The Abdus Salam International Centre for Theoretical Physics

School in Computational Condensed Matter Physics: From Atomistic Simulations to Universal Model Hamiltonians

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Trieste, Italy

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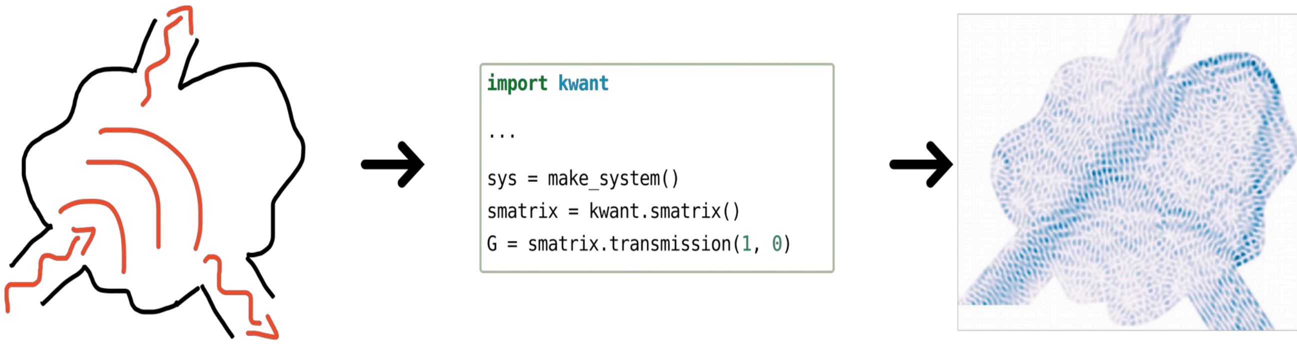
NUMERICAL QUANTUM TRANSPORT

1. **Introduction to numerics for quantum transport**
   - What is quantum transport? What are nanostructures or mesoscopic systems?
   - Open quantum systems: scattering wave function
   - Conductance, Landauer formula, scattering matrix
   - Tight-binding models, finite difference methods, graphs and matrices
   - Band structure
   - Numerics: super-large sparse linear systems, nonlinear eigenvalue equations (sounds complicated, but is surprisingly simple!)
   - Survey of prominent quantum transport phenomena that you can compute in the hands-on tutorial

2. **Hands-on tutorial using python and kwant**
   - Super-brief introduction to scientific computing with python
   - Defining tight-binding systems in kwant, play with complicated geometries and Hamiltonians
   - Computing scattering wave functions and the conductance
   - Projects in groups/pairs/own your own: simulate prominent examples such as quantum point contacts, quantum billiards or quantum Hall effect. For those who already know more about these topics, there will also be more advanced projects on topological insulators, spin physics, …

When you make condensed matter systems very small and very cold, quantum effects start to dominate. In order to do experiments, you need to probe these nanostructures from the outside and hence one deals with open quantum systems[1]. A particularly prominent experimental probe is to pass a current through the nanostructure – this is the realm of quantum transport.

In this course you will learn basics about quantum transport phenomena in nanostructures, and how to efficiently simulate them on a computer. In the hands-on session you will learn to use python and kwant to this end, and be able to do first simulations yourself.



In this course, you will learn basics about quantum transport (left), how to do numerical simulations (middle), and compute physical properties such as the conductance of a nanostructure (right).

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1 This course will, in contrast to many other lectures in Trieste, only deal with non-interacting systems. In open systems interactions can in the majority of cases be neglected.