy
    $\rightarrow$ bound state of a pair of electrons



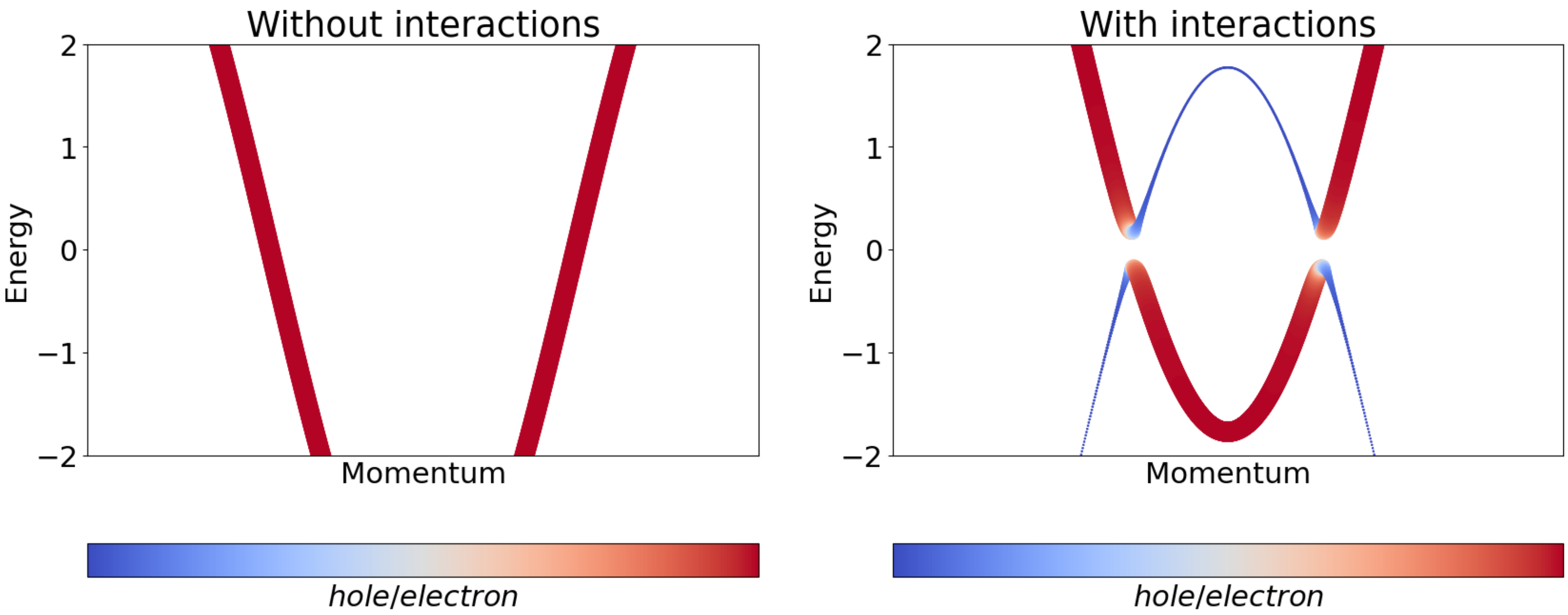
Background: Measuring Superconductivity

- Superconducting states are described by $\langle c_{\uparrow i}^{\dagger} c_{\downarrow i}^{\dagger} \rangle = f(k)$ where
  - $f(k)$ is a pairing between particles
  - $c_{\uparrow i}^{\dagger}$ and $c_{\downarrow i}^{\dagger}$ are creation operators, that create a pair of electrons with opposite spins at the same location
  - $\langle c_{\uparrow i}^{\dagger} c_{\downarrow i}^{\dagger} \rangle$ is the expectation value of a Cooper pair at site i

$\rightarrow$ cannot be directly measured

- Materials can be imaged at the atomic level by using scanning tunnelling microscopy (STM)
  - Differential conductance dI/dV can be obtained
  - This reveals the electronic structure, but the nature of the pairing mechanism is very hard to see

Background: gap formation



Background: Mathematical representation

- Superconducting states represented with Hamiltonians (total energy operators):

$$H = \sum_{ij} t_{ij}(c_{i\uparrow}^{\dagger}c_{j\uparrow} + c_{i\downarrow}^{\dagger}c_{j\downarrow}) + \sum_{i} U c_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow} \quad ; \quad U < 0$$

- Four fermion model is not solvable
  - approximated using two fermions:

$$H \approx \sum_{ij} t_{ij}(c_{i\uparrow}^{\dagger}c_{j\uparrow} + c_{i\downarrow}^{\dagger}c_{j\downarrow}) + \sum_{i} \langle c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}\rangle c_{i\uparrow}c_{i\downarrow} + h.c.$$

Where $\Delta = \langle c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}\rangle$ is the superconducting order

- t_{ij} represents hopping between sites i and j, i.e. the kinetic energy gained or lost
- U is the interaction term, U<0 for superconductivity

Goals & scope

- Creating a machine learning algorithm for recognising unconventional superconductivity from real space conductance

- Comparing different types of superconducting with different pairing mechanisms
- Seeing how these affect real space conductance

Methods and tools

- Simulating data with the pyqula-Python library
- Building ML models using Keras

Schedule

- **Feb.-March**: Getting familiar with the topic
- **20.03.2024**: Topic presentation
- **March-April**: Building ML implementation and analyzing results
- **May**: Finishing the thesis

References

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- V. P. Mineev, K. V. Samokhin (1999). ”Introduction to Unconventional Superconductivity”, Gordon and Breach Science Publishers
- Bruus, H. & Flensberg, K. (2002). ” Introduction to many-body quantum theory in condensed matter physics”.