Introduction to TranSIESTA

Simulating voltage in SIESTA

Pol Febrer (EPFL), SIESTA advanced workshop 2025

INTRODUCTION TO TRANSIESTA: One talk, four questions

QUESTION 1. What is TranSIESTA?

QUESTION 2. Why do we need TranSIESTA?

QUESTION 3. How does TranSIESTA work?

QUESTION 4. How does TranSIESTA integrate with SIESTA?

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Differences between SIESTA and TranSIESTA

…as illustrated by AI

Q1. WHAT IS TRANSIESTA? — AI illustrations

Here are some SIESTA logos proposed by AI…

Q1. WHAT IS TRANSIESTA? — AI illustrations

…and here is the same AI proposing TranSIESTA logos.

Q1. WHAT IS TRANSIESTA? — The simple answer

TranSIESTA is:

SIESTA
ELECTRODES APPLY VOLTAGE

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A method to do voltage calculations in SIESTA.

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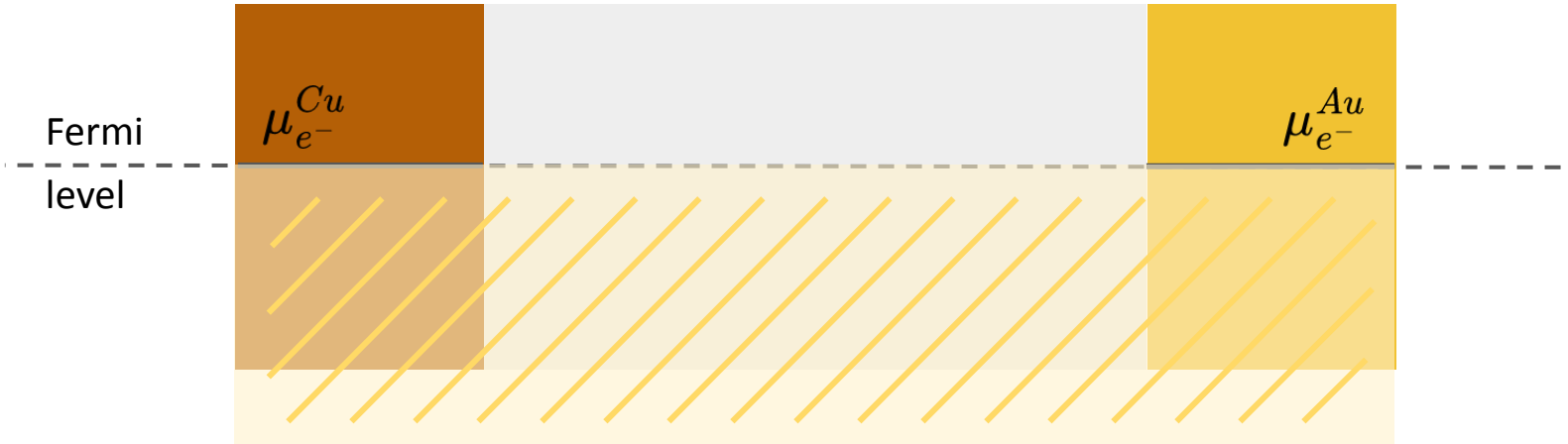
Q2. WHY DO WE NEED TRANSIESTA? — The complexity of applying voltage

In the most common DFT simulations,
we **fill states up until the Fermi Level**.



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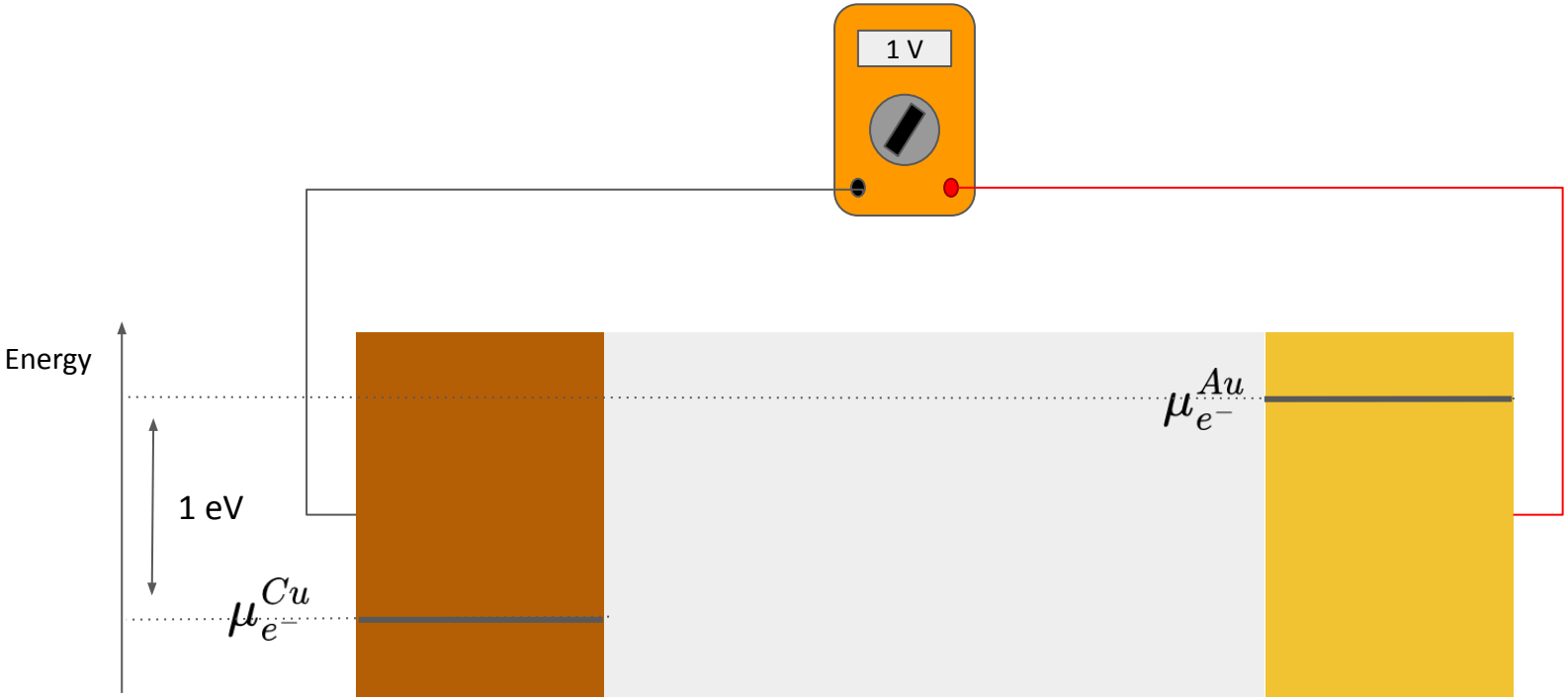

When you apply voltage, you create a **difference in fermi levels**.

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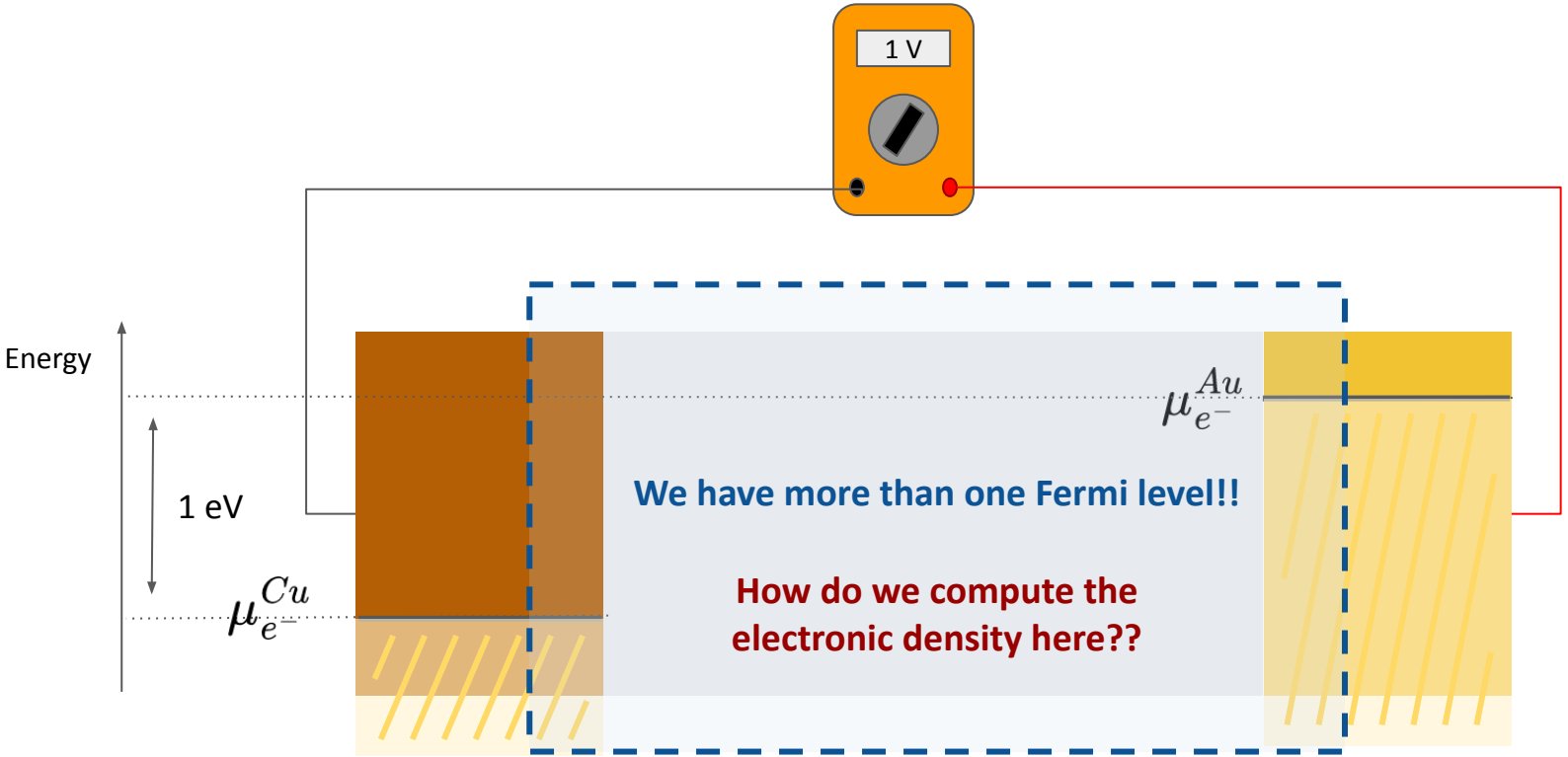

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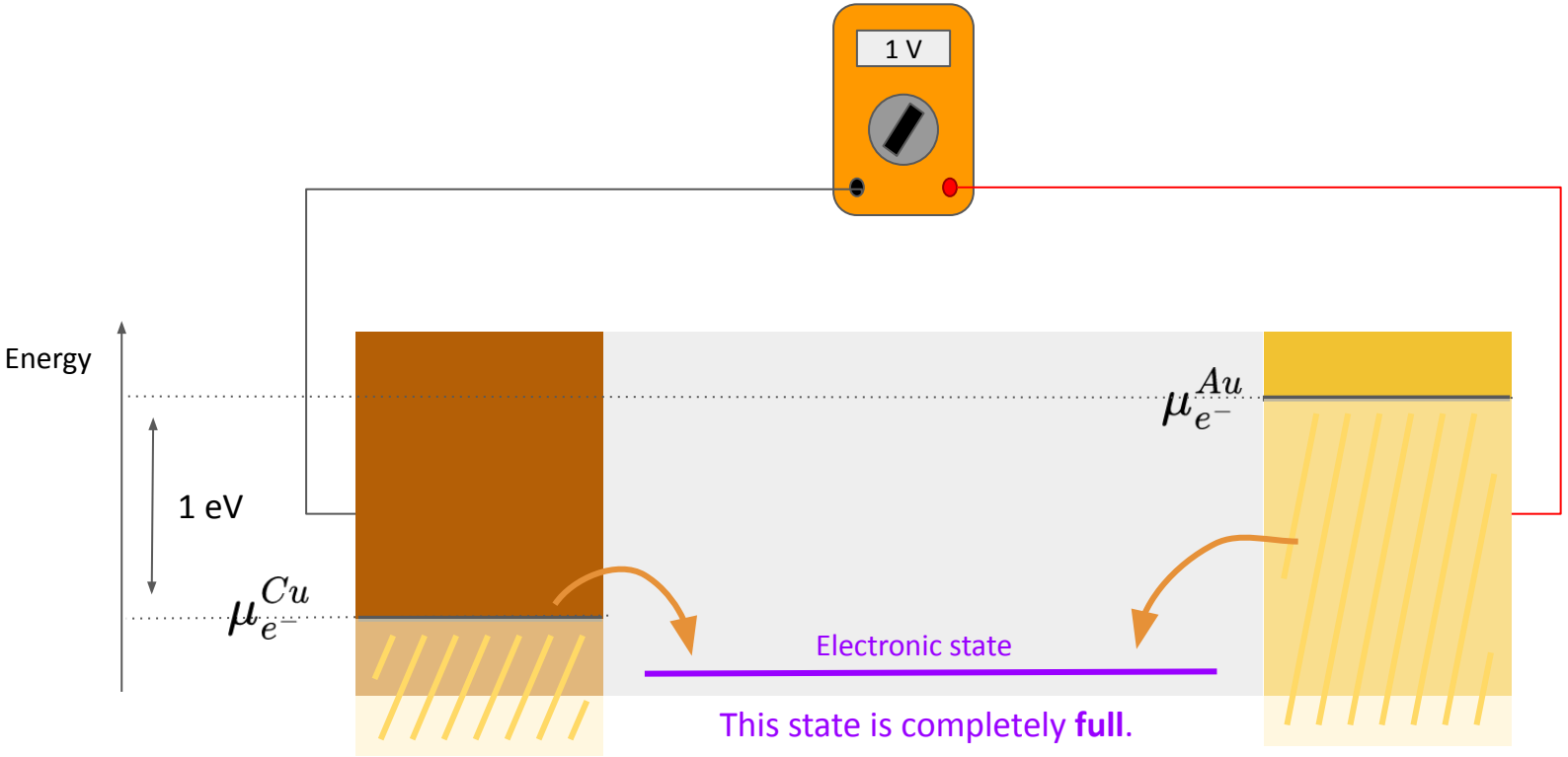

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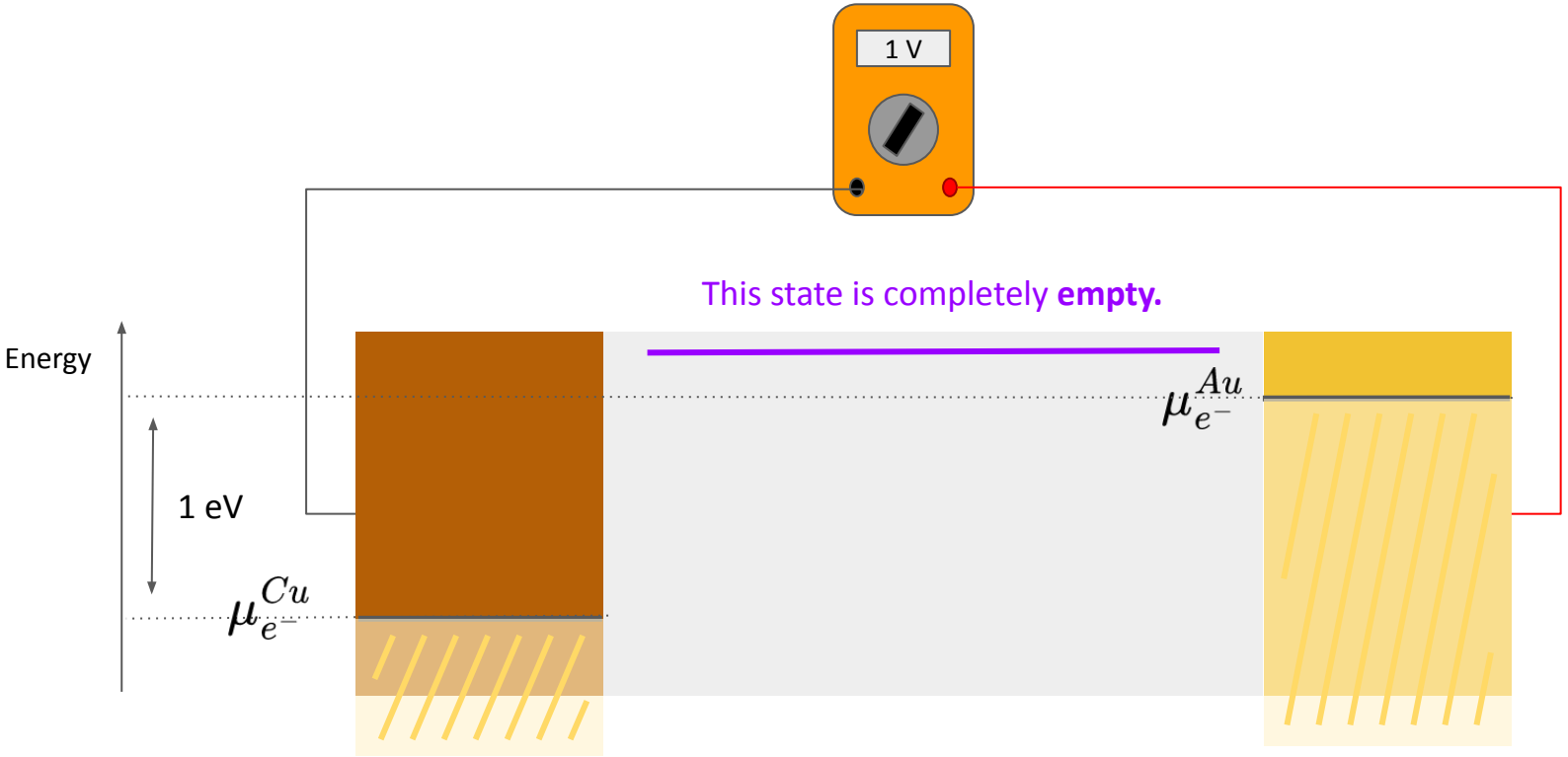

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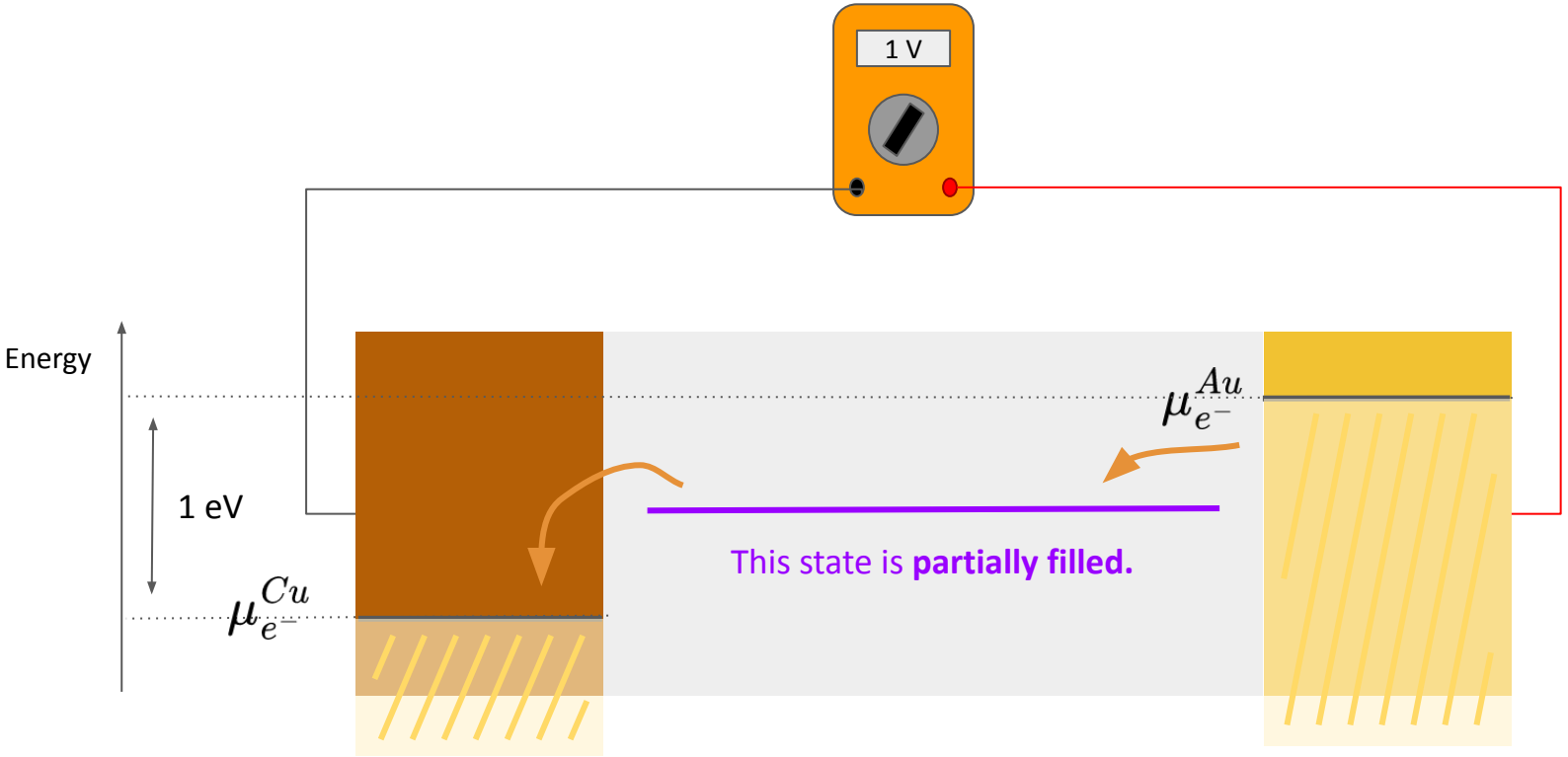
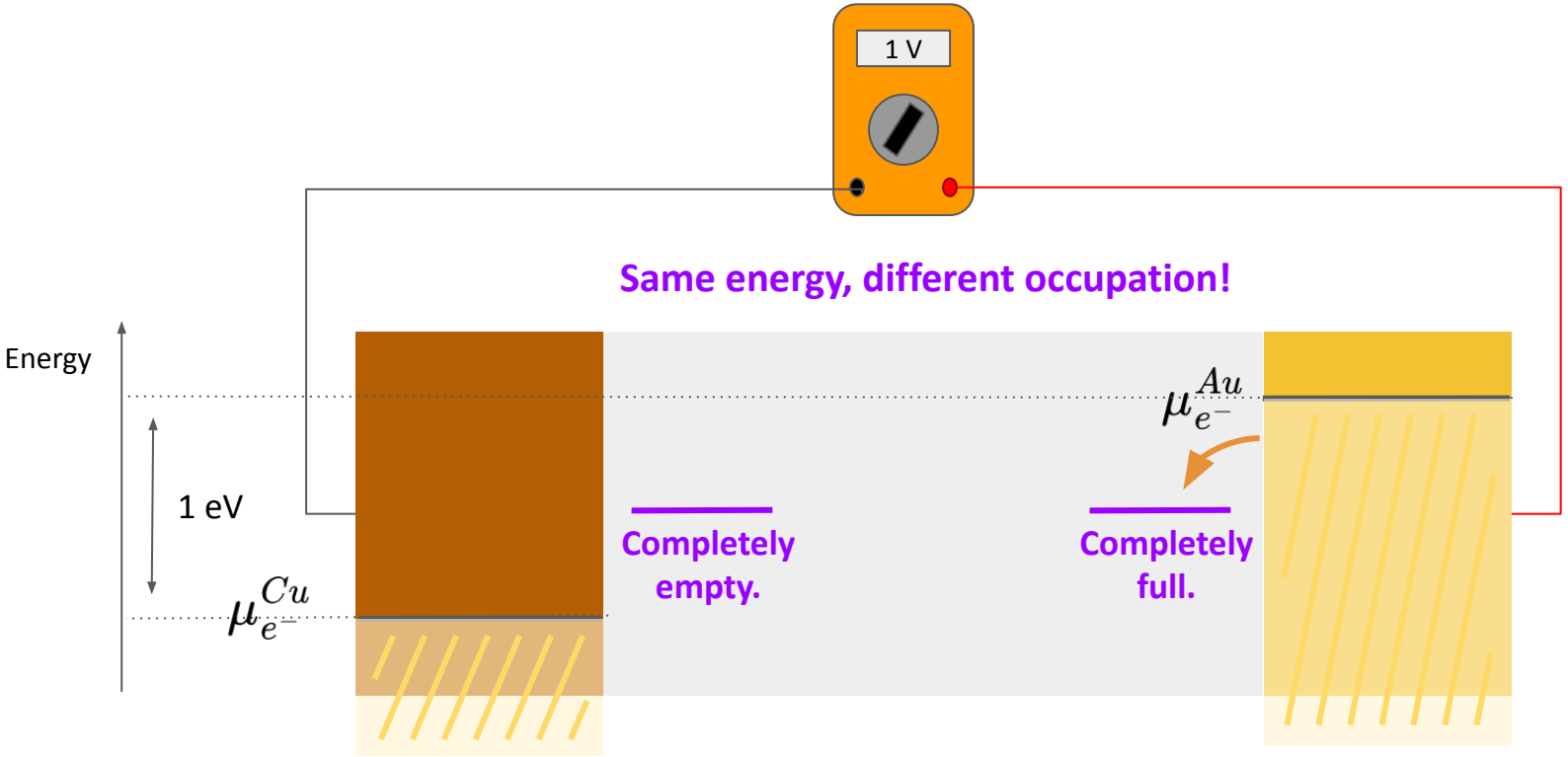


The occupation depends on
how connected is the state to each electrode.

Q2. WHY DO WE NEED TRANSIESTA? — The complexity of applying voltage



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INTRODUCTION TO TRANSIESTA: One talk, four questions

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A method to do voltage calculations in SIESTA.

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Because we need special methods to occupy states if there are multiple Fermi levels.

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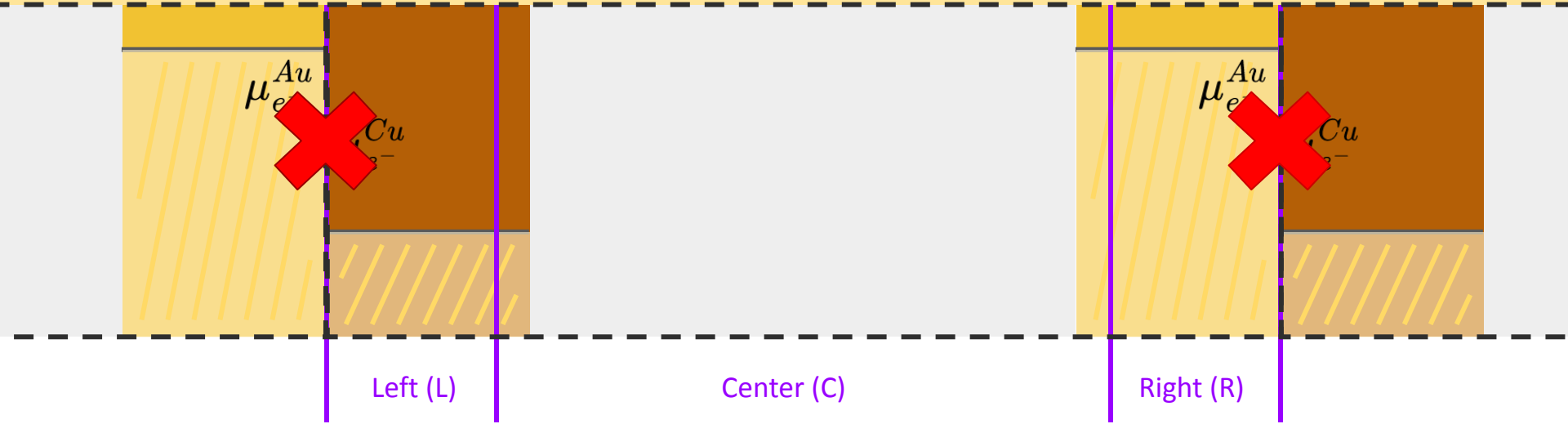
Q3. HOW DOES TRANSIESTA WORK? — Boundary conditions



Periodic boundary conditions have **catastrophic consequences!**

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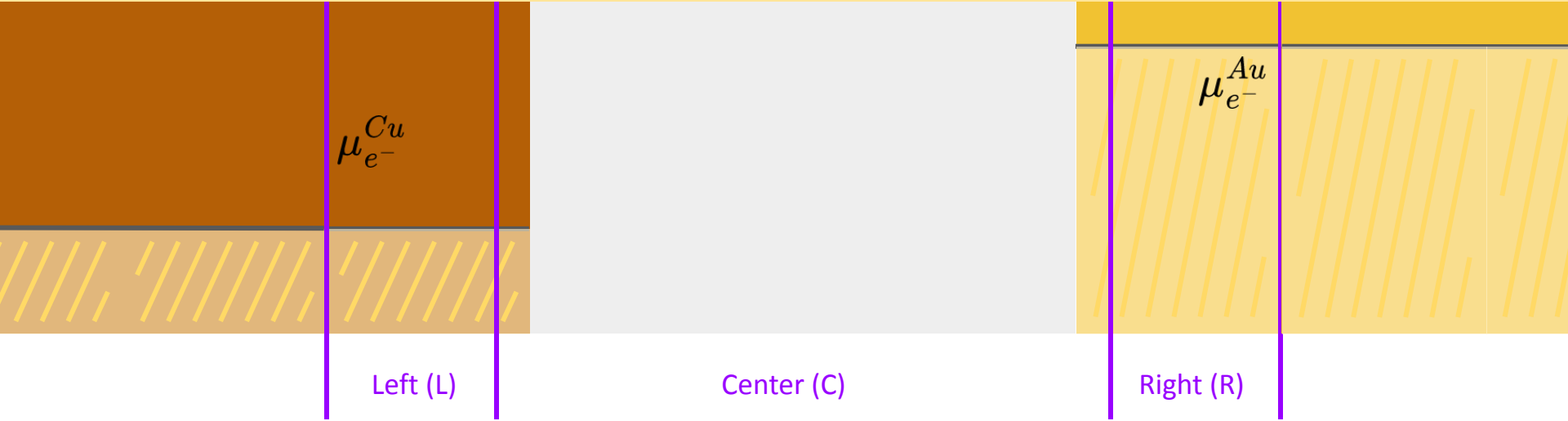

Periodic boundary conditions

Semi-infinite electrodes

We must use semi-infinite electrodes.

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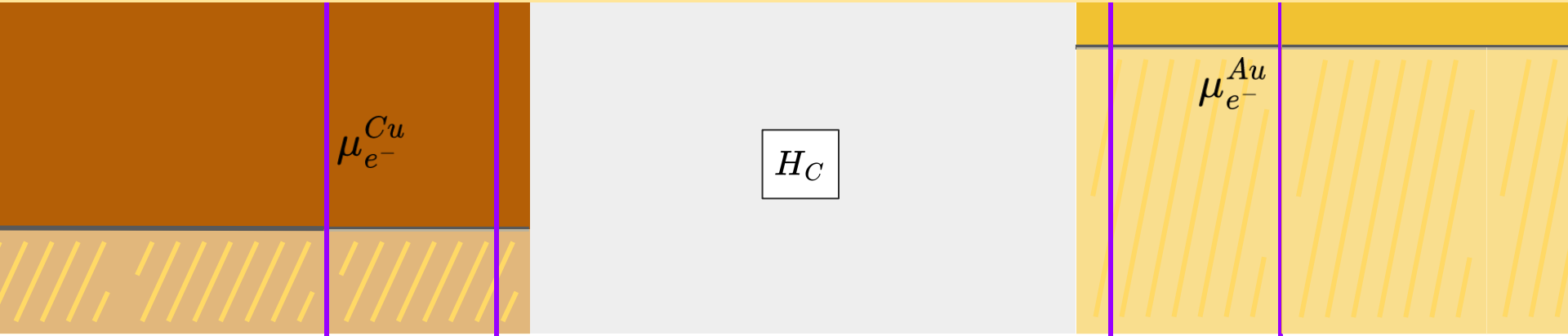

$$H = \begin{bmatrix} \dots & \dots & 0 & 0 & 0 \\ \dots & H_L & V_L & 0 & 0 \\ 0 & V_L^\dagger & H_C & V_R & 0 \\ 0 & 0 & V_R^\dagger & H_R & \dots \\ 0 & 0 & 0 & \dots & \dots \end{bmatrix}$$

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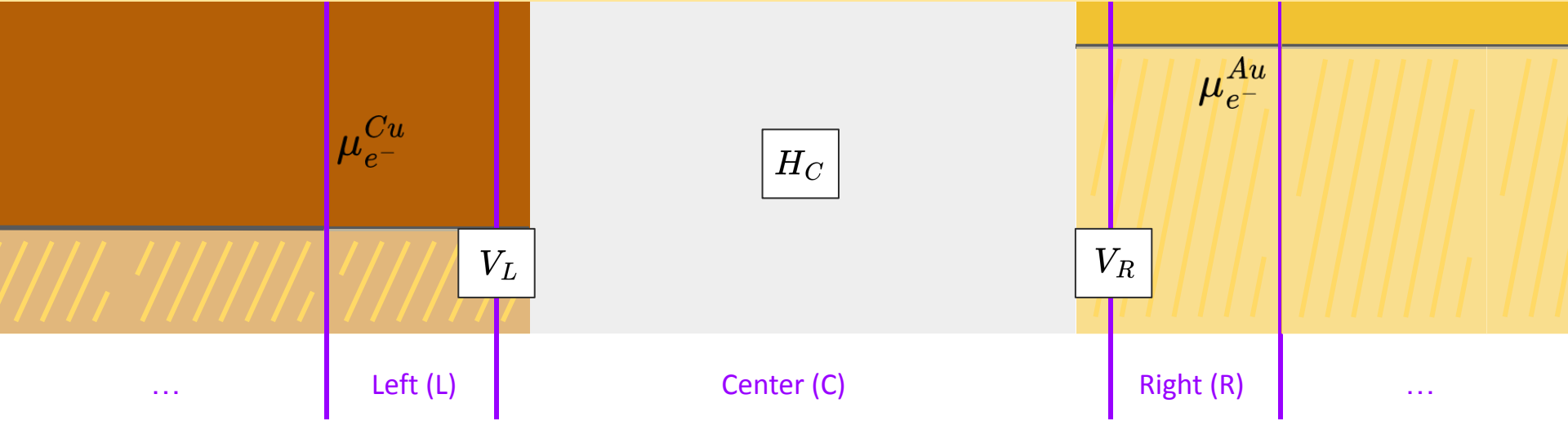

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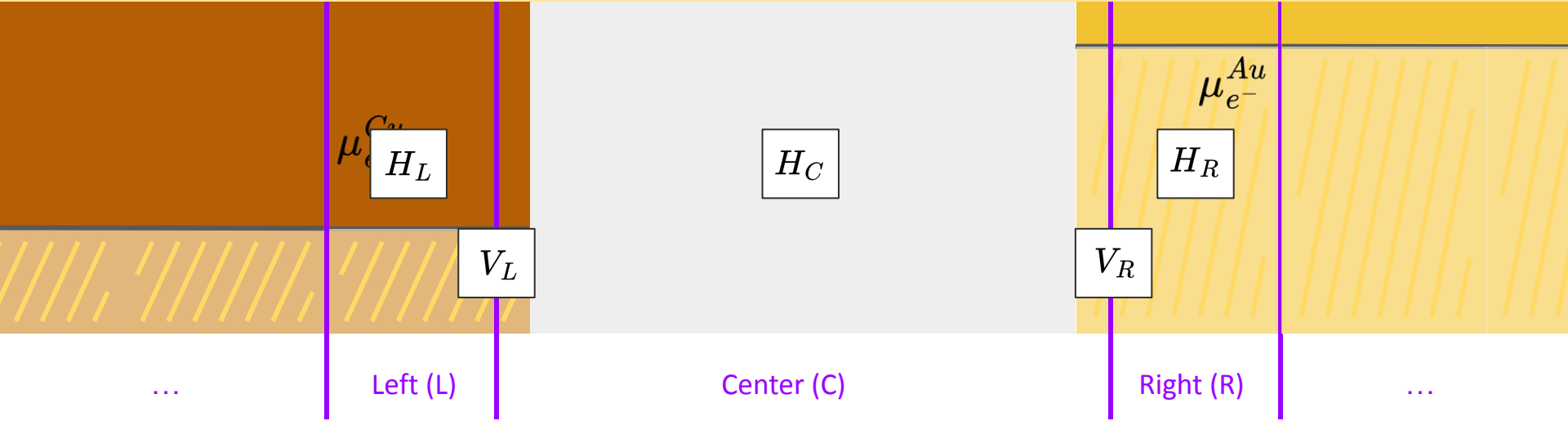

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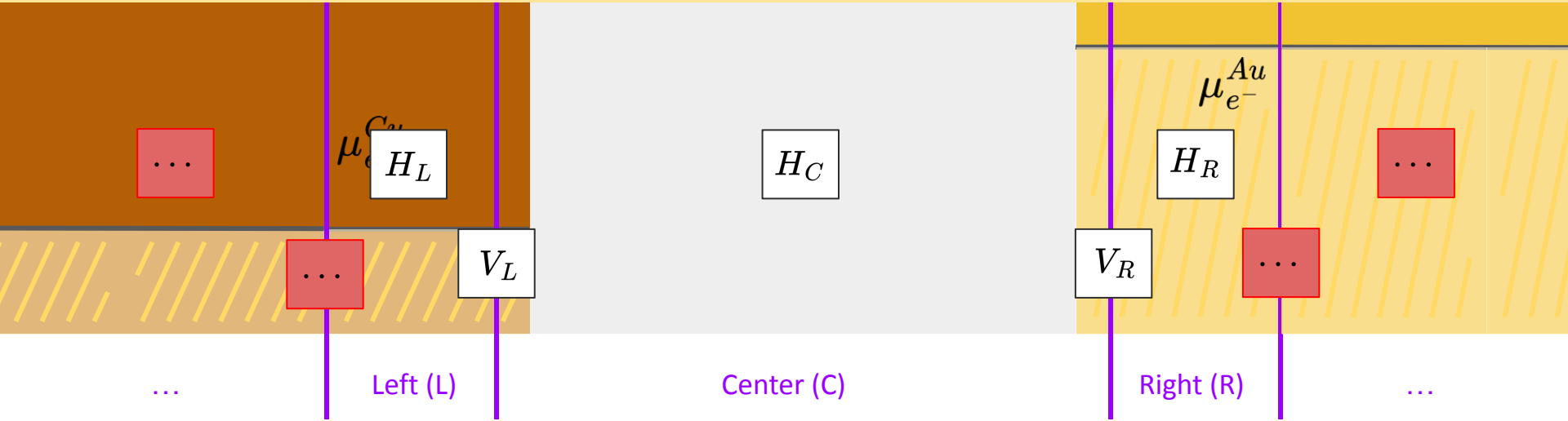

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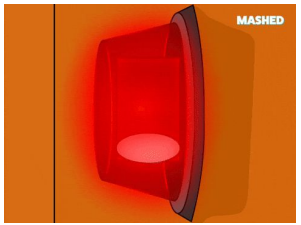
Infinite Hamiltonian alert!



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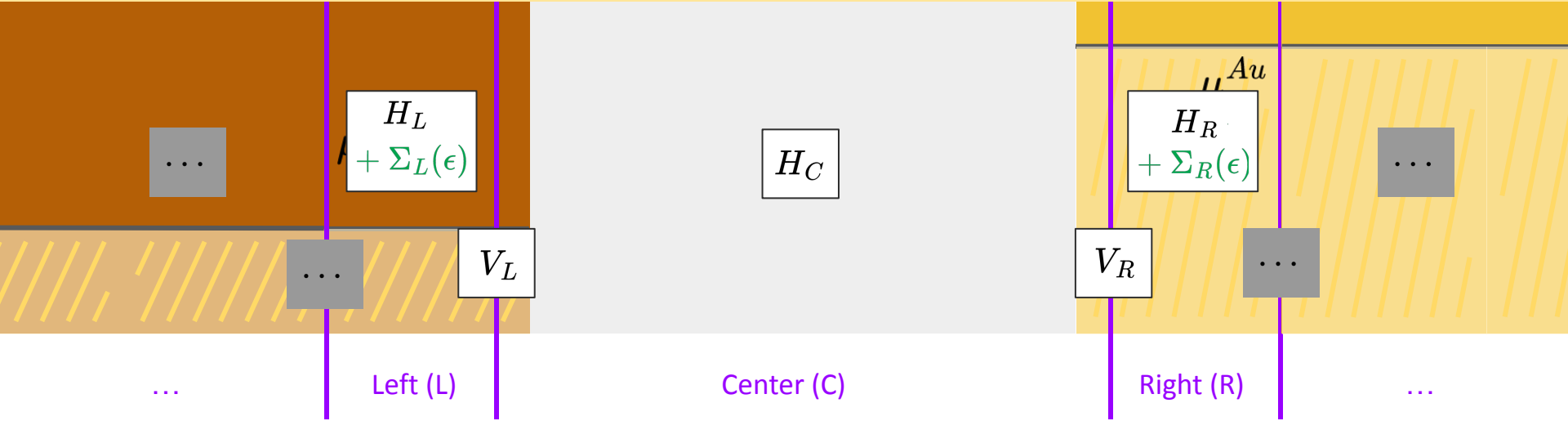

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Self-energies account for the effect of the rest of the electrode.

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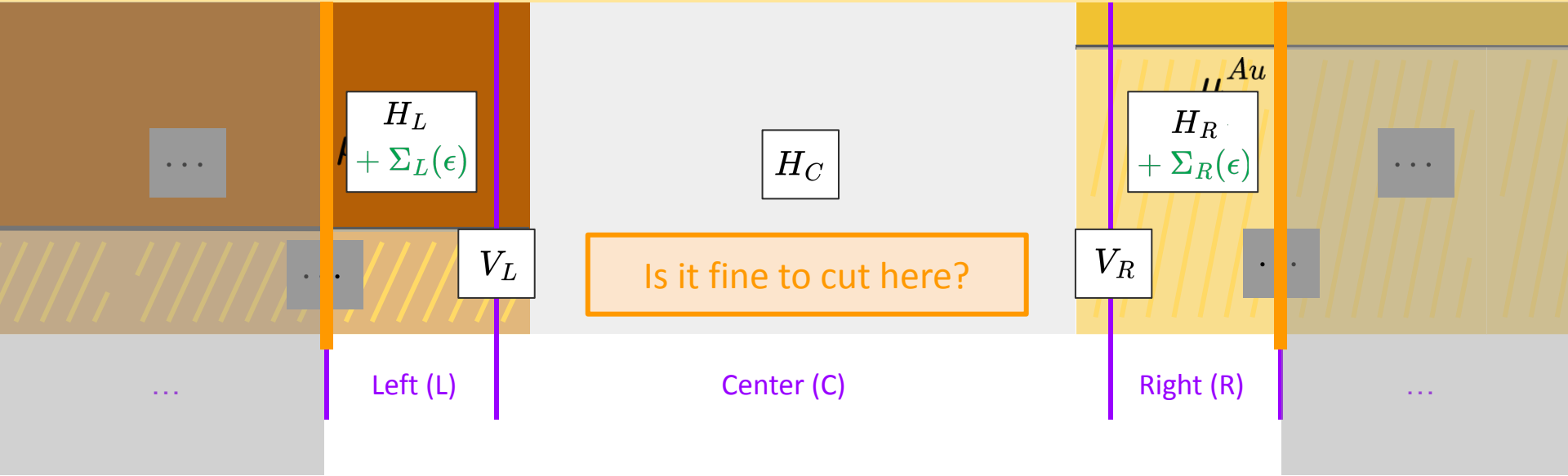

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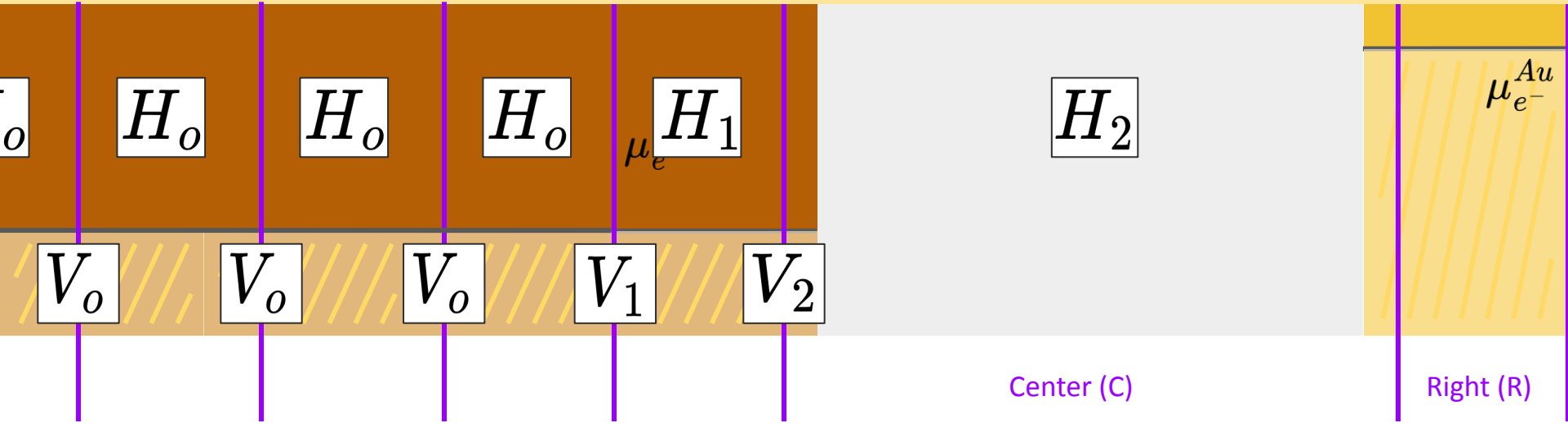

The system needs to be cut at a place where the coupling (V) is still the bulk one.

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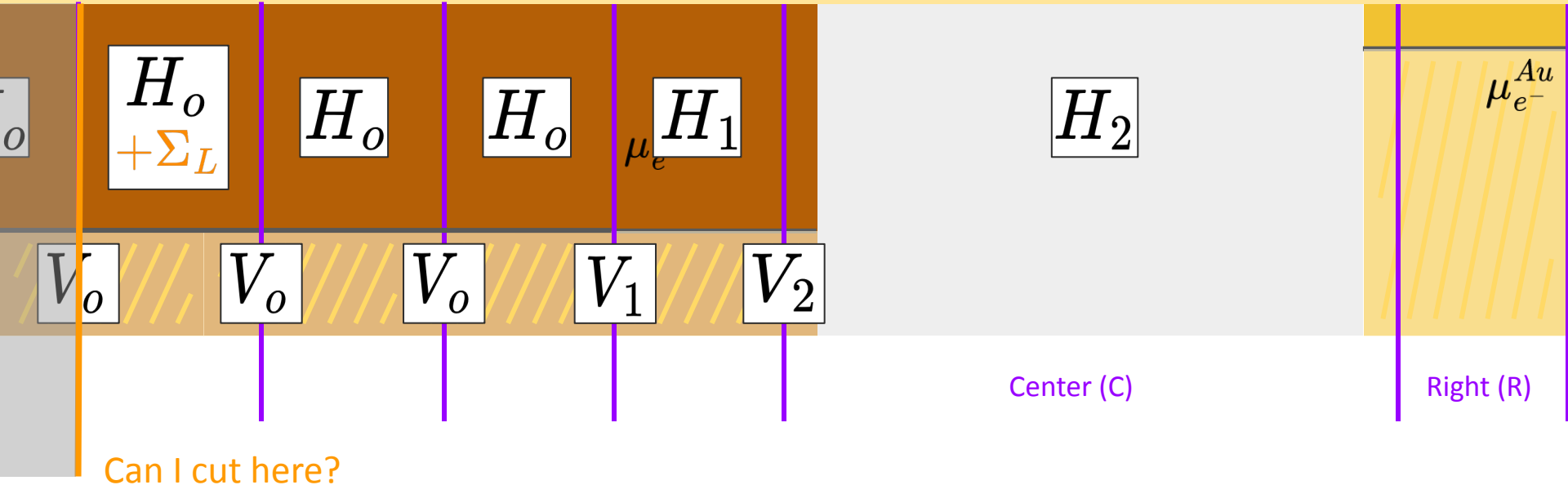

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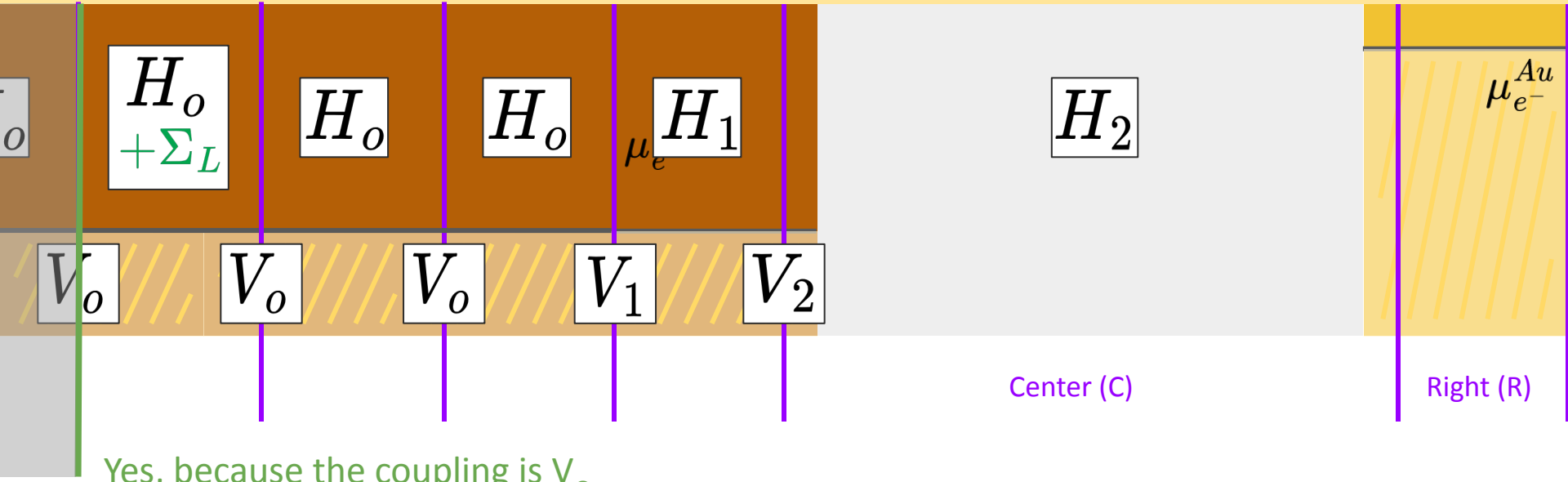

Yes, because the coupling is V_o

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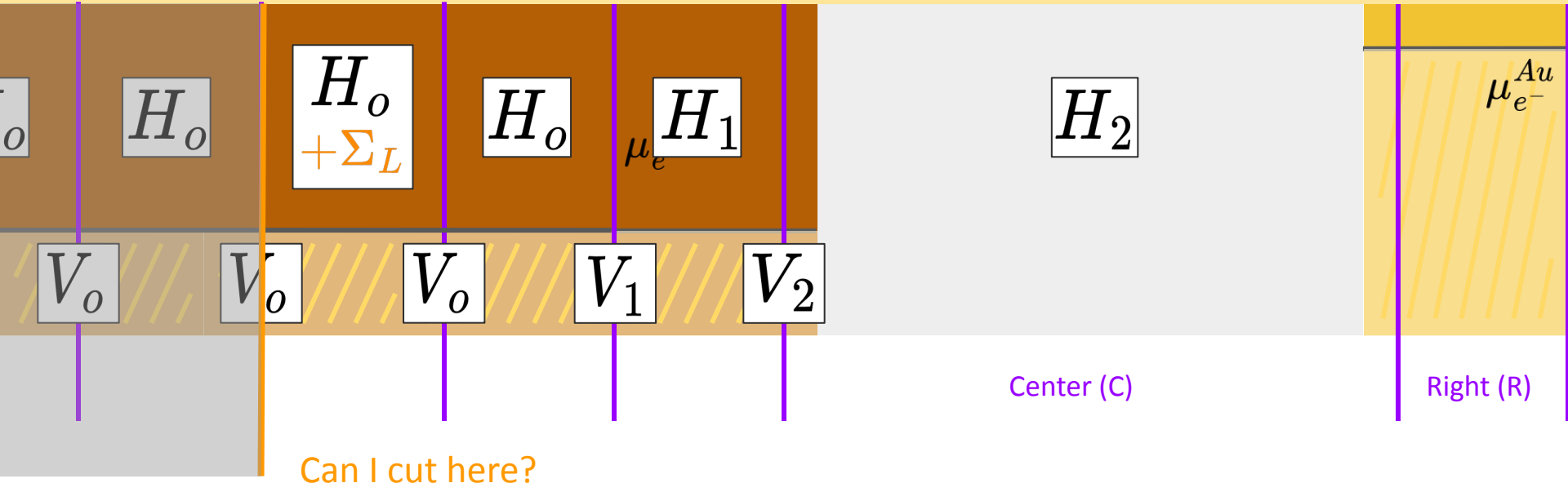

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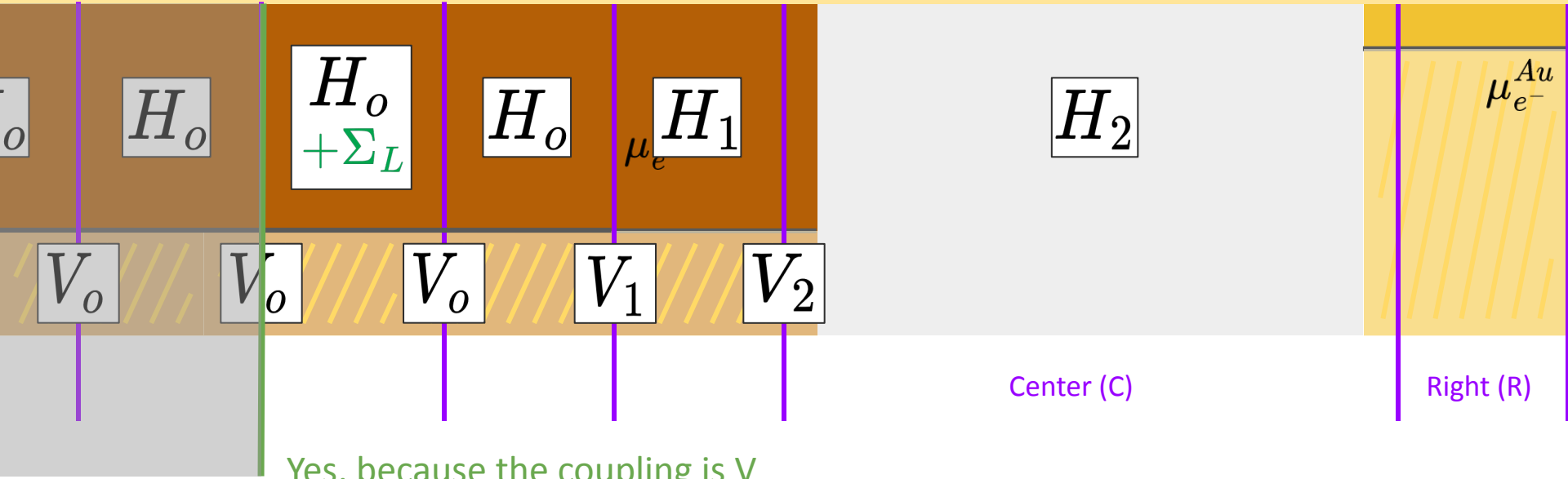

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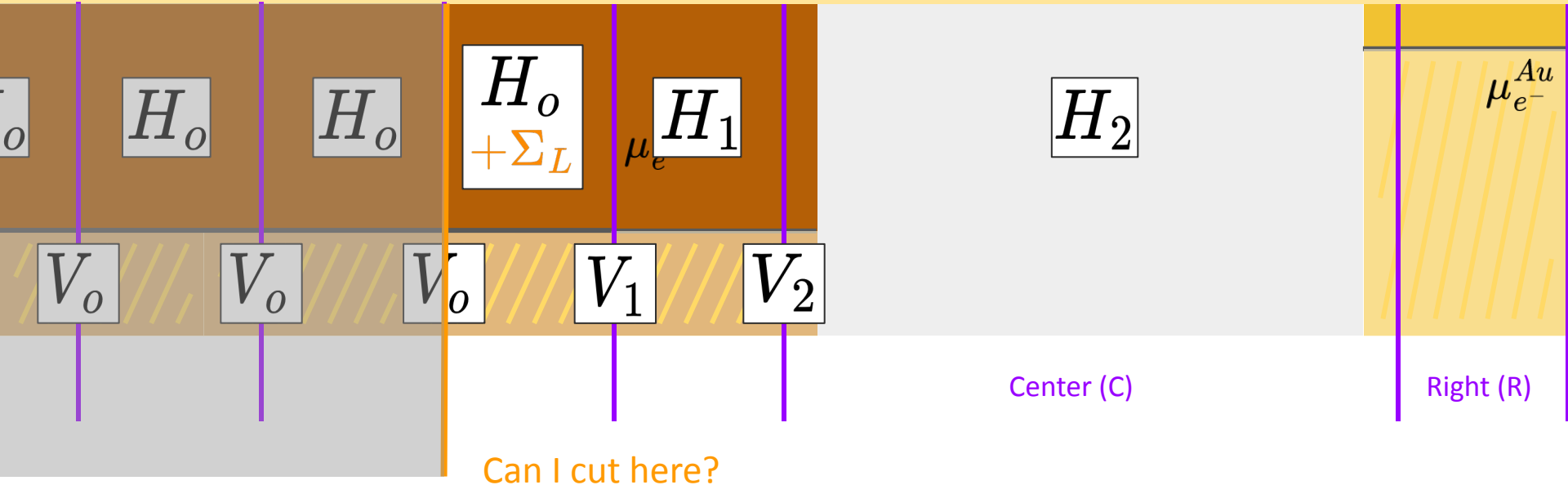

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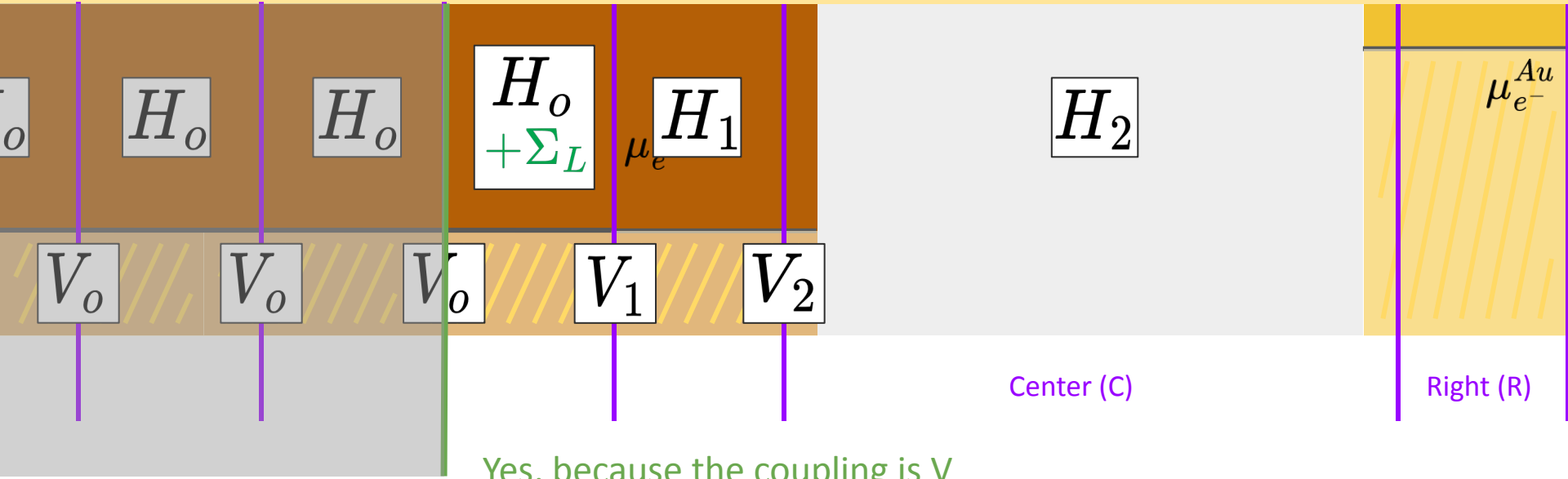

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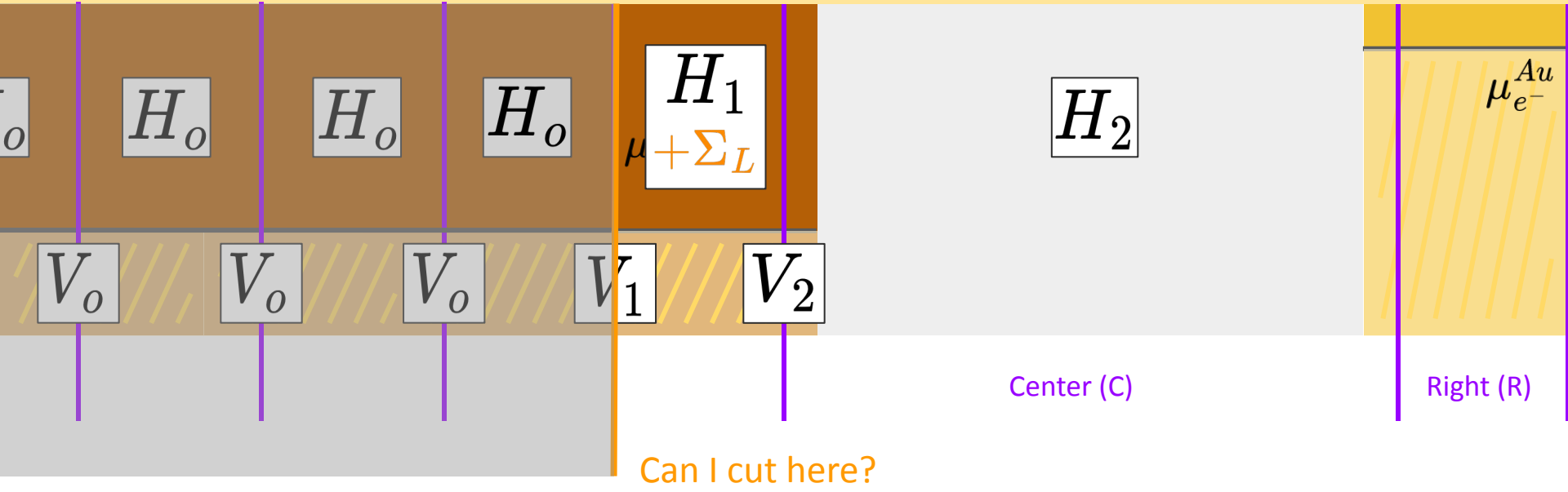

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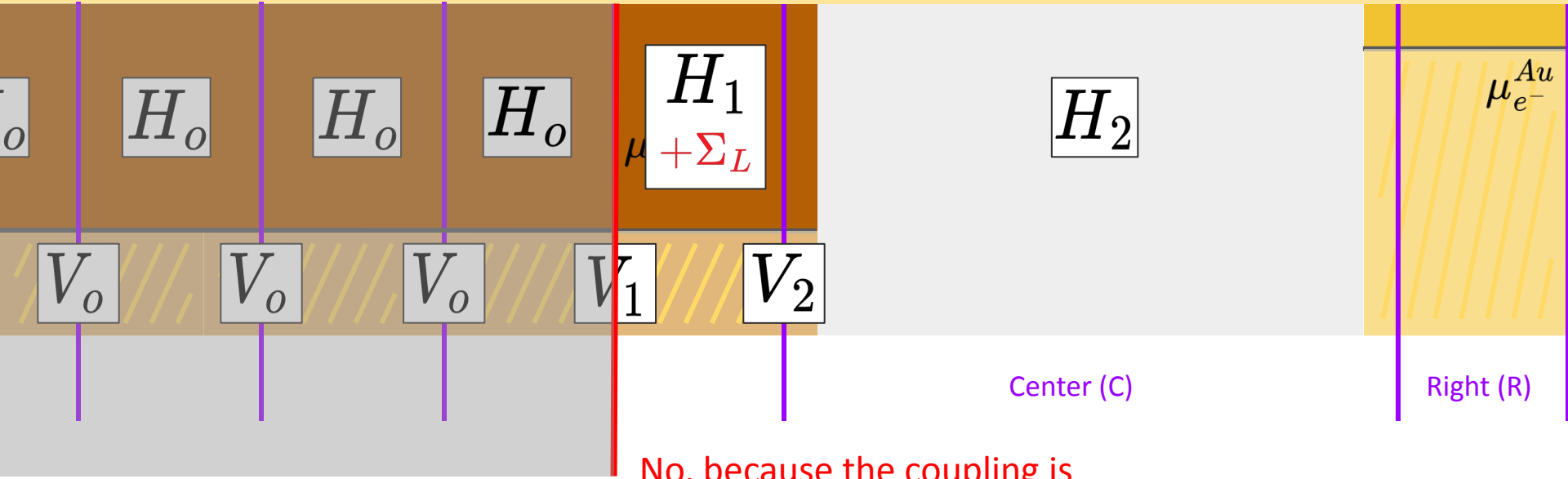

No, because the coupling is not the bulk coupling!!

The system needs to be cut at a place where the coupling (V) is still the bulk one.

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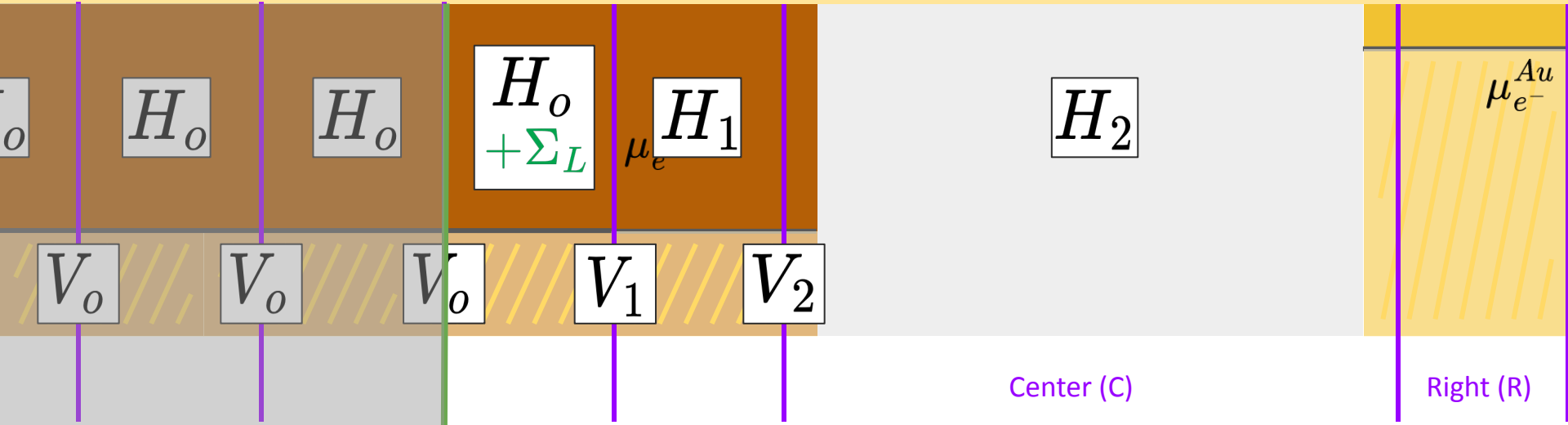


I will choose to cut here, because it gives me the **smallest system that is correct.**

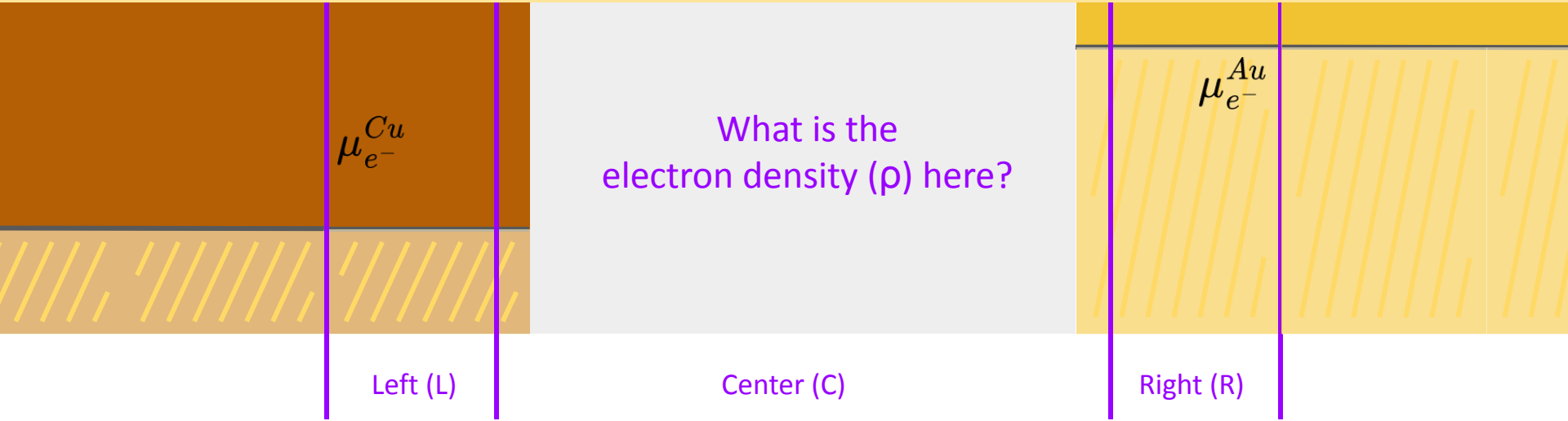
The system needs to be cut at a place where the coupling (V) is still the bulk one.

NON-EQUILIBRIUM GREEN'S FUNCTIONS

The theory behind TranSIESTA.

NOTE: I will be intentionally sloppy in some equations to prioritize conceptual understanding.
For a fully formally correct derivation see:
Mads Brandbyge et al., Phys Rev B (March 2002)
Nick Papior et al. Computer Physics Communications 212 (2017)

Q3. HOW DOES TRANSIESTA WORK? — The scattering states approach



The goal is to **split the density** of the central (C) region into contributions from the left (L) and right (R).

$$\rho_C = \rho_L + \rho_R$$

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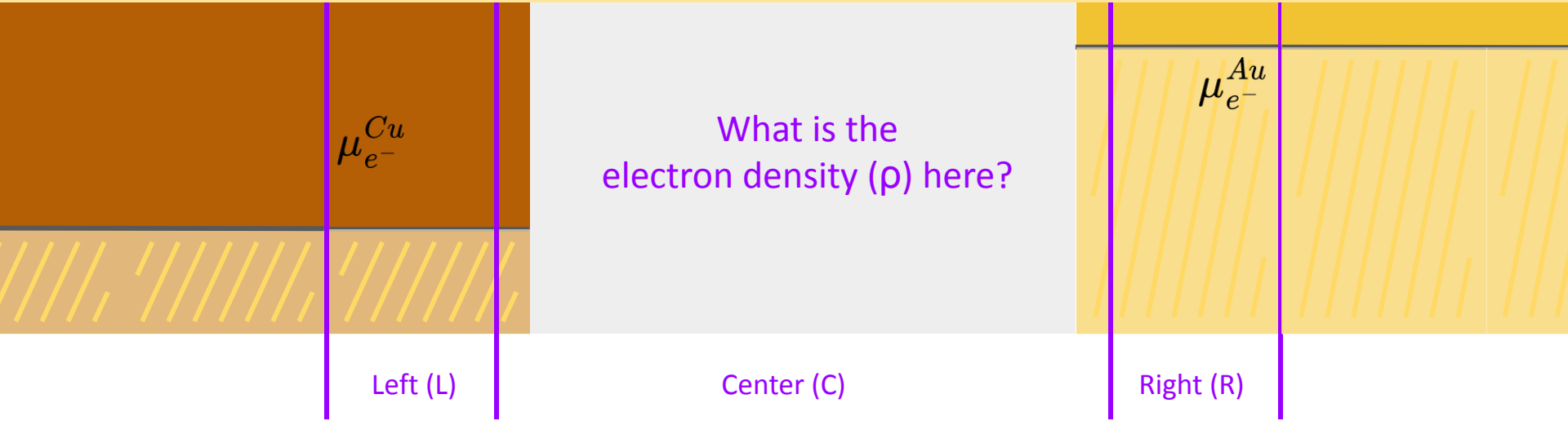

The goal is to **split the density** of the central (C) region into contributions from the left (L) and right (R).

$$\rho_C = \int \rho_L(E) n_L(E) dE + \int \rho_R(E) n_R(E) dE$$

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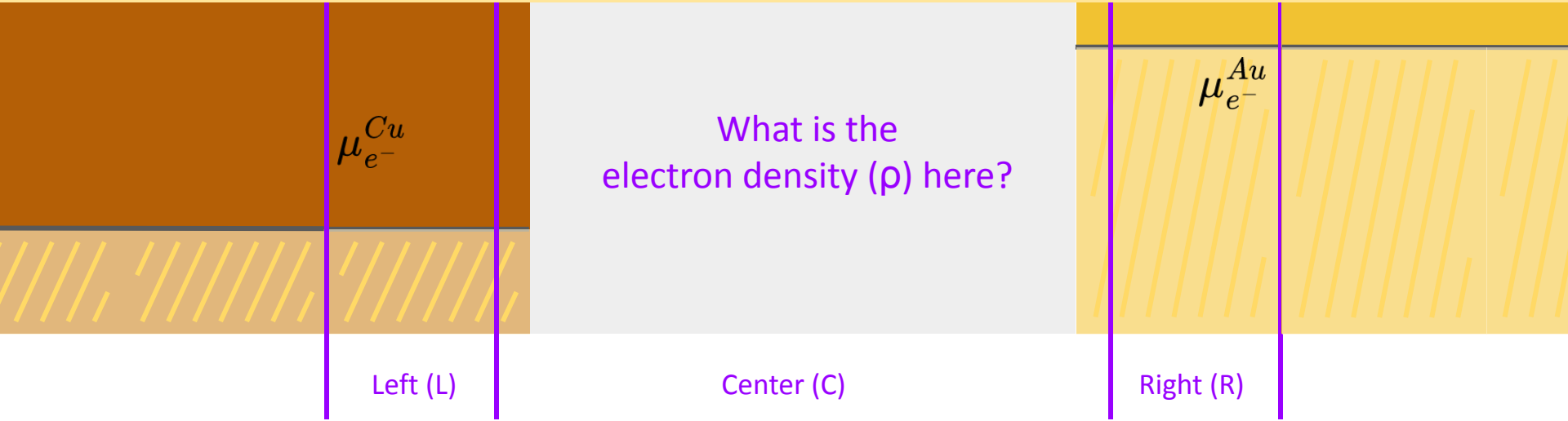

Density of states coming from left side

It gets occupied with the Fermi level of the left side.

$$\rho_C = \int \rho_L(E) n_L(E) dE + \int \rho_R(E) n_R(E) dE$$

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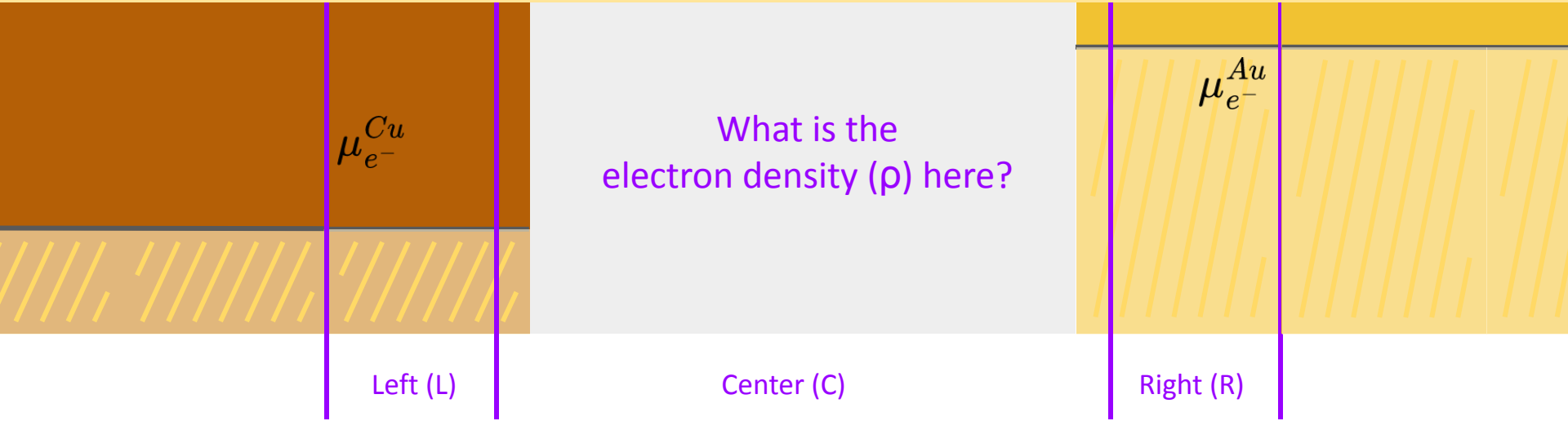

We need to find these.

$$\rho_C = \int \rho_L(E) n_L(E) dE + \int \rho_R(E) n_R(E) dE$$

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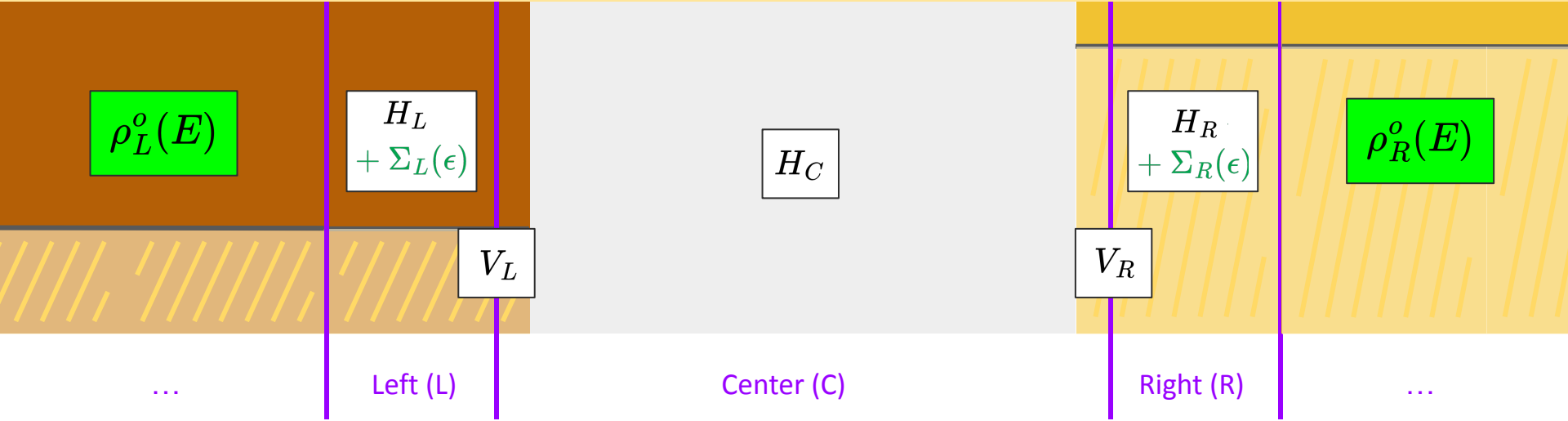

We have the Hamiltonian:

$$H = \begin{bmatrix} H_L + \Sigma_L(\epsilon) & V_L & 0 \\ V_L^\dagger & H_C & V_R \\ 0 & V_R^\dagger & H_R + \Sigma_R(\epsilon) \end{bmatrix}$$

And we can also compute the
bulk density of states of the electrodes

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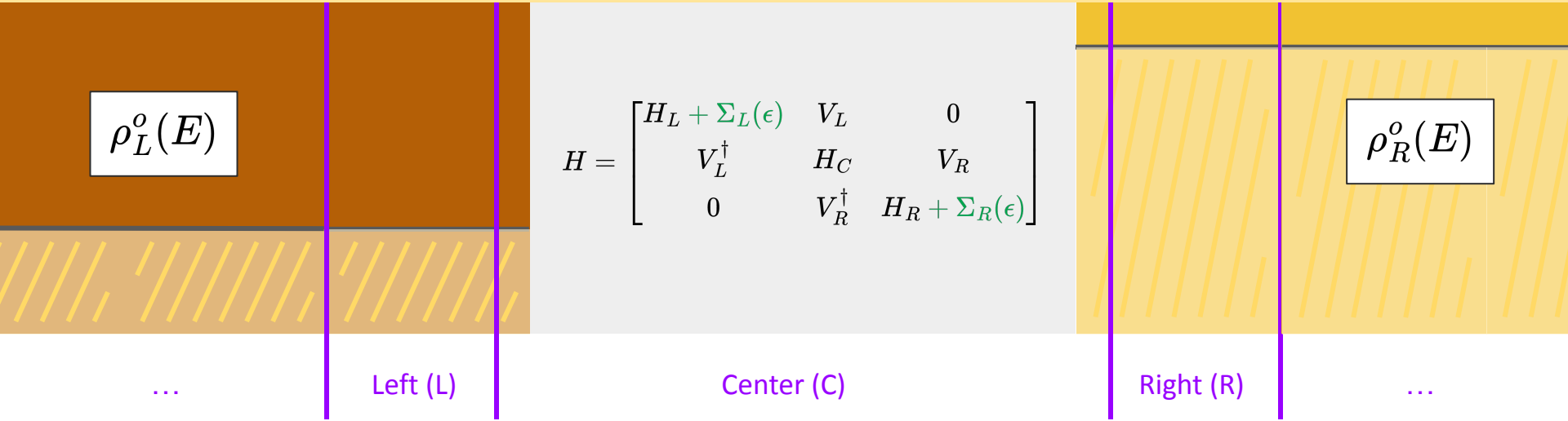

The **Green's Function**:

$$G(E) = (E - H)^{-1}$$

gives us the **response of the system** to an incoming wave.

Wavefunction: $|\psi_L\rangle = G(E)\,|\psi^o_L\rangle$

Density of states:

$$\rho_L(E) = G(E)\rho^o_L(E)G^\dagger(E)$$

Q3. HOW DOES TRANSIESTA WORK? — NEGF electron density equation

$$\rho = \frac{1}{\pi} \sum_{e} \int G(\epsilon)\Gamma_e(\epsilon)G^{\dagger}(\epsilon)n_e(\epsilon)d\epsilon$$

Response of the system

DOS of the bulk electrode.

DOS of the system

Electronic density of the system

Q3. HOW DOES TRANSIESTA WORK? — NEGF electron density equation

Response of the system

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DOS of the bulk electrode.

DOS of the system

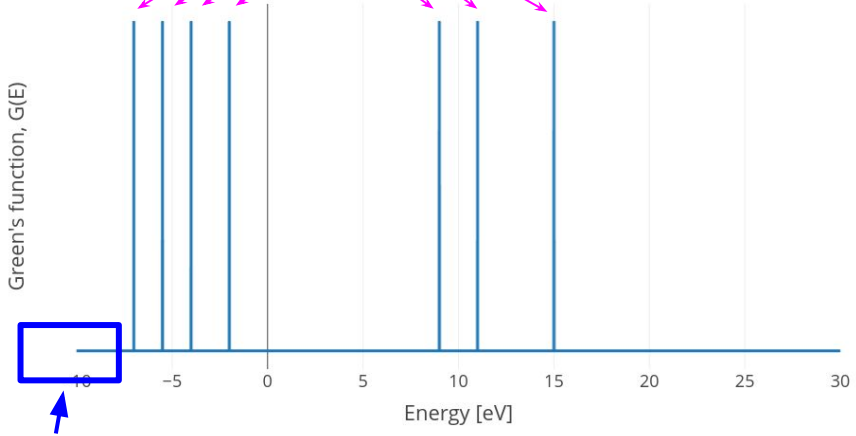
Electronic density of the system

Performing this integral is not trivial

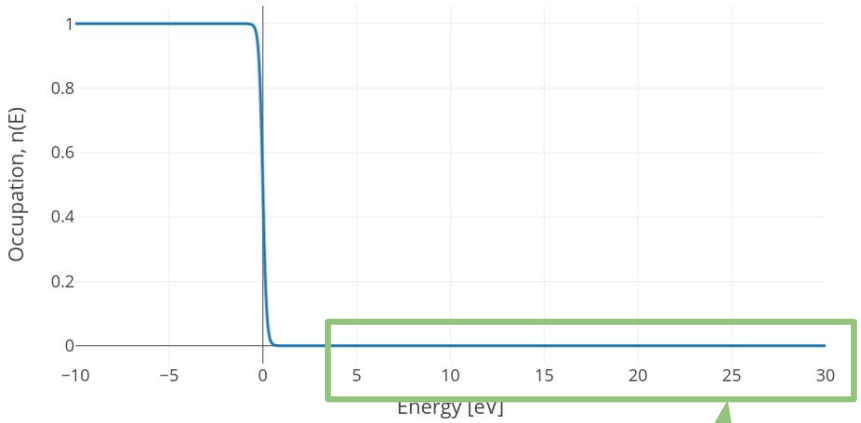
Q3. HOW DOES TRANSIESTA WORK? — NEGF electron density, a dificult integral

$$\int_{-\infty}^{\infty} G(\epsilon)\Gamma_e(\epsilon)G^{\dagger}(\epsilon)n_e(\epsilon)d\epsilon$$

System's eigenvalues



No states with lower energy

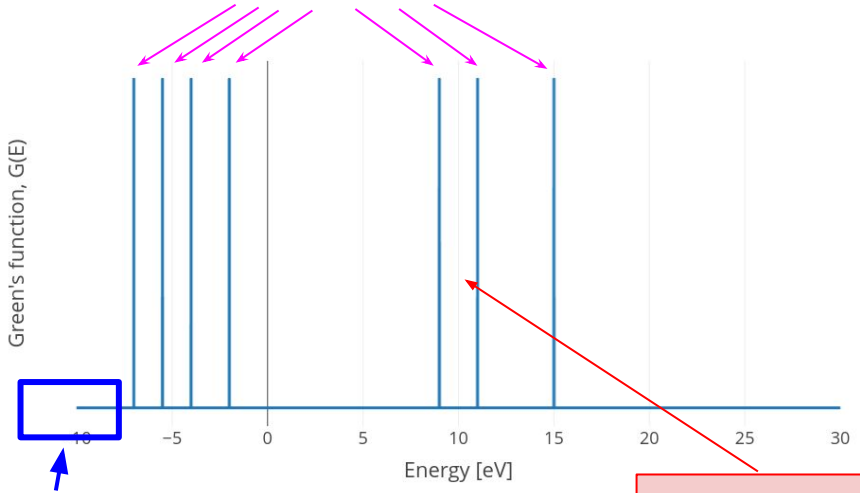


Occupation function becomes 0

Q3. HOW DOES TRANSIESTA WORK? — NEGF electron density, a dificult integral

$$\int_{lowest\ eigenvalue}^{E_f+margin(T)} G(\epsilon)\Gamma_e(\epsilon)G^{\dagger}(\epsilon)n_e(\epsilon)d\epsilon$$

System's eigenvalues



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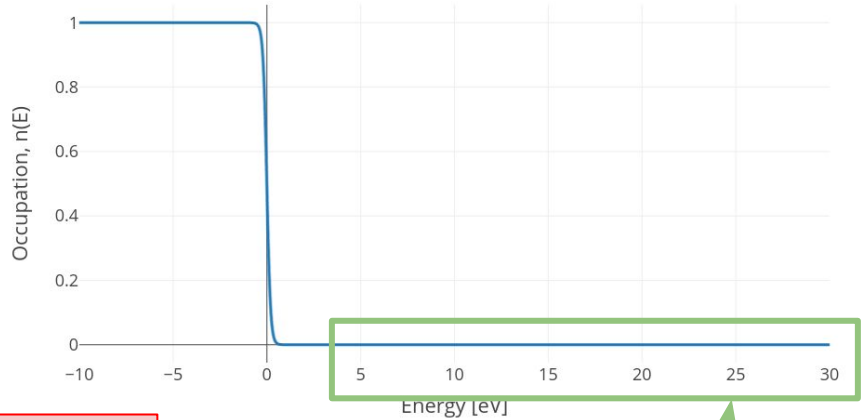
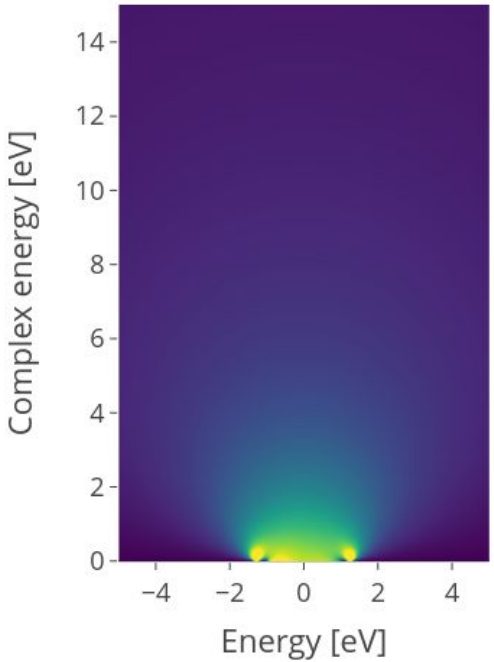


Occupation function becomes 0

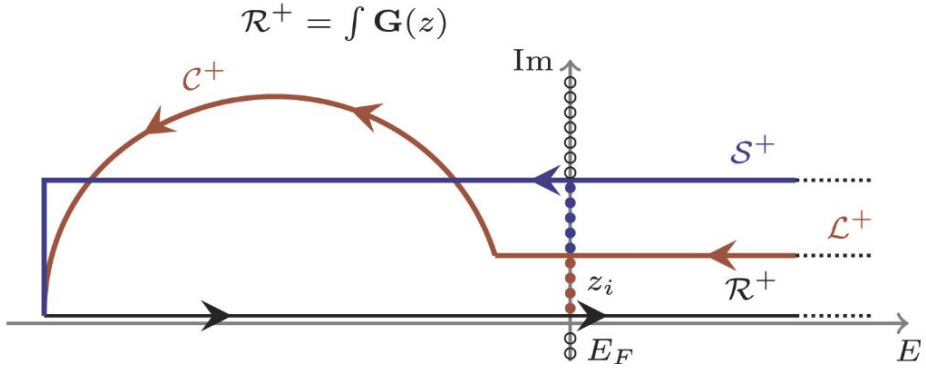
Not smooth!!!

Q3. HOW DOES TRANSIESTA WORK? — NEGF electron density, a dificult integral

The Green's function is much smoother on the complex plane:



The integral is always done through some kind of contour that goes through complex values of E.



N. Papior et al., Computer Physics Communications, Vol. 212, March 2017

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INTRODUCTION TO TRANSIESTA: One talk, four questions

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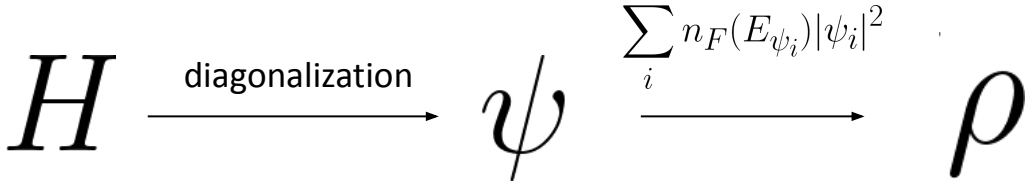
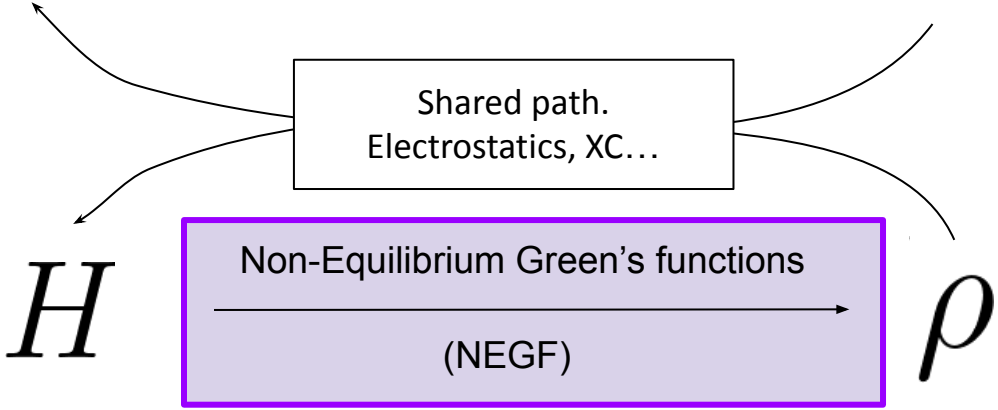
Q4. HOW DOES TRANSIESTA INTEGRATE WITH SIESTA? — A solution method

A single fermi level:

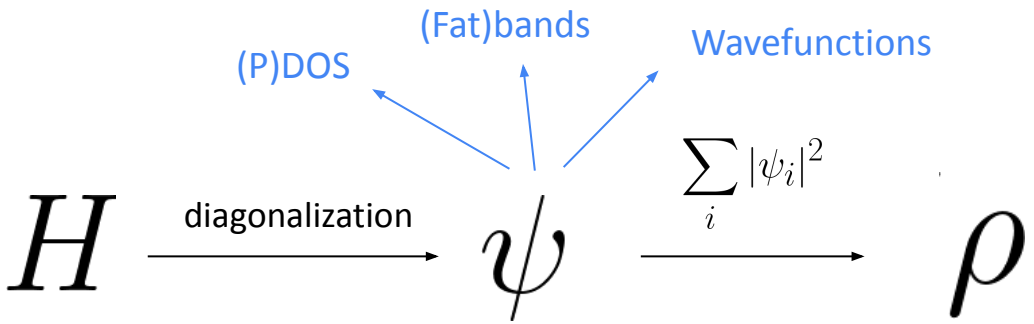




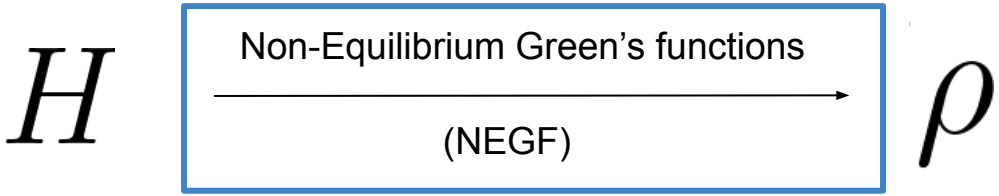
This is what we know as TranSIESTA

Q4. HOW DOES TRANSIESTA INTEGRATE WITH SIESTA? — Postprocessing

A single fermi level:

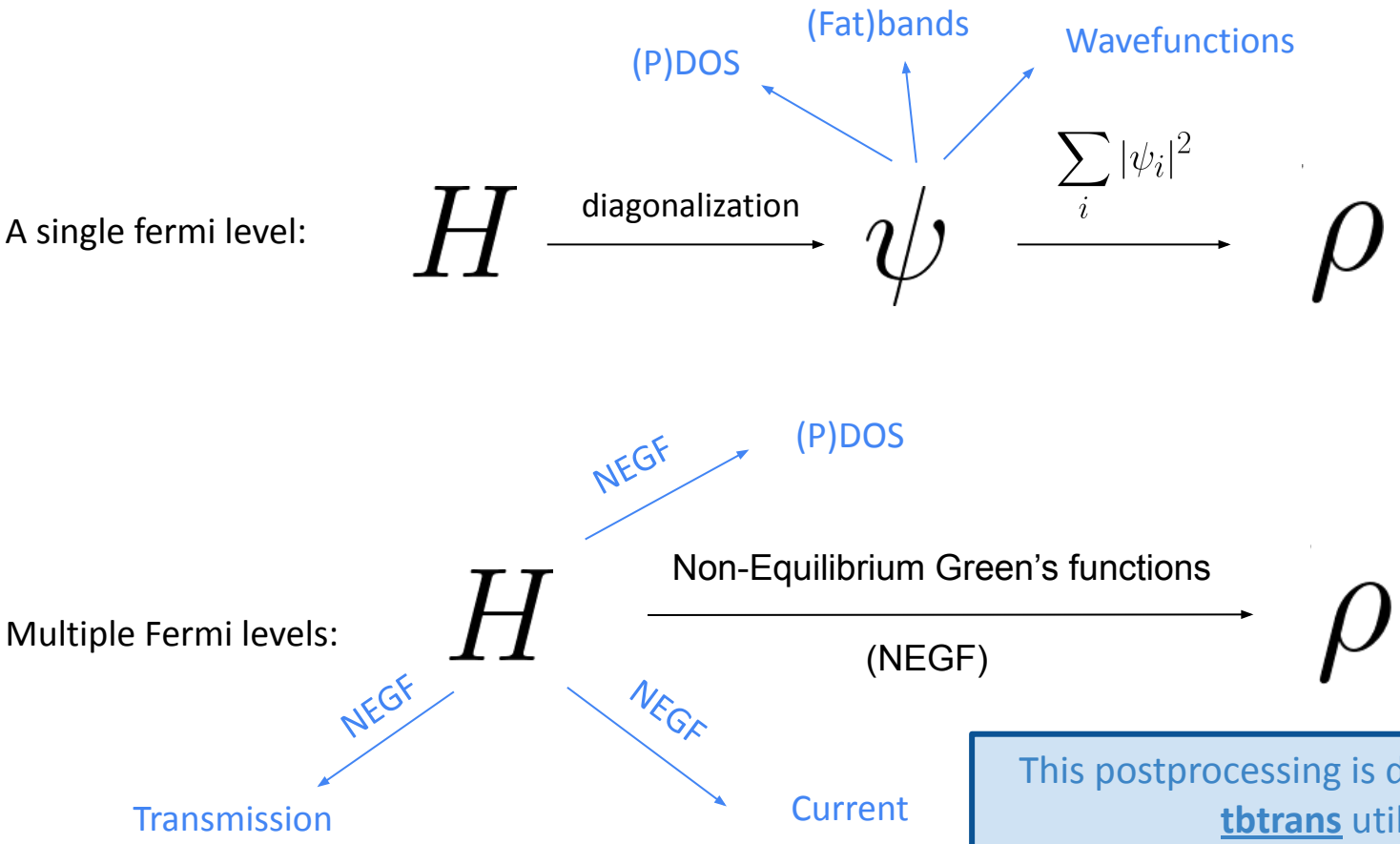


Multiple Fermi levels:



What do we do if we don't have eigenstates??

Q4. HOW DOES TRANSIESTA INTEGRATE WITH SIESTA? — Postprocessing



This postprocessing is done with the **tbtrans** util.

A bit of history…

Q4. HOW DOES TRANSIESTA INTEGRATE WITH SIESTA? — The history.

PREHISTORY

2002 (year -1)

Density-functional method for nonequilibrium electron transport

Mads Brandbyge[1,*], José-Luis Mozos[2], Pablo Ordejón[2], Jeremy Taylor[1], and Kurt Stokbro[1]

HISTORY

2003 (year 0)

TranSIESTA: a spice for molecular electronics

Kurt Stokbro [1], Jeremy Taylor, Mads Brandbyge, Pablo Ordejón

2016 (year 13)

Improvements on non-equilibrium and transport Green function techniques: The next-generation TRANSIESTA

Nick Papior [a], Nicolás Lorente [b, c], Thomas Frederiksen [c, d], Alberto García [c], Mads Brandbyge [a]

FUTURE (?)

2025 (year 22)

Quantum Transport with Spin Orbit Coupling: New Developments in TranSIESTA

Nils Wittemeier, Nick Papior, Mads Brandbyge, Zeila Zanolli, Pablo Ordejón

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TranSIESTA is a solution method inside SIESTA. It has an associated util: TBtrans.