



# FYS2160

Fall, 2018

OVERVIEW ON THERMAL AND STATISTICAL PHYSICS

20.08.2018

# Thermodynamics

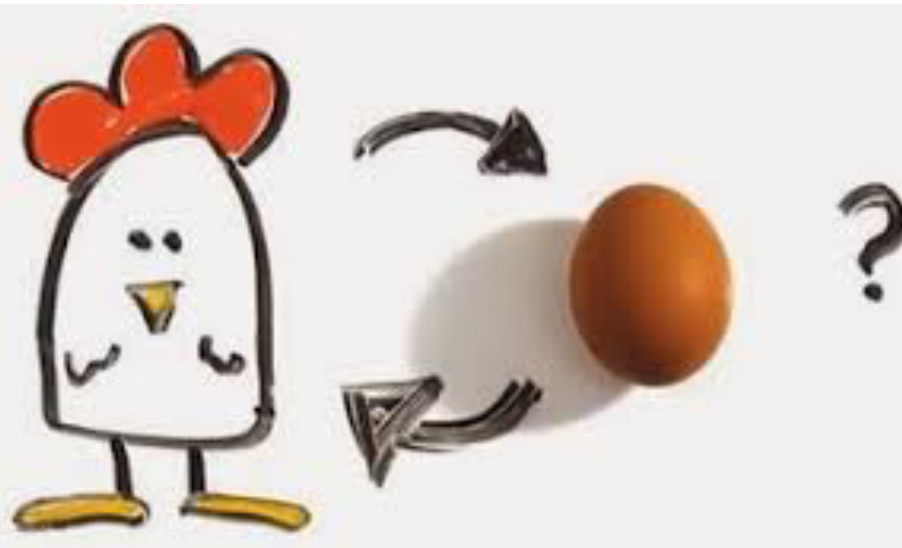
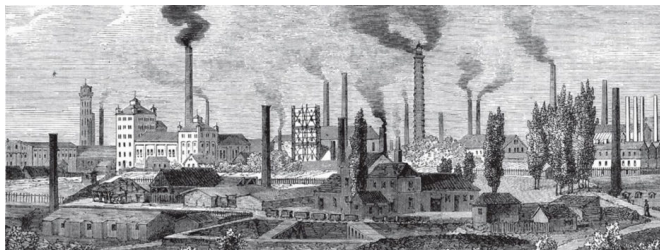
«A theory is more impressive, the greater the simplicity of its premises is, the more different kinds of things it relates and the more extended is its area of applicability. Therefore the deep impression that classical thermodynamics made upon me. It is the only theory of universal content concerning which I am convinced that, within the framework of applicability of its basic concepts, it will never be overthrown.»

*Einstein (taken from Martin J. Klein «Thermodynamics in Einstein's thought», Science , 1967, Vol.157(3788), p.509)*

# Thermodynamics—Theory of principle

The science that deals with heat  $Q$  and work  $W$  and properties of matter that relate to  $Q$  and  $W$

- *invention* and *trigger* of the Industrial Revolution (1800→..)



$$\Delta U = Q + W$$

$$T\Delta S \geq \Delta U + P\Delta V$$

$$PV = nRT$$

# Thermodynamics—Theory of principle

- Based on few empirically observed general properties elevated as thermodynamic principles

- ❖ 0<sup>th</sup> law → defines temperature (T)

- ❖ 1<sup>th</sup> law → defines energy (U) and energy transformation

- ❖ 2<sup>th</sup> law → defines **ENTROPY** (S)

- ❖ 3<sup>rd</sup> law → fixes the value of ENTROPY at  $T = 0$  Kelvin

- These laws are UNIVERSALLY VALID

# Thermodynamic systems—Everywhere



# What is a thermodynamic system?

- **Systems:** *the part of the Universe that we choose to study*
- **Surrounding or environment:** *the rest of the Universe*
- **Boundary:** *the surface separating the System from the Surrounding*

A System relative to its surroundings can be:

- **Open:** System can exchange both mass and energy with the Surroundings
- **Closed:** System can exchange only energy with the Surroundings, but NOT mass
- **Isolated:** Neither Mass nor Energy can transfer between the System and the Surroundings

# What is a thermodynamic system?

- **Systems:** *the part of the Universe that we choose to study*
- **Surrounding or environment:** *the rest of the Universe*
- **Boundary:** *the surface separating the System from the Surrounding*

How do we describe the system:

- A few macroscopic properties:  
pressure, temperature, volume, molar volume, ...
- Homogeneous or Heterogeneous
- State of the system:  
equilibrium or non-equilibrium
- Number of components:  
pure system or composite system

# Statistical mechanics – Constructive theory

Invented to *explain* the principles of thermodynamics based on the **atomistic** description of matter – kinetic theory of gases (1870→)

## Thermodynamics:

Heat *always* flows *spontaneously* from **hot** to **cold** until the same *temperature* is reached

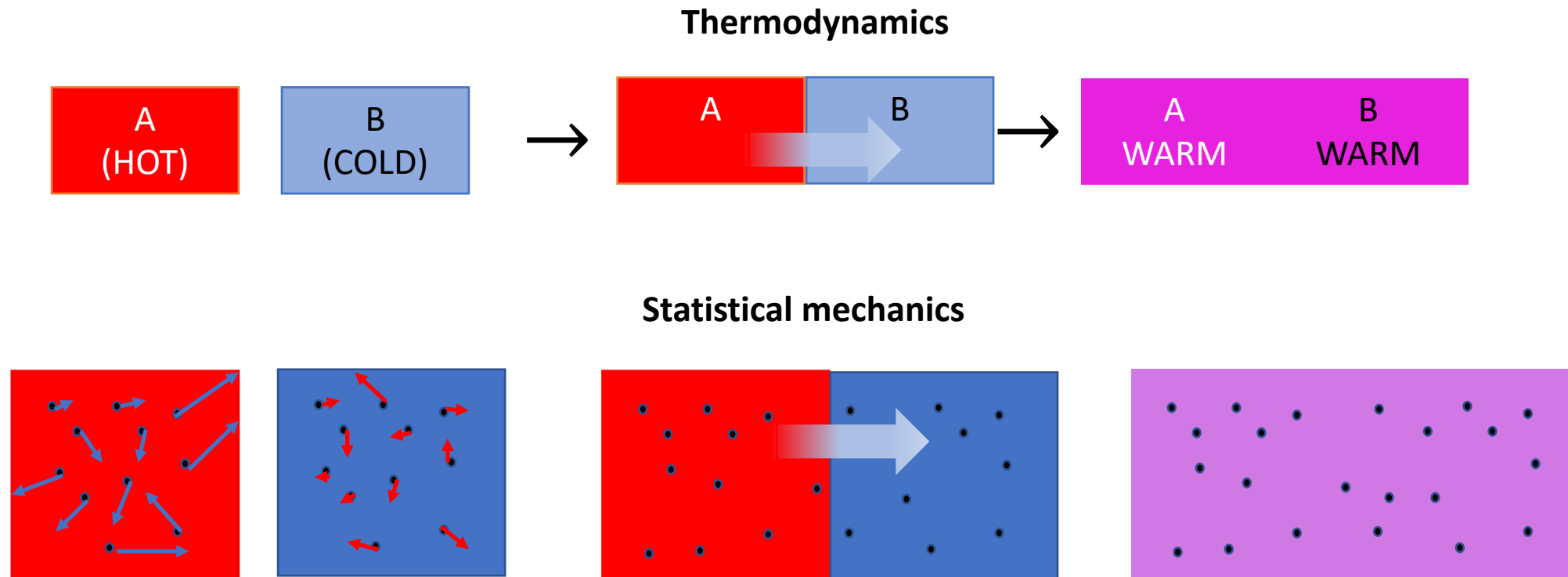
## Statistical mechanics:

**Most likely**, heat flows spontaneously from hot to cold because the atoms of the **hot** system have more kinetic energy. Therefore there is a natural tendency that, by mutual collisions, «**hot**» atoms loose some of their energy while «**cold**» atoms gain some kinetic energy until everyone has *the same kinetic energy*, **on average**



# Statistical mechanics – Constructive theory

Invented to *explain* the principles of thermodynamics based on the atomistic description of matter



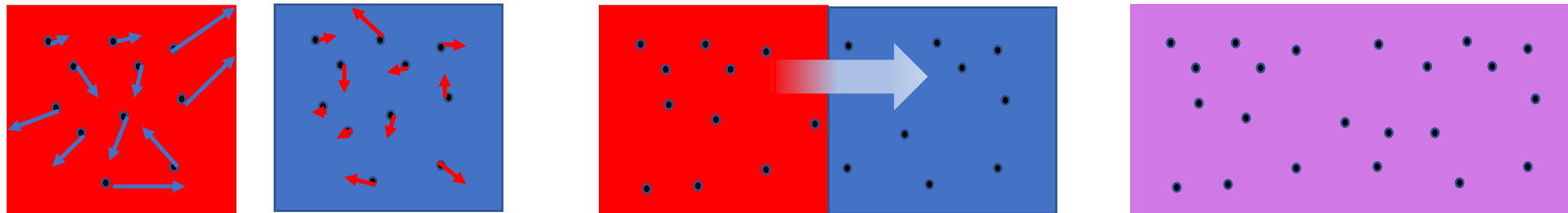
# Statistical mechanics – Constructive theory

Invented to *explain* the principles of thermodynamics based on the atomistic description of matter

*Thermodynamic process*: Spontaneous relaxation to **thermal equilibrium**



Spontaneous *heat diffusion* until they reach the **equipartition of energy**



# Statistical mechanics – Constructive theory

- Frames the validity of the thermodynamic principles

*Importance of statistical fluctuations*

- New discoveries:

*exotic new states of matter Bose-Einstein condensation, superconductors...*

- Based on particle *modelling*

*Statistical Models of matter: Ideal gas model, molecular dynamics, Ising model..*

# Thermodynamics--Statistical mechanics: Correspondence

- «Atoms» = microscopic particles, neutral atoms, electrons, photons, phonons, M&Ms ...so *particles* in general

Thermodynamic system (T,P,V,N..)	Ensemble of particle configurations at (T,P,V,N...)
Equilibrium state (macrostate)	Number of configurations (multiplicity of microstates)
Free energies	Partition functions: weighted sum over the number of microstates





# Prototype Models in statistical mechanics

Gases: Ideal gas

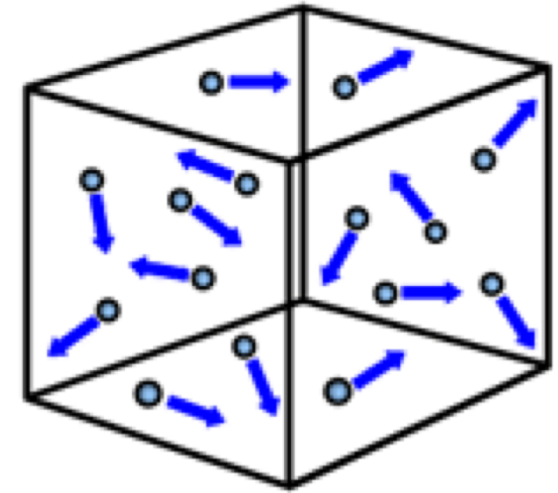
Solid crystals: Einstein model

Magnetism: Ising spin model

Cosmic radiation: Black body radiation model

# *Dilute* gases in a box: Ideal gas model

- Low density of particles
- Newtonian particles
- No interaction forces
- Perfect collisions

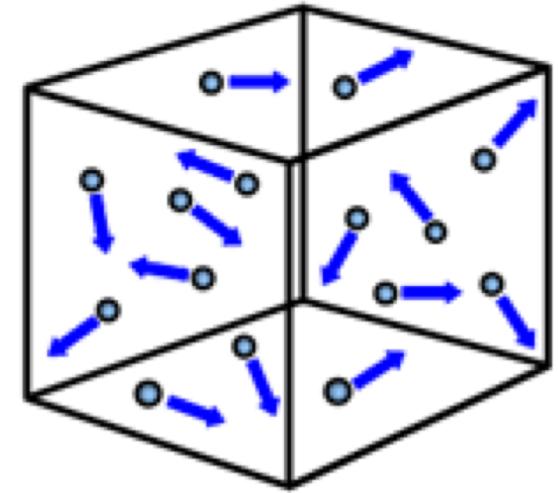




# *Dilute* gases in a box: Ideal gas model

## Predictions from the model

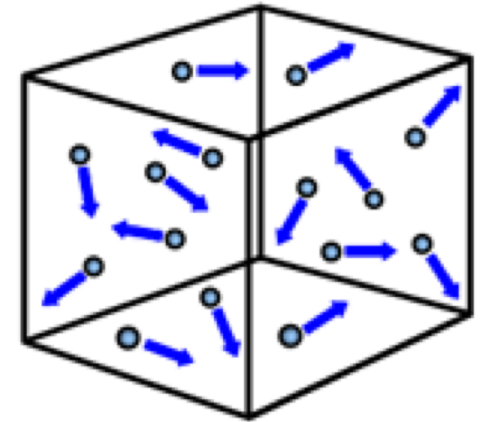
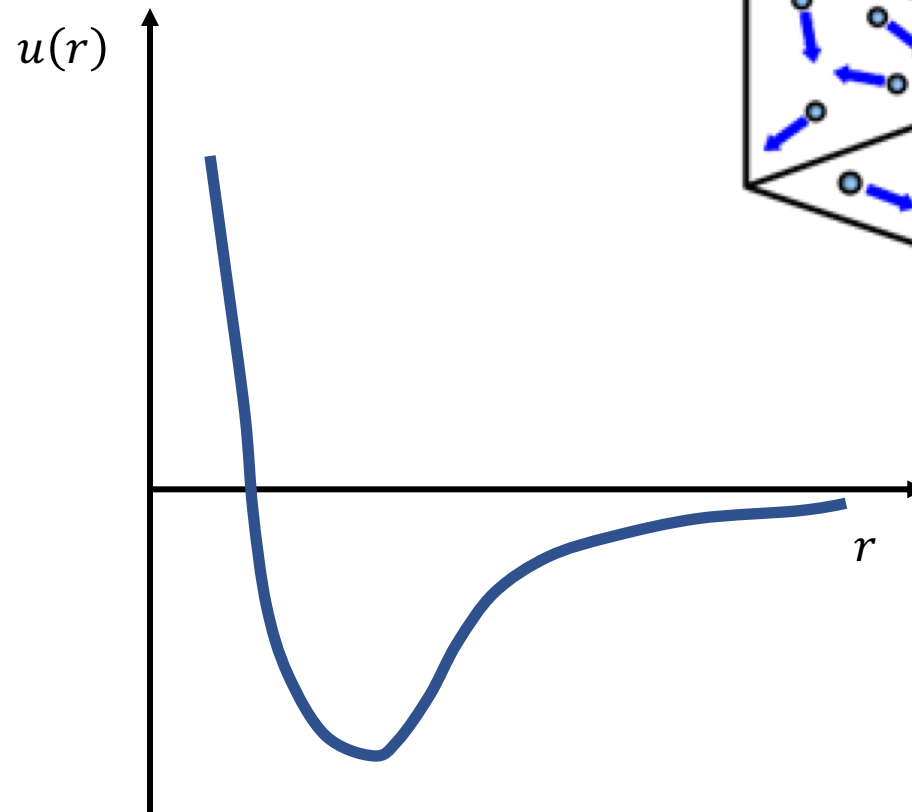
- Pressure, Temperature and the equation of state
- What is the **entropy** of the gas
- How does the gas responds to external forces?



# *Real* gases in a box: Van der Waal gas model

- Newtonian particles
- Weak interaction
- Lenard Jones potential (1924)

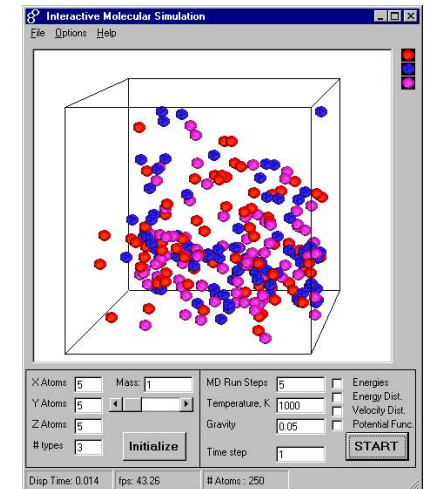
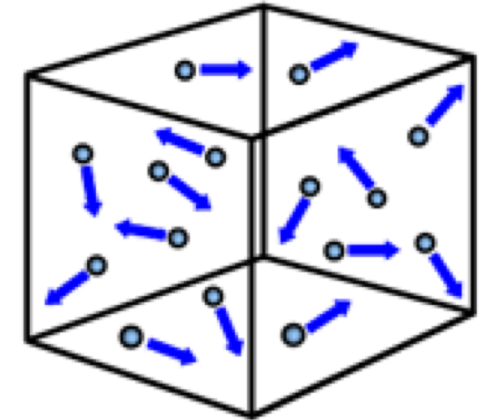
$$u(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$



# *Real* gases in a box: Molecular dynamics

- Newtonian particles
- Weakly interaction
- Lenard Jones potential (1924)

$$u(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

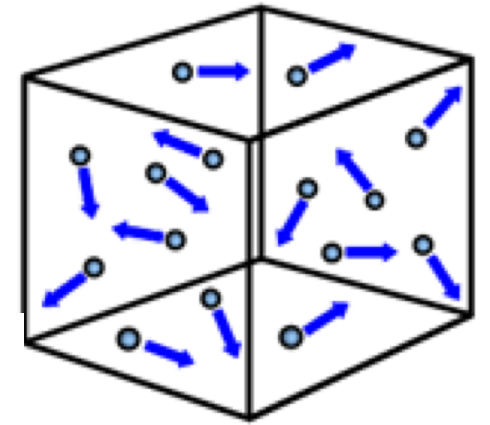
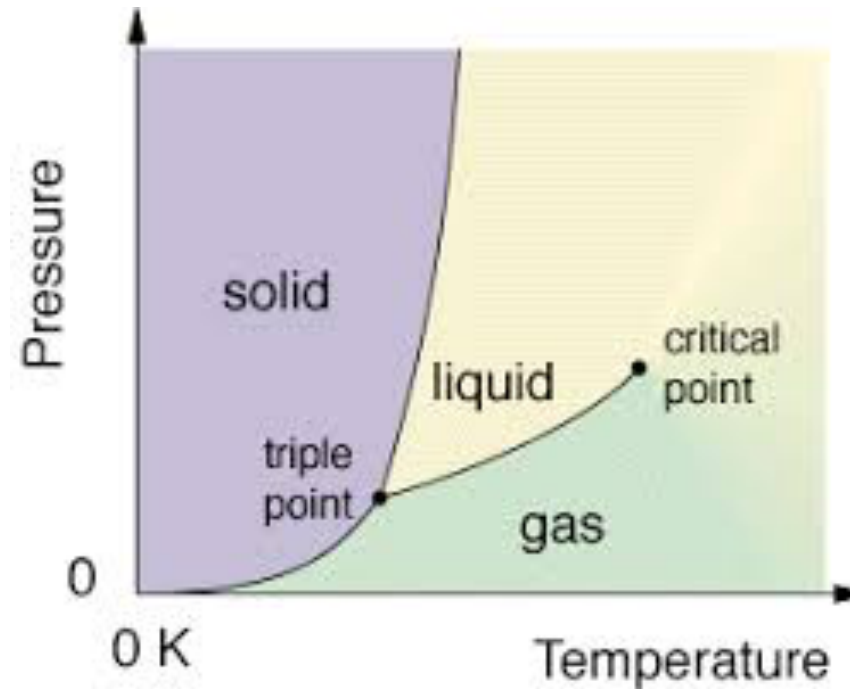


<http://physics.weber.edu/schroeder/md/InteractiveMD.html>

# *Real* gases in a box: Van der Waal gas model

## Model Predictions

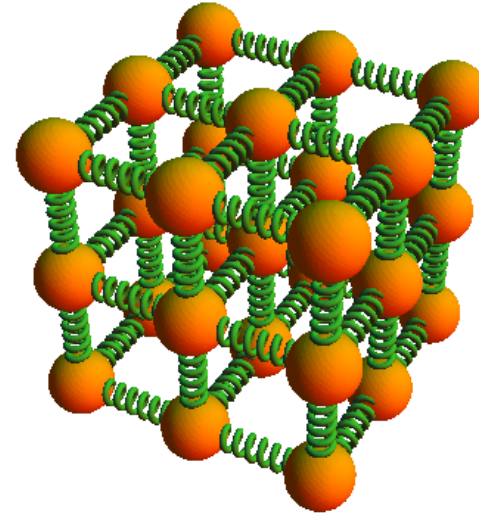
Liquid-gas phase transition





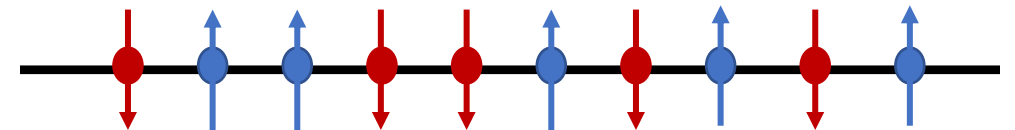
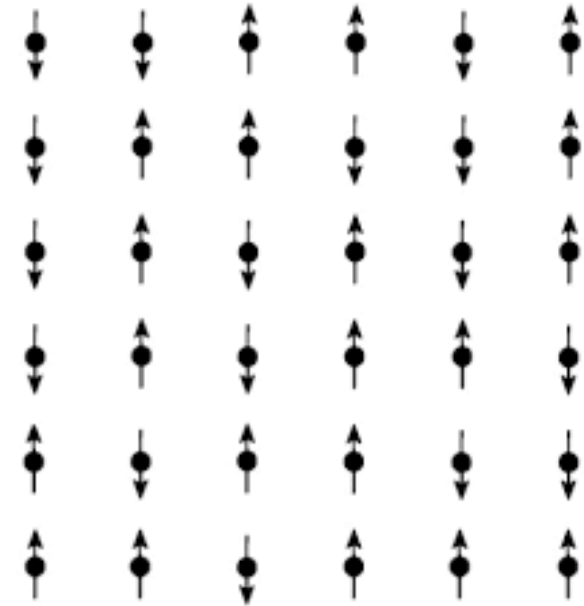
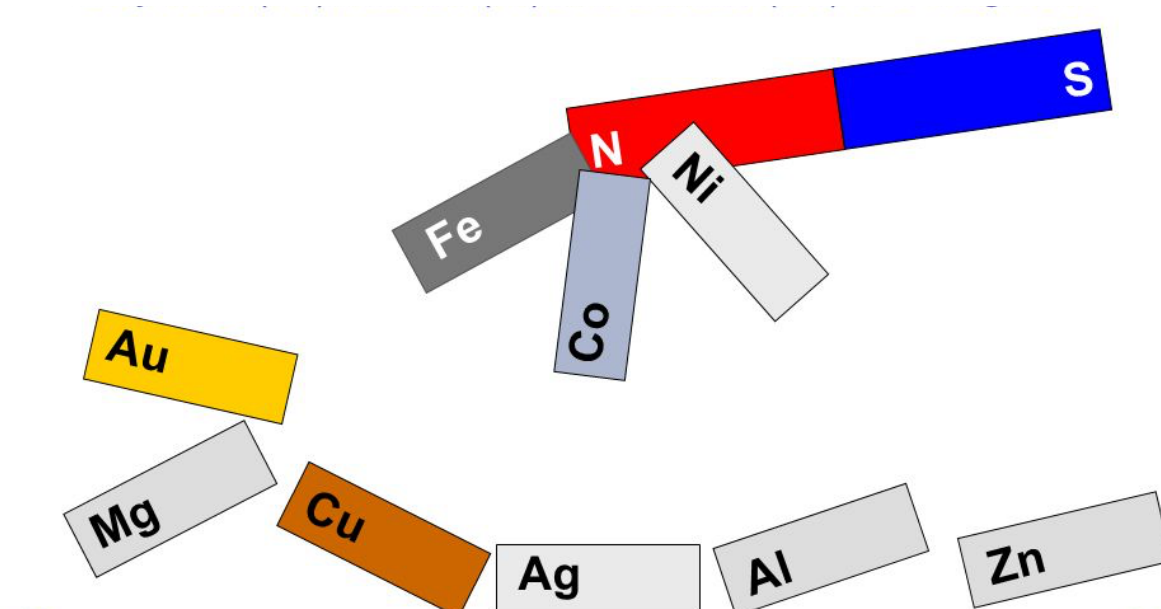
# *Solids*: Einstein model

- Particles can oscillate independently along each lattice direction
- Harmonic oscillators





# Magnetism: Ising Spin Model

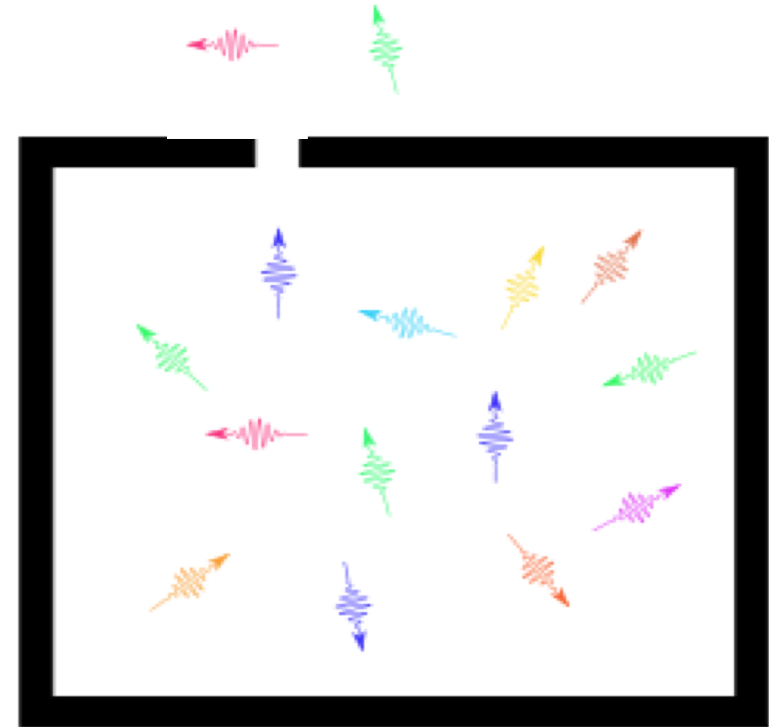






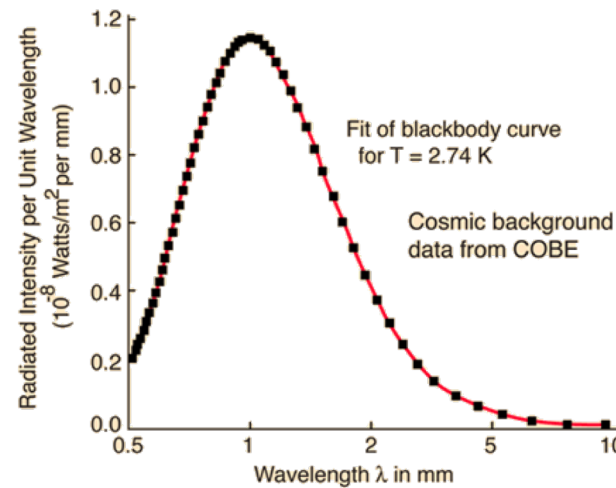
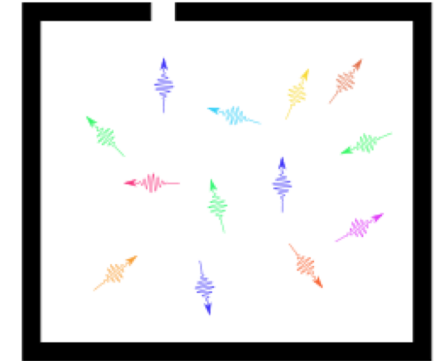
# *Cosmic radiation:* Black-body radiation

- Quantum ideal gas of photons
- Quantum harmonic oscillator



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