

## Section 15

# Introduction to Non-Equilibrium

Gerhard Klimeck

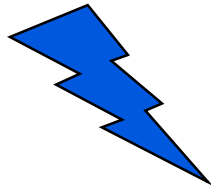
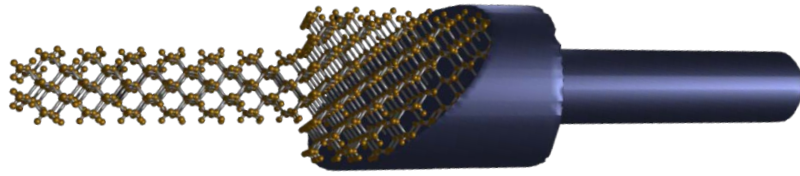
[gekco@purdue.edu](mailto:gekco@purdue.edu)



School of Electrical and  
Computer Engineering

# Section 15

## Introduction to Non-Equilibrium

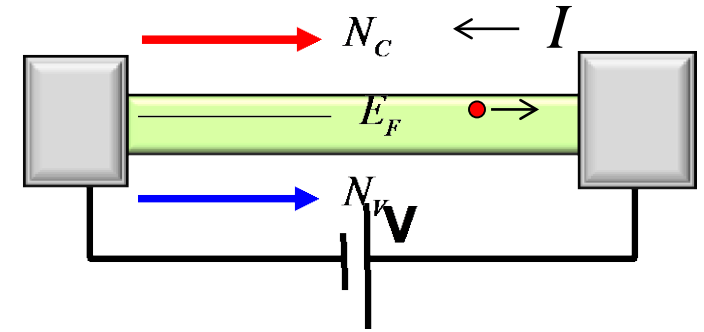


How does the system go BACK to equilibrium?

$$I = G \times V$$

$$= q \times n \times v \times A$$

↑ charge density   
 ↑ density   
 ↑ velocity   
 ↑ area



- Materials, composition, crystals
- Tabulated for **“known” bulk materials**
- ⇒ Quantum Mechanics
- Concepts of **density of states and masses**
- ⇒ Equilibrium Statistical Mechanics

- **Occupation factors**

**Transport with scattering, non-equilibrium Stat. Mech.**

- Drift-diffusion equation with recombination-generation

Understanding transport in devices

- Diodes, BJT/HBT, MOS

• 15.1 Steady State, Transient, Equilibrium

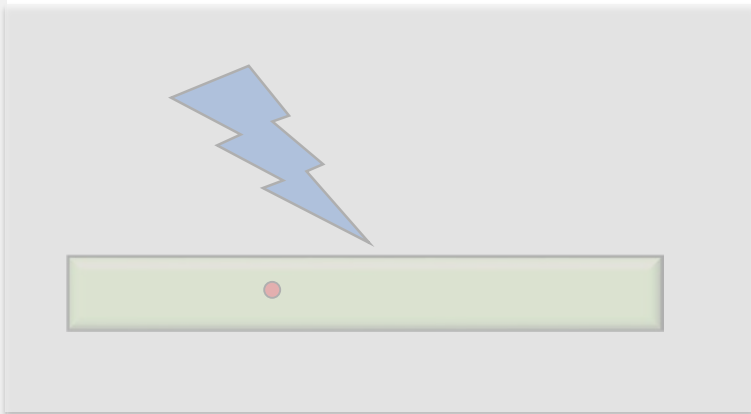
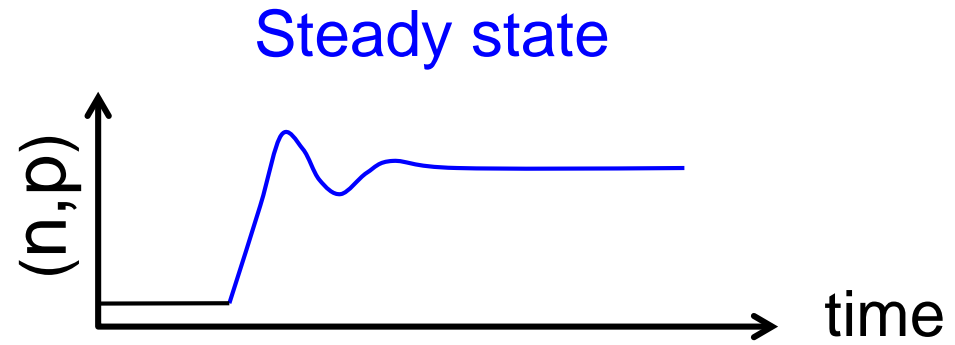
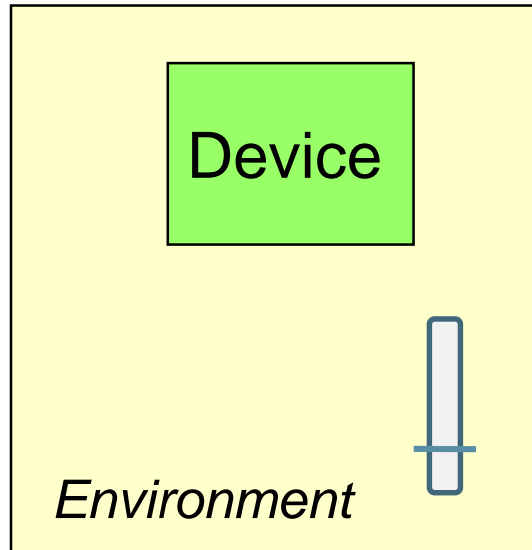
• 15.2 Recombination & Generation Overview

Video

Video

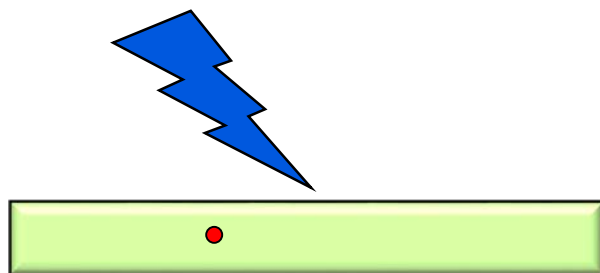
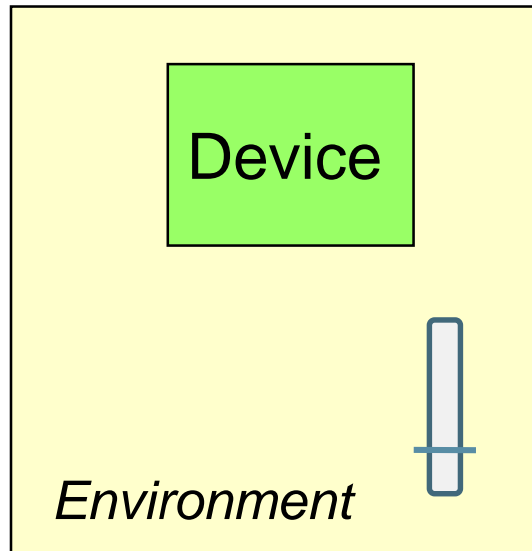
# Equilibrium, Steady state, Transient

## Equilibrium

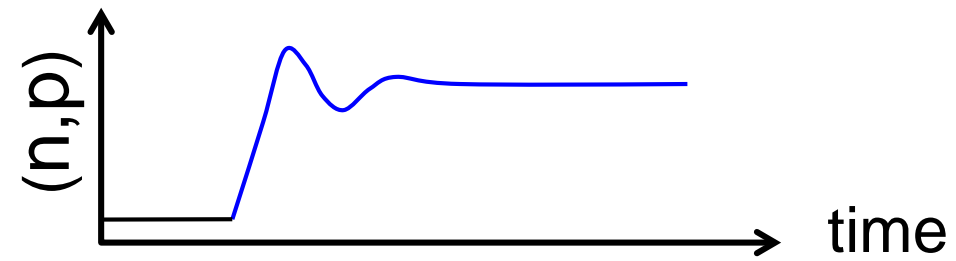


# Equilibrium, Steady state, Transient

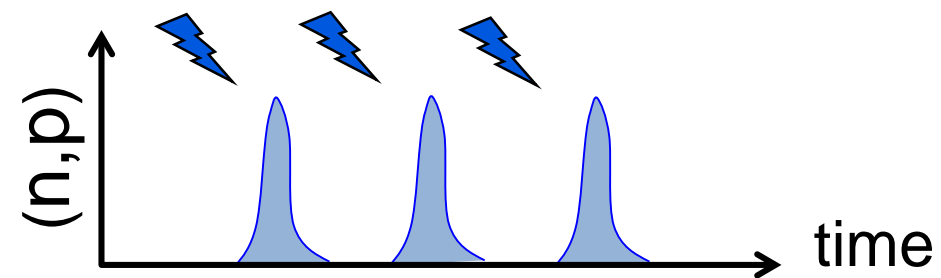
## Equilibrium



## Steady state

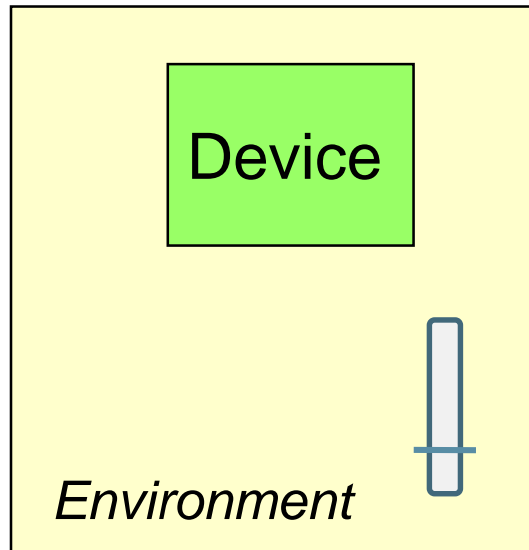


## Transient



# Detailed Balance: Simple Explanation

## Equilibrium



Equilibrium is a very active place

typical semiconductor device there are  $1e17$  to  $1e20$  electrons in the conduction band. All electrons carry charge and are occupying their respective DOS.

Fermi-Dirac distribution demands exploration of allowed states

**In equilibrium each process is balanced by its counter process**

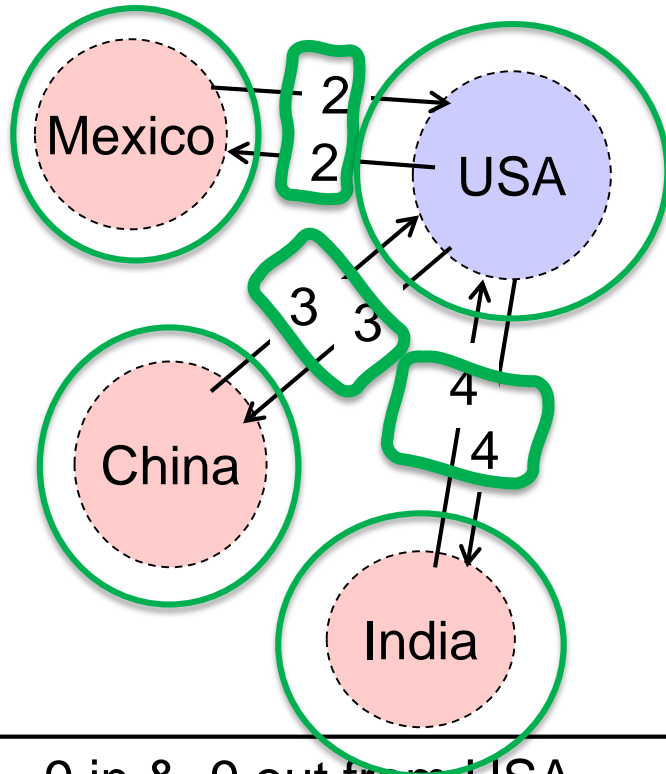
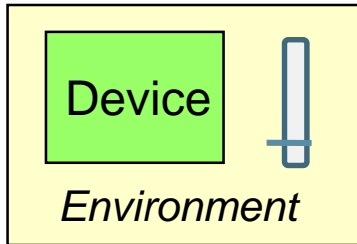
**=> Detailed Balance**

=> Externally it looks as if nothing is happening.

This is different from steady state!!!

# Detailed Balance: Simple Explanation

## Equilibrium



9 in & 9 out from USA  
All numbers are people/unit time.

Equilibrium is a very active place

Fermi-Dirac distribution demands exploration of allowed states

**In equilibrium each process is balanced by its counter process**

**=> Detailed Balance**

=> Externally it looks as if nothing is happening for each site.

**This is different from steady state!!!**

The rates of exchange of people (particles) between every pair of countries (energy levels) is balanced. Hence the name "Detailed Balance".

Detailed balance is the property of equilibrium

The population of each of the countries (energy levels) remains constant under detailed balance.

The concept of detailed balance is powerful, because it can be used for many things

- derive particle distributions Fermi-Dirac, Bose-Einstein
- reduce the number of unknown rate constants by half

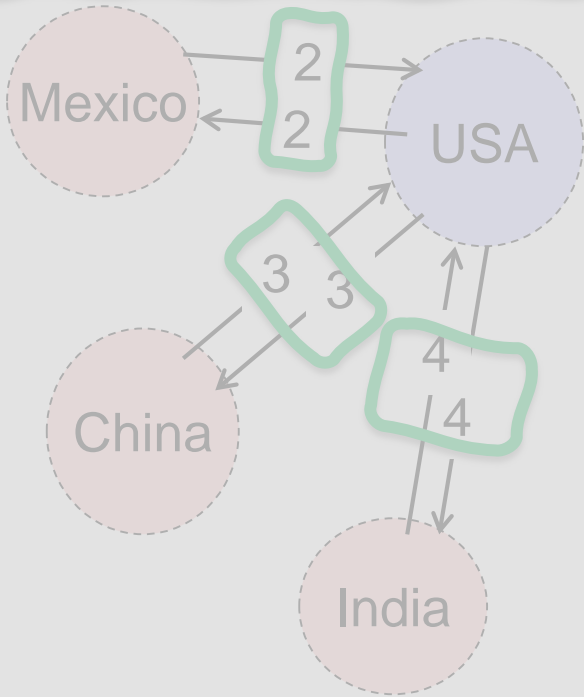
# Steady State Response

In equilibrium each process is balanced by its counter process

=> Detailed Balance

=> Externally it looks as if nothing is happening for each site.

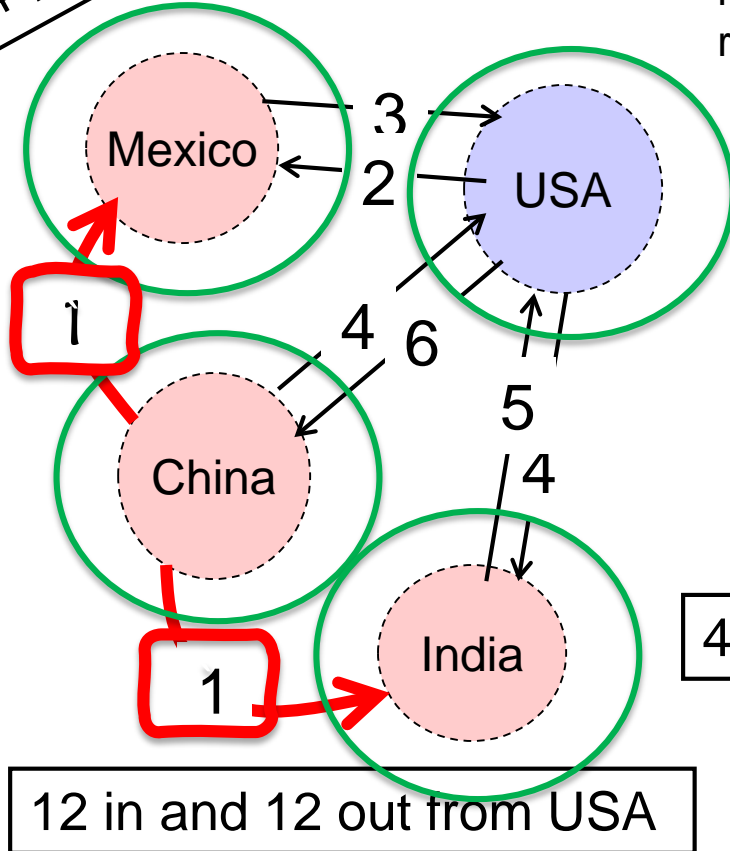
This is different from steady state!!!



9 in & 9 out from USA

All numbers are people/unit time.

2+1 in and 3 out from Mexico



12 in and 12 out from USA

4+1 in and 5 out from India

Disturbing the detailed balance requires non-equilibrium conditions (needs energy).

Unidirectional forces (red lines) can create such Non-equilibrium conditions

The population of a country (energy level) remains constant with time after steady state is reached.

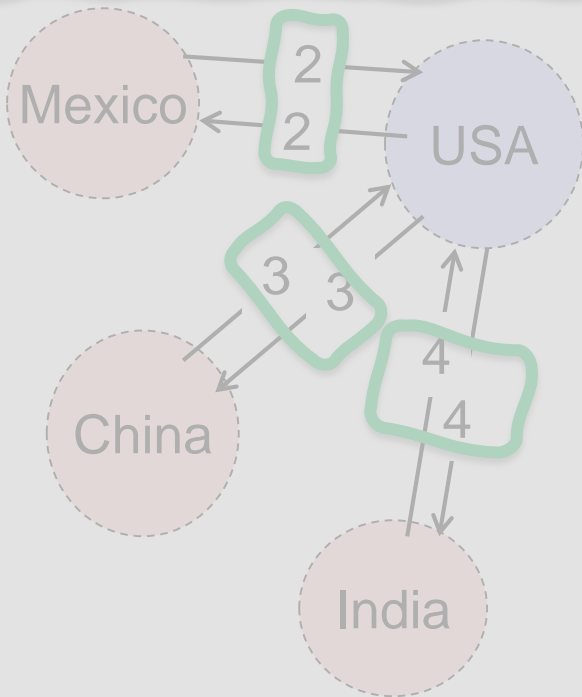
# Steady State Response

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9 in & 9 out from USA

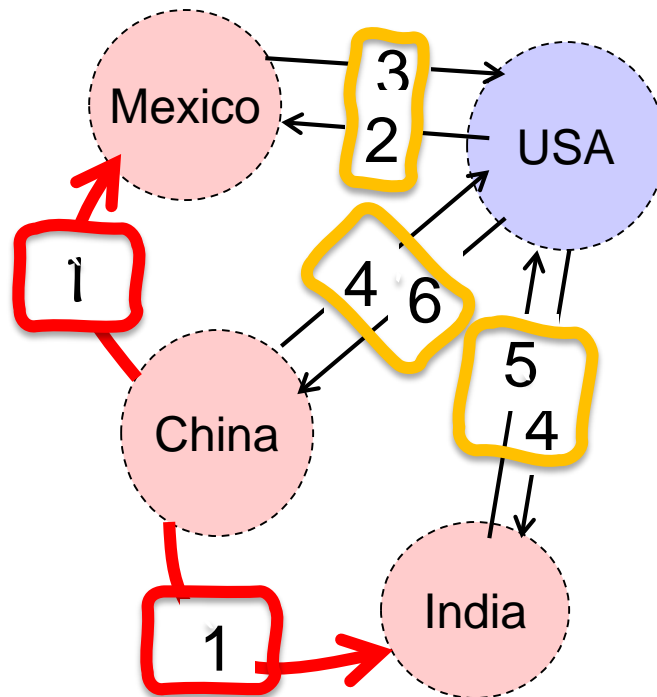
All numbers are people/unit time.

Disturbing the detailed balance requires non-equilibrium conditions (needs energy).

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The population of a country (energy level) remains constant with time after steady state is reached.

The rates of exchange of people (particles) between every pair of countries (energy levels) is NOT balanced.



12 in and 12 out from USA



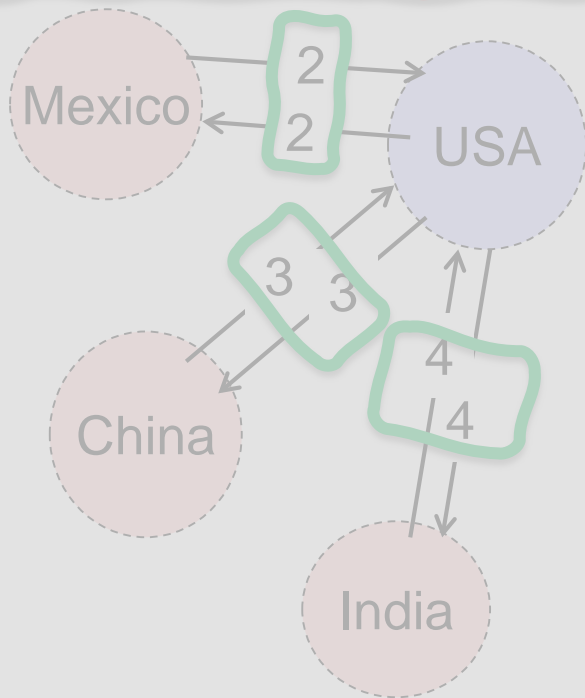
# Steady State Response

In equilibrium each process is balanced by its counter process

=> Detailed Balance

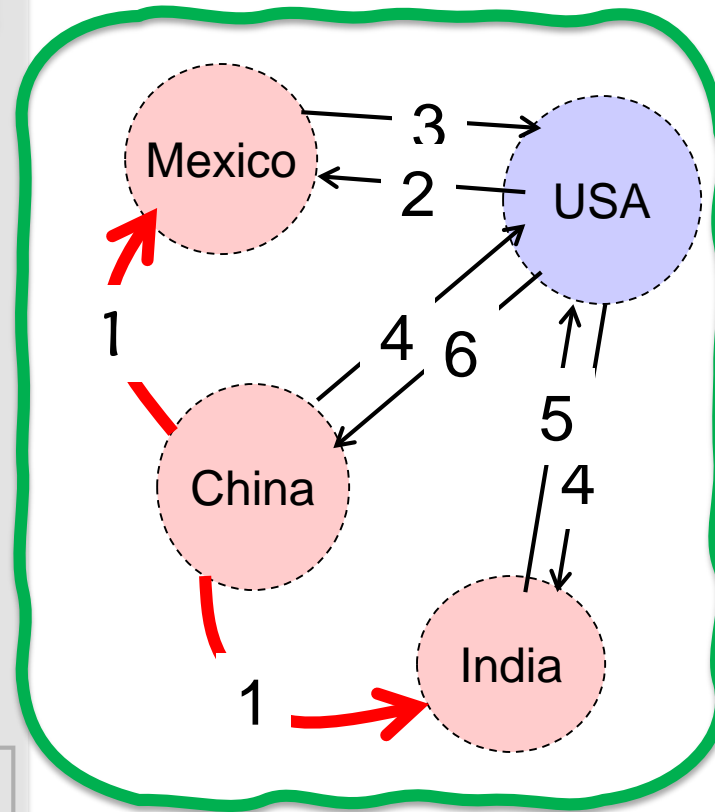
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9 in & 9 out from USA

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The flux at steady state is balanced overall,

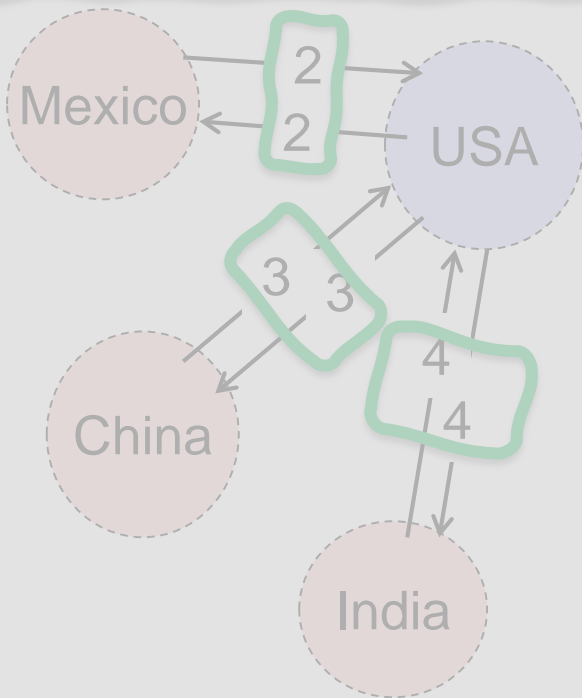
# Steady State Response

In equilibrium each process is balanced by its counter process

=> Detailed Balance

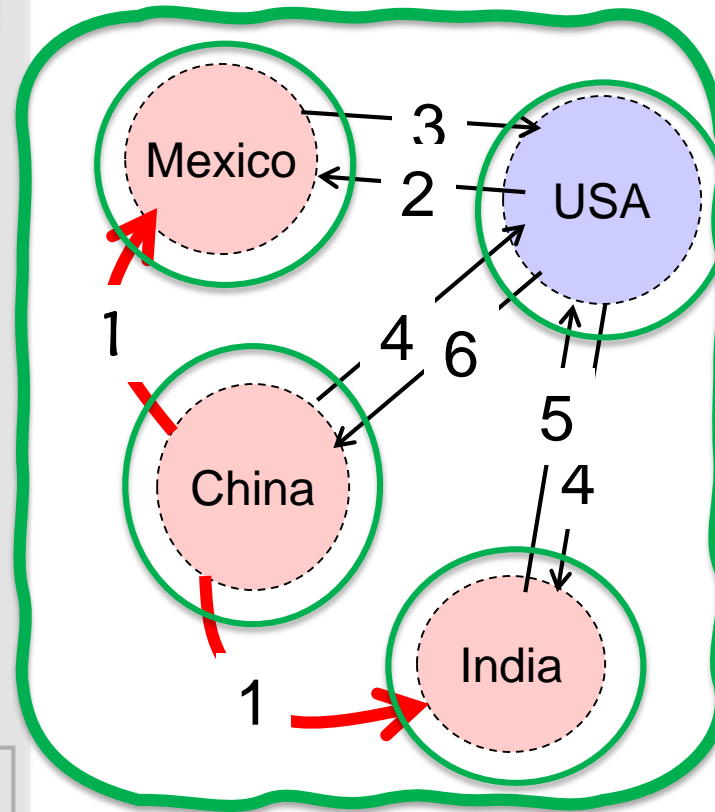
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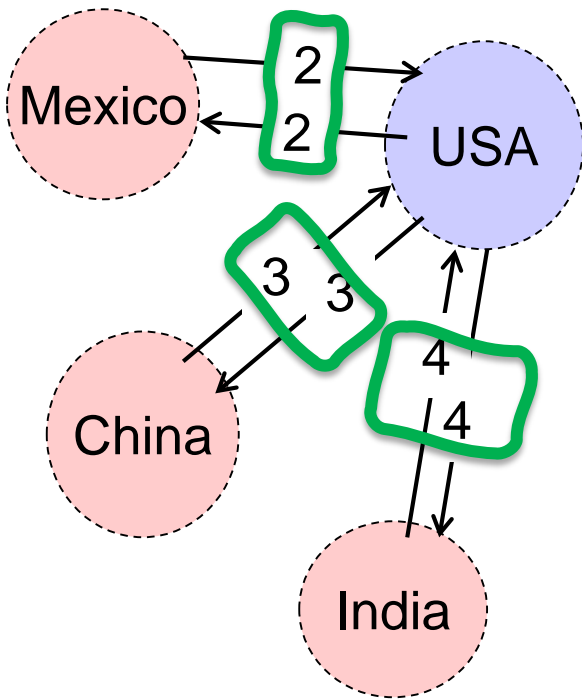
One can use the requirement that net flux at steady state be zero to calculate steady state population of a country

# Transient Response

In equilibrium each process is balanced by its counter process

=> **Detailed Balance**

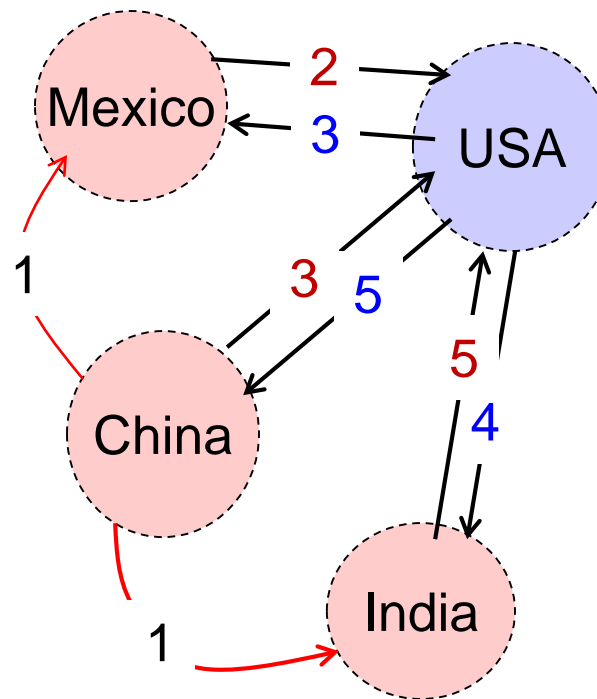
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9 in & 9 out from USA

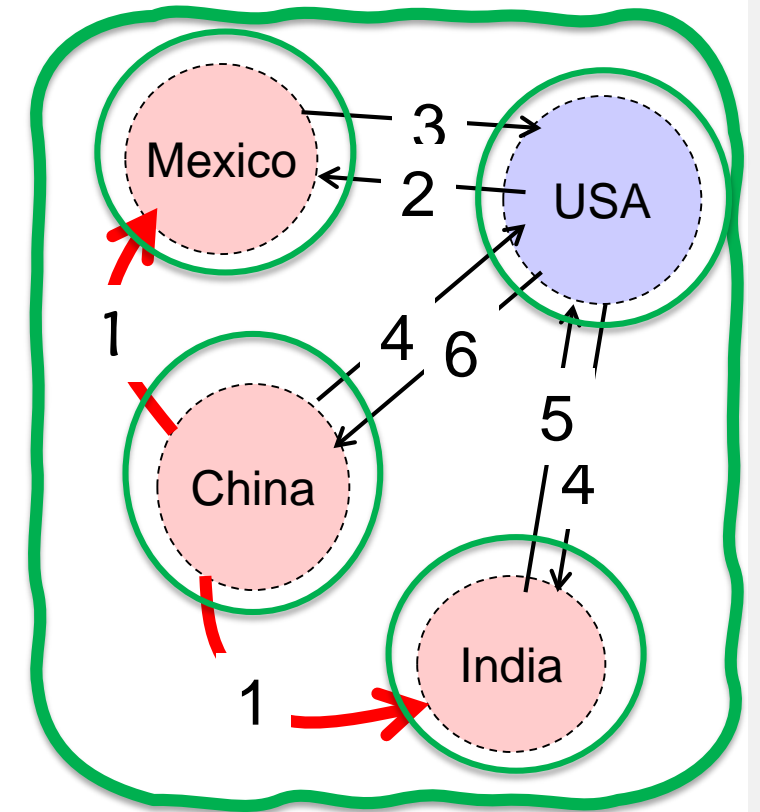
All numbers are people/unit time.

Forced unidirectional connections (red lines) disturbs equilibrium (e.g. 10 in/12 out at time t1 local populations not conserved, but global population is .... Transient populations



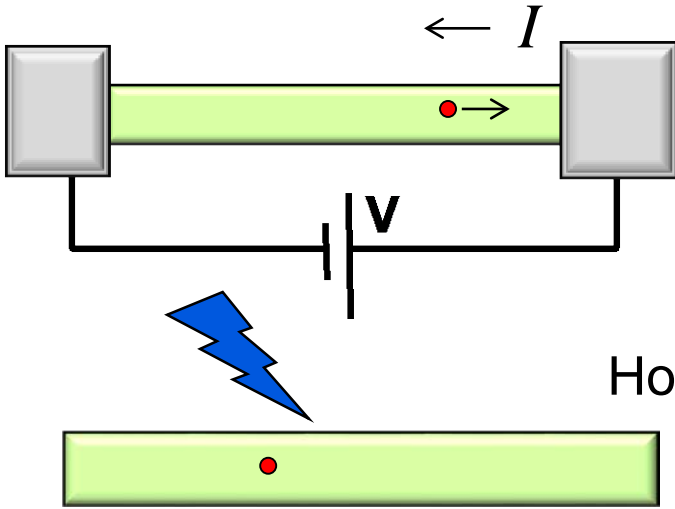
**steady state**

=> Externally it looks as if nothing is happening for the **overall system.**



# Section 15

## Introduction to Non-Equilibrium



$$I = G \times V$$

$$= q \times n \times v \times A$$

↑ charge density   
 ↑ density   
 ↑ velocity   
 ↑ area

How does the system go BACK to equilibrium?

- Materials, composition, crystals
- Tabulated for **known bulk materials**
- ⇒ Quantum Mechanics
- Concepts of **density of states and masses**
- ⇒ Equilibrium Statistical Mechanics
- **Occupation factors**

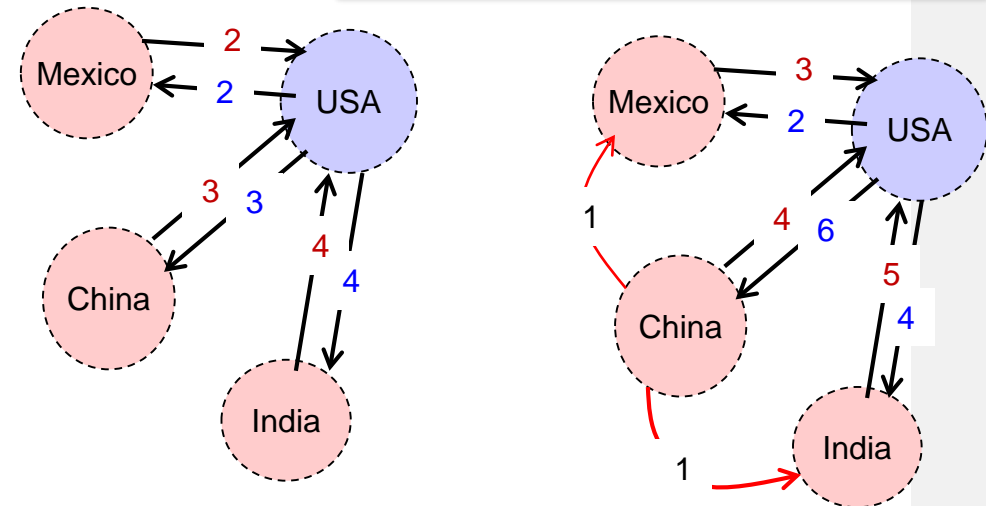
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Understanding device transport

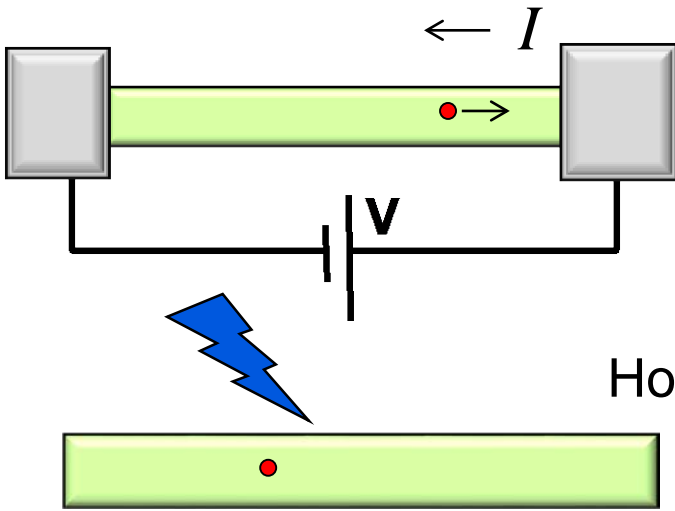
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- 15.1 Steady State, Transient, Equilibrium
  - »Critical conceptual differences!
  - »Need to understand these!
- 15.2



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$$I = G \times V$$

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$q$ : charge  
 $n$ : density  
 $v$ : velocity  
 $A$ : area

How does the system go BACK to equilibrium?

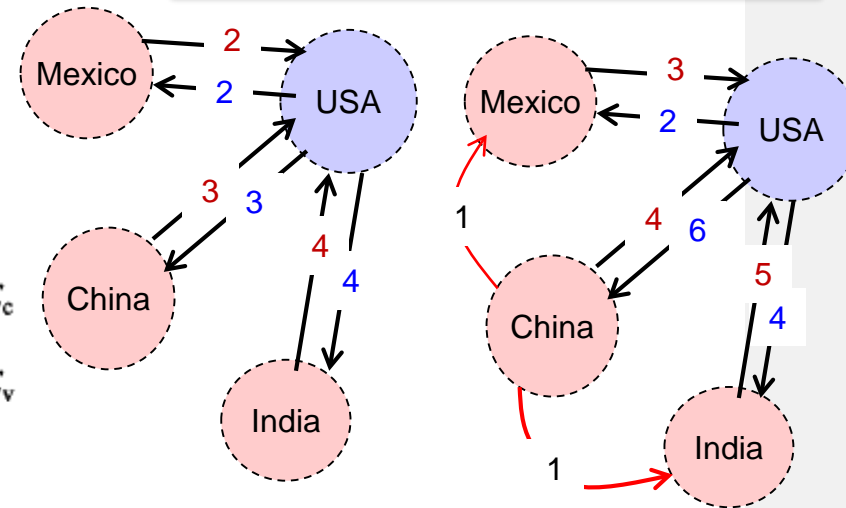
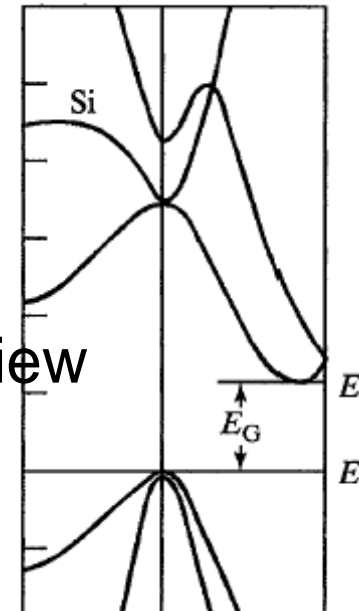
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Video1

Video2