Quantum Transport Simulations with Tight-Binding Models

Hamiltonian : A mathematical desc. of the total energy of a system
↳ KE + PE

very important - allows us to solve the Shrodinger eqn.

Shrodinger eqn. : calculates how the system will evolve or change in time.
↑ basically tells us everything useful we would like to know

Now:

What is the Tight-Binding Model (TBM)?

→ It's an approximation
→ Used in solid state physics,
→ To describe how electrons move in a material

Assumptions of the TBM :

(like atoms in a lattice)

1.) Electrons are tightly bound to atomic sites
2.) Electrons can hop to neighboring states w/ a probability determined by a param, "<u>hopping amplitude</u>" (t).
3.) Each site has an <u>on-site</u> <u>potential</u> that represents the energy of an electron at that site

1D tight-binding Hamiltonian:

$$H = \sum_i \varepsilon_i \overbrace{c_i^\dagger c_i}^{\text{Number Operator}} + \sum_{\langle i,j \rangle} t_{ij} \overbrace{c_i^\dagger c_j}^{\text{Hopping Term}}$$

$\varepsilon_i c_i^\dagger c_i$ represents the on-site energy of an e^- at site i

$t_{ij} c_i^\dagger c_j$ represents the hopping term, which allows an e^- to move between neighboring sites i and j

Where:

→ $c_i^\dagger$ and c_i are $\boxed{\text{creation}}$ and $\boxed{\text{annihilation}}$ operators for electrons at site i.

→ ε_i is the on-site energy (potential E @ site i)

→ t_{ij} is the hopping amplitude btw sites i and j

An Aside on Creation and Annihilation Operators:

→ These operators describe how particles (like e^-s) are added or removed from a quantum system

$\boxed{\text{Creation Operator } c_i^\dagger}$ → Adds a particle (e^-) to site i

$\boxed{\text{Annihilation Operator } c_i}$ → Removes a particle (e^-) from site i

Mathematically, they act on quantum states in the following way:

$$c_i^\dagger |0\rangle = |1\rangle$$

$$c_i |1\rangle = |0\rangle$$

where: $|0\rangle$ = No e^- at site i

$|1\rangle$ = An electron is present at site i

These ops. obey the anti-commutation relations (due to Pauli Exclusion Principle):

$$\{c_i, c_i^\dagger\} = c_i c_i^\dagger + c_j^\dagger c_i = \delta_{ij}$$

$$\{c_j, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0$$

which enforce fermionic behavior (e^-s are fermions and obey the Pauli Exclusion Principle, meaning two e^-s cannot occupy the same quantum state.

Breaking Down the Hamiltonian:

→ $c_i^\dagger c_i$ (Number Operator)

- Counts whether there is an e^- at site i
- If there is an e^- at site i, the system has energy ε_i

→ $c_i^\dagger c_j$ (Hopping Term)

- Moves an e^- from site j to site i
- The hopping amplitude $\boxed{t_{ij}}$ determines how strongly e^-s move between sites.

Physical Meaning of the TBM

→ Imagine an array of atoms where e^-s can hop between neighboring sites.

* site 1 — site 2 — site 3 — site 4 ...

→ if $t_{ij} = 0$, e^-s are localized at their sites

→ if $t_{ij} \neq 0$, e^-s can spread out and move b/w sites

- The energy spectrum of this system depends on the hopping strength and boundary conditions

⇒ In our 1D TBM, the <u>leads</u> allows e^-s to enter and exit the system, enabling quantum transport

$\boxed{\text{Apparatus of 1D Tight Binding Chain}}$

* Left Lead → Scattering Region → Right Lead

(Electron Source) — injects e^-s into system

(Finite Chain of atomic sites) — where quantum effects (e.g., interference, tunneling) occur.

(Electron Drain) — allows e^-s to exit the system

* Leads are modeled as infinite conductors, providing a well defined boundary condition.

Overview: How does Quantum Transport Work in this System?

1.) An e^- wave enters the system from left lead

2.) This e^- propagates through finite chain

3.) Some part of the wave transmits through to the right lead, and some part reflects back.

→ The <u>conductance</u> (electron flow) is computed using the $\boxed{\text{Landauer}}$ formula:

$$G = \frac{2e^2}{h} T(E)$$

where $T(E)$ is the transmission probability at energy E

Now, let's add some disorder to our System.

↳ Anderson Localization

→ What is it??

- In a perfect system, e^-'s propagate freely through the lattice
- If we introduce random disorder (on-site potential variations), electron waves interfere <u>destructively</u>, leading to this localization effect.
- In 1D systems, even weak disorder can cause

localization, meaning e^-s stop propagating and conductance stops

- Expected results of adding disorder (remember, this is just on-site potential variations)
  - w/o disorder → conductance remains at $1.0\,e^2/h$
  - w disorder → sharp dips in conductance appears due to localized states
  - Stronger disorder → conductance may drop to 0 in some energy ranges

What happens if we add a magnetic field to a 2D version (lattice)?

→ Quantum Hall Effect (QHE)

↳ What is it?

- when you apply a magnetic field (B) ⊥ to a 2D material, e^-s move in cyclotron orbits instead of straight paths
- In a TBM, we introduce a magnetic phase factor ($\boxed{\text{Peierls phase}}$) to simulate the effect of a magnetic field.
- This breaks time-reversal symmetry and leads to the formation of $\boxed{\text{Landau levels}}$.

Edge states emerge, carrying current w/o backscattering definitions aside

"Peierls Phase" → refers to a phase factor introduced in condensed matter physics to account for the effect of a magnetic field on the hopping of electrons in a lattice

↳ essentially represents the additional phase an e^- acquires when moving through an magnetic field

"Landau Levels" are just the quantized energy levels of e^-s in a magnetic field.

Going back to QHE ... How do we implement a magnetic field in kwant?

→ Modify hopping term to introduce a magnetic phase using Peierls substitution:

$$\boxed{t_{ij} \rightarrow t_{ij} e^{i 2\pi \phi_{ij}}}$$

* where ϕ_{ij} is related to the magnetic flux per plaquette

- So ϕ represents the magnetic flux per unit cell
- $e^{i2\pi\phi}$ modifies the hopping term to introduce a phase shift

What to expect when adding the magnetic field

→ W/o a magnetic field $(\phi = 0)$ → conductance remains unchanged

→ w a magnetic field $(\phi > 0)$:

- Shifts in conductance plateaus (energy levels due to cyclotron orbits)
- Gaps where conductance drops (formation of Landau levels)
- Stronger fields lead to well-separated plateaus

Conductance will show plateaus at integer multiples of e^2/h

Now... what happens if we add disorder to this QHE system?

→ Two competing effects:

A. Landau Levels and Quantum Hall Plateaus

→ w/o disorder, e^-, form landau levels, leading to conductance plateaus

→ As disorder increases, localized states appear b/w landau levels.

B. Anderson Localization

→ Weak disorder → quantum hall plateaus remain intact

→ Strong disorder → States b/w landau levels become localized, meaning e^-s become trapped instead of conducting

→ very strong disorder → localization dominates, and the QHE breaks down

So: by gradually increasing disorder strength, we can observe the transition from quantum hall transport to localized insulating behavior.

Expected Results:

Disorder Strength = 0.0

→ Sharp conductance plateaus at integer multiples of e^2/h

Weak Disorder ~1.0

→ slight rounding of plateaus, but QHE remains intact

Moderate Disorder ~2.0

→ Some conductance dips appear due to localized states

Strong disorder > 3.0

→ Conductance breaks down, as all states become localized

→ quantum hall plateaus disappear, and the system becomes more like an insulator

Lets Compare the Hamiltonians for the 1D and 2D TBMs

1D:

w/o magnetic phase factor

$$\boxed{H = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{(i,j)} t_{ij} c_i^\dagger c_j}$$

- where ε_i is on-site energy at sit i
- $c_i^\dagger$, c_i are creation / annihilation operators for e^-'s at site i
- t_{ij} is the hopping amplitude btw neighboring sites

- So system consists of single row sites
- Electrons only hop left or right (nearest-neighbor hopping)
- Dispersion relation:

$$E(k) = \varepsilon - 2t \cos(k)$$

- The bandwidth is $4t$ (since energy varies from $-2t$ to $2t$)

2D : Allow hopping in both x and y directions

$$\boxed{H = \sum_{x,y} \varepsilon_{x,y} C^{\dagger}_{x,y} C_{xy} + \sum_{(x',y')} t_{x',y'} e^{i\phi_{x',y'}} C^{\dagger}_{x',y'} C_{x,y}}$$

Where :

- $\varepsilon_{x,y}$ is the on-site energy at each site (x,y)
- $C^{\dagger}_{x,y}$, $C_{x,y}$ are creation / annihilation
- hopping now occurs in x and y directions
- A magnetic phase factor $e^{i\phi}$ is introduced in the y-direction to simulate magne tic field.

So :

- e^-s now hop in both x and y directions
- Peierls phase $e^{i\phi}$ modifies hopping in the y direction (introducing the cyclotron motion in a magnetic field)
- Dispersion relation is more complex bc of Landau Levels :

$$E(k_x, k_y) = \varepsilon - 2t(\cos k_x + \cos k_y)$$

- The magnetic field quantizes the energy into landau levels which are missing in 1D .

Next Step in Experimentation:

$$\boxed{\text{Compute the energy spectrum to observe Landau quantization}}$$

$$\boxed{\text{Extend the system to a honeycomb lattice} \rightarrow \text{Graphene QHE}}$$