
Work, Energy, and Power

Agenda: Energy Conversion and Transformation

Work and other Energy Forms

- Potential and kinetic energy,
- Molecular binding and rearrangement energies,
- pV work, kinetic energy equilibration, heat flow,
  Mechanical equivalent of heat,
  Basic fluid dynamics, laminar & turbulent flow,

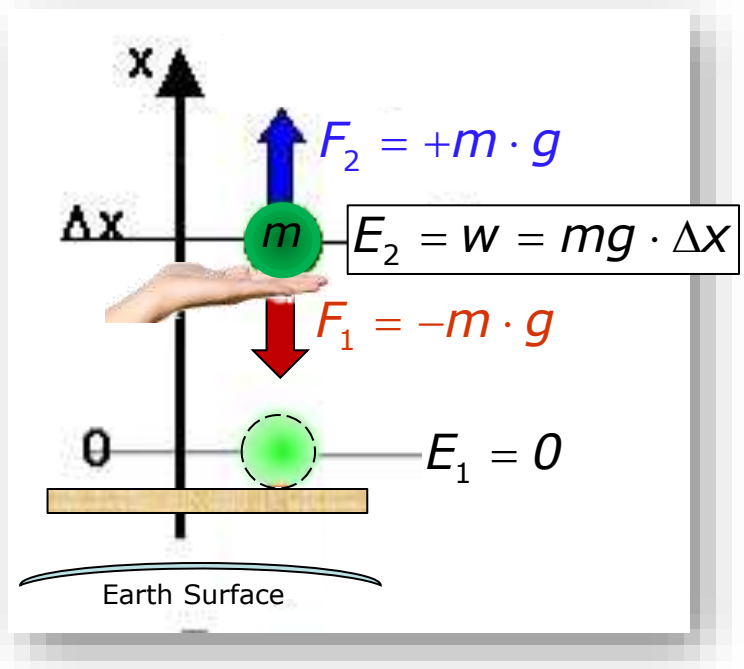
Basic Electricity

- Static electro-magnetic phenomena, electrical current laws,
  Electromagnetic induction, generators, transformers, AC/DC transmission,
- Electronic circuits, reactance,

Principles of Thermodynamic Processes

- Laws of Thermodynamics, state functions, reversible processes,
- Carnot and other TD cycles, steam engines, gas turbines,
- Electro-chemistry, batteries, hydrolyzers & fuel cells.

Mechanical Work & Energy: Weightlifting



Only differences ΔE in energy E *are* measureable →
→ arbitrary energy-zero, $E=0$.

Newton's Law→ Motion of massive bodies:

$$Force = Mass \cdot Acceleration$$

Balancing gravitational force F_1 requires an equal force F_2 in the opposite direction.

$$\vec{F}_2 = -\vec{F}_1 = -m \cdot g$$

Applying $\boldsymbol{F}_2$ over an altitude change $\boldsymbol{\Delta x}$ requires work $\boldsymbol{w}$

$$w = +F_2 \cdot \Delta x \; = -F_1 \cdot \Delta x = m \cdot g \cdot \Delta x$$

This increases the intrinsic (potential) energy of the body (= system) by

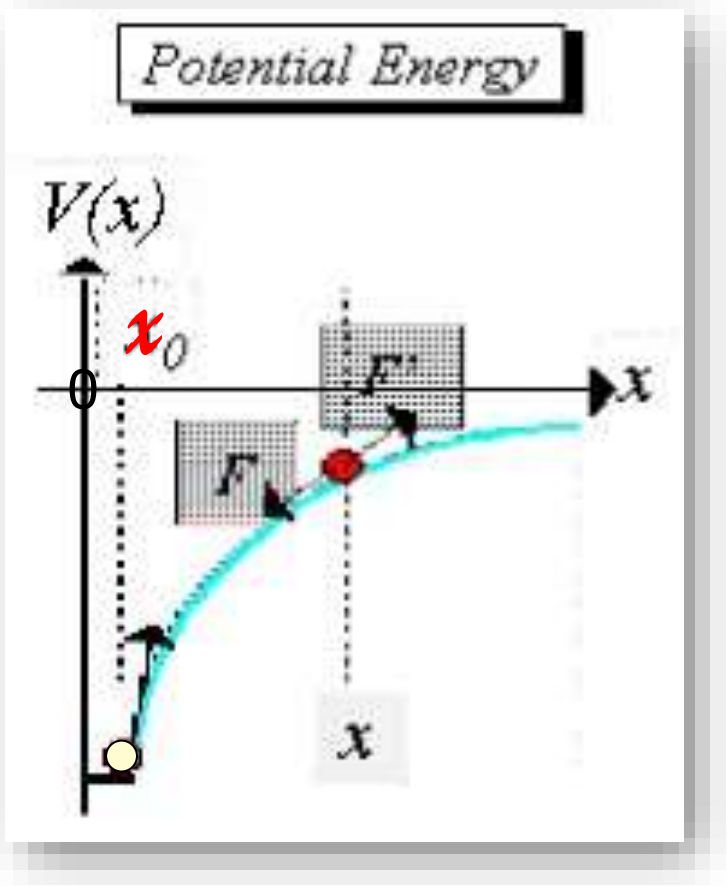
$$\Delta E = m \cdot g \cdot \Delta x \rightarrow w \equiv \Delta E$$

If the work $\boldsymbol{w}$ is done during time Δt, the mean power applied is

$$\Delta P = \Delta E / \Delta t = m \cdot g \cdot (\Delta x / \Delta t)$$

The body gains, as internal energy, the difference in gravitational potential energies at different heights x. Body can do work $w=-mg\Delta x$.

Work Against a Variable Force



Variable force F'(x), differential work:
Sum over (infinitely) many differentials *dw*

Lifting: $dw = F'(x)\cdot dx = -F(x)\cdot dx > 0$

→ Total work ***done on*** particle
in terms of potential energy difference:

$$\mathbf{w} = \int_{x_0}^{x} dw(x') = \int_{x_0}^{x} F'(x')\cdot dx' = -\int_{x_0}^{x} F(x')\cdot dx' \mathbf{>0}$$

$$w = -\int_{x_0}^{x} F(x')\cdot dx' = \int_{x_0}^{x} \frac{dV(x')}{dx'}\cdot dx' = V(x) - V(x_0) = \Delta V$$

In 3D components: $F \to \vec{F} = \begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix}$; $x \to \vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$

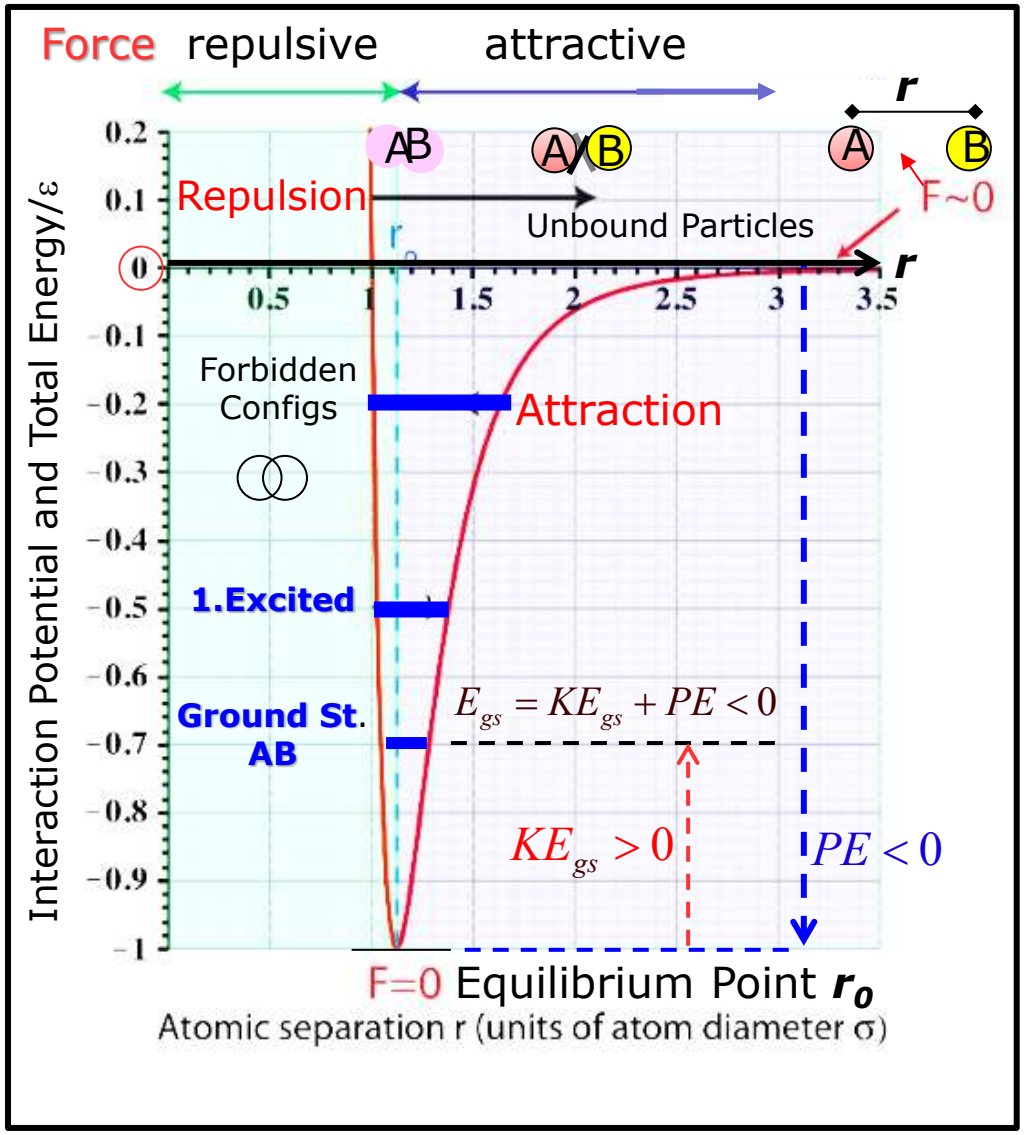
$$w = -\int_{\vec{r}_0}^{\vec{r}} \vec{F}(\vec{r})\cdot d\vec{r} = \int_{\vec{r}_0}^{\vec{r}} \vec{\nabla} V(\vec{r})\cdot d\vec{r} = V(\vec{r}) - V(\vec{r}_0)$$

Force =
Negative gradient: $F(x) = -\frac{dV(x)}{dx} \to 3D:$ $\vec{F}(\vec{r}) = -\vec{\nabla} V(\vec{r}) = -\begin{pmatrix} dV(\vec{r})/dx \\ dV(\vec{r})/dy \\ dV(\vec{r})/dz \end{pmatrix}$

Del or ***Nabla*** **Operator**

Potential Interaction Energy Between 2 Neutral Atoms

Lennard-Jones Interaction Potential



$$Potential\, V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$Force\, F(r) = -\frac{d}{dr}V(r)$$

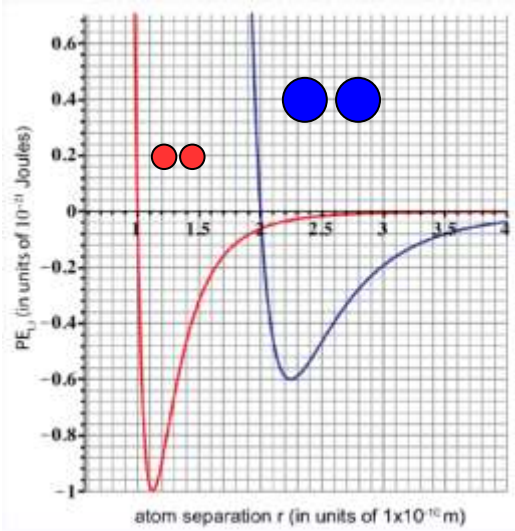
Separation distance r

Atom diameter σ

Dept of potential well ε (J)

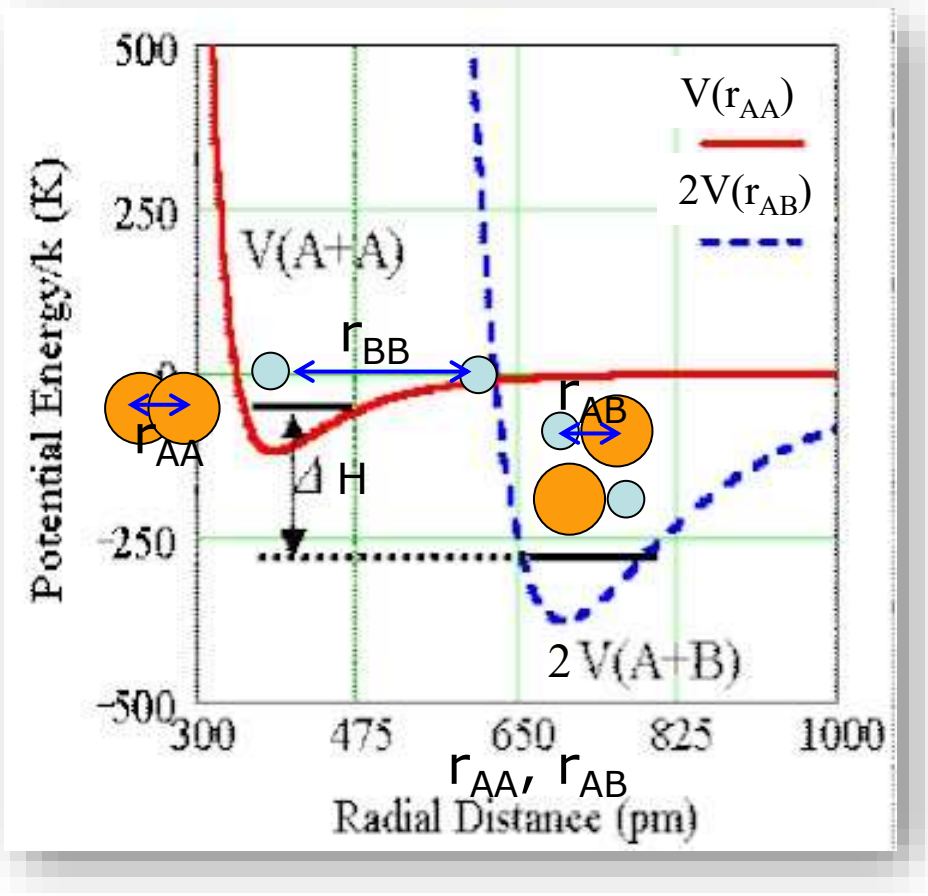
Discrete bound states E_i

Different Dimers

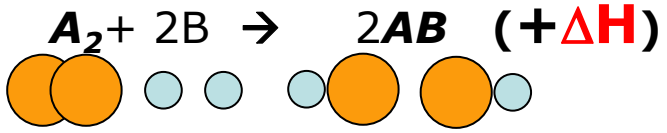


Energy Gain in Chemical Configuration Changes

Example: Covalent bonding
(Lennard-Jones potential)



Consider schematic reaction between one bound molecule ***A_2*** and 2 unbound atoms ***B*** forming 2 bound molecules ***AB***:



Enthalpy ΔH < 0: energy released from the molecular system (2***AB***)

Since *B* are individual atoms and not bound together, $V(B)=V_{B+B}=0$.

→ Reaction takes place if

$$2V_{A+B} < V_{A+A} + \underbrace{V_{BB}}_{=0} = V_{A2}$$

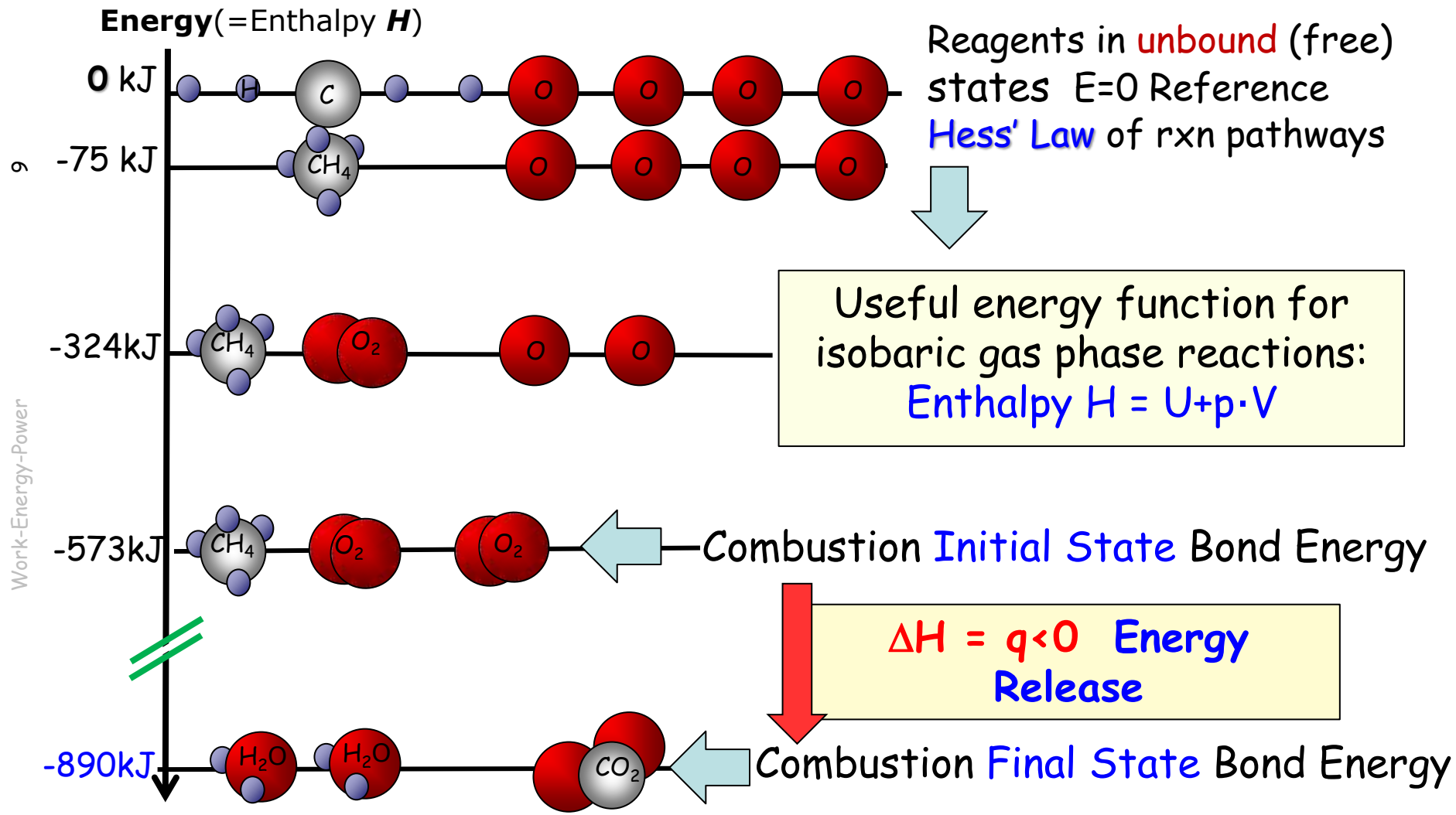
Reaction is exo-thermic (final system is more strongly bound).

Rearrangement of individual constituents of ensemble of atoms and molecules is associated with changes in interaction potential (bonding) energy.

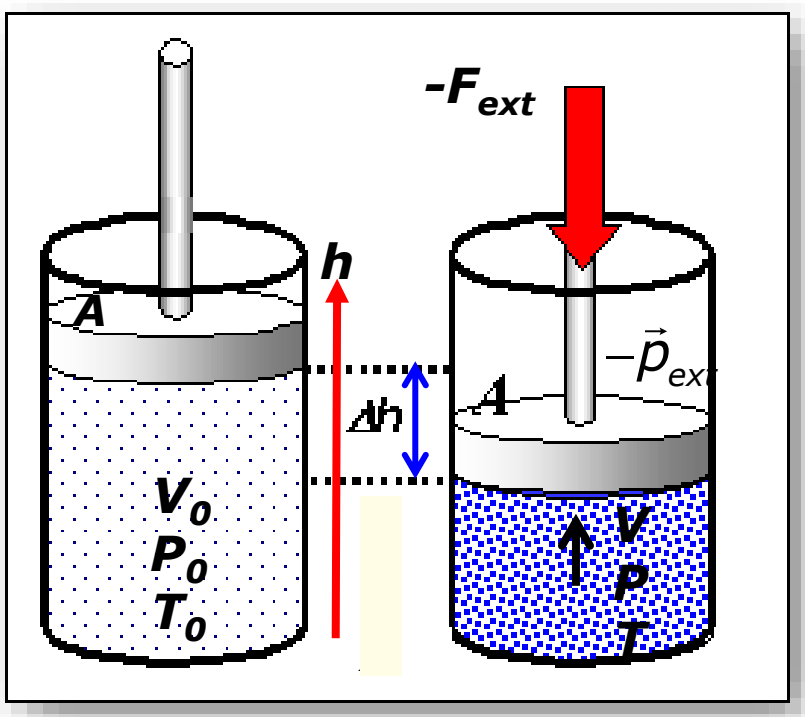
Example: Chemical Bond Changes in CH_4 Combustion

Example: burning natural gas $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O$ *(not spontaneous)*

Methane



Physical Kinetic Energy Changes in Compression



Gas=equilibrated ***system of independent particles moving in random directions.***

Compression of a gas volume *V* with a constant force *F* (e.g., weight) on a constant area *A*:

→ Pressure *p* = Force *F*/Area *A*,

at $p = p_{ext}$ =const.

(external, not internal)

$$p = \frac{-F_{ext}}{A} = p_{ext} \rightarrow \Delta V = A \cdot \underbrace{\Delta h}_{<0} < 0$$

Compression work done on system

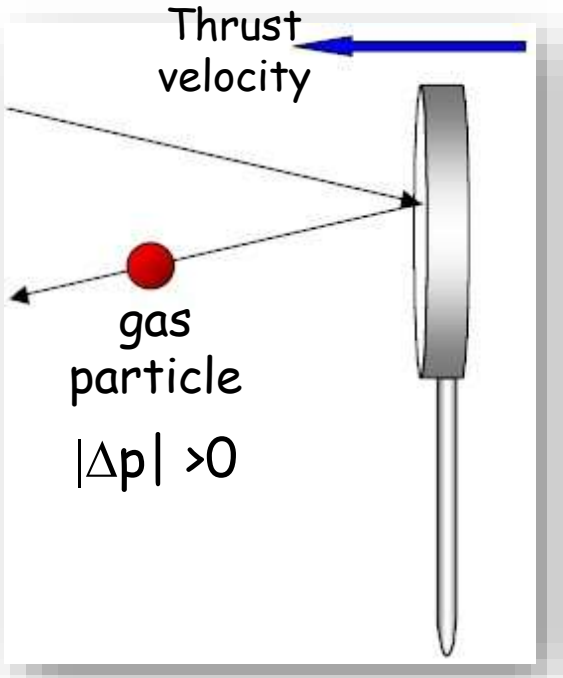
$$w = -F_{ext} \cdot \Delta h = -\left(p_{ext} \cdot A\right) \cdot \Delta h = -p_{ext} \cdot \underbrace{\Delta V}_{<0} > 0$$

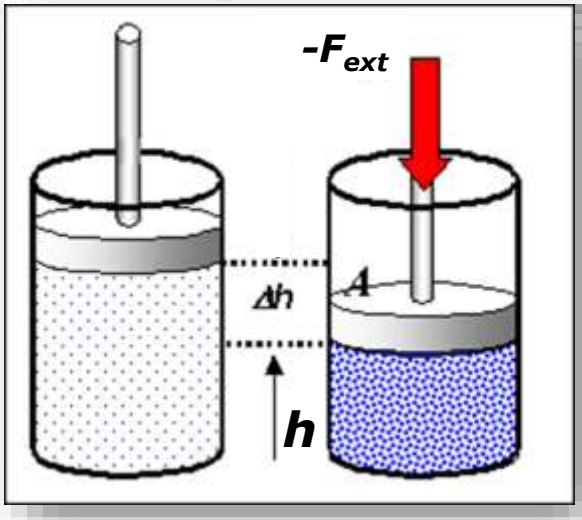
Sign Convention: Compressional work on a gas volume (=system) increases the internal energy ***E*** of the gas . → Temperature $T_0 \rightarrow T$

Therefore, work $w > 0$ is counted as positive (done on gas), Energy content increased.

Compression Work as Energy Transfer Mode

Energy and momentum are transferred to gas particles hit by a (collectively) moving piston, with magnitude depending on the relative velocity between piston and gas particle.





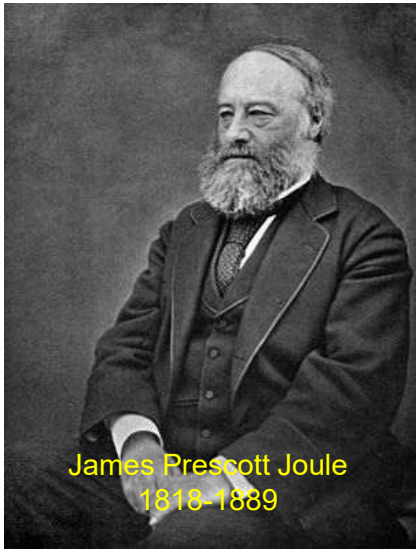
The effect is similar to that driving a tennis ball with a racket.

Thermally insolated system (cylinder with gas)

Compressed gas has more energy in random motion than before.

Transfer directed collective → random motion = dissipation of collective energy into heat.

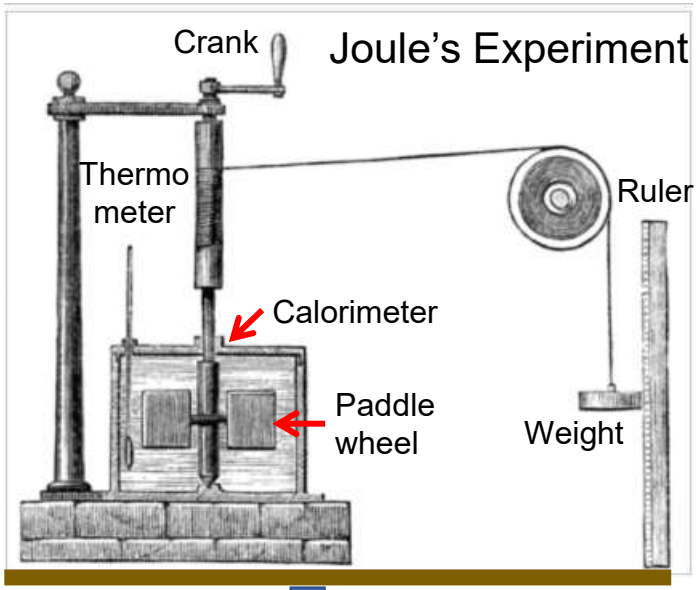
Mechanical Equivalent of Heat



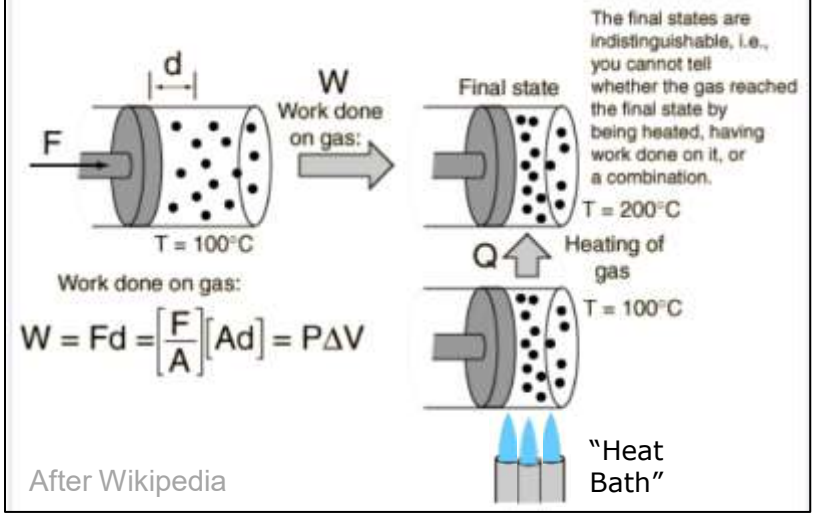
"An Experimental Enquiry Concerning the Source of the Heat which is Excited by Friction", (1798), Philosophical Transactions of the Royal Society p. 102

Work W $\propto$ *Q Heat*

$$W = J \cdot Q,\ J = 4.186 \frac{kJ}{kcal}$$



P-V Work equivalent to Heat



Specific Heat → Energy (ΔT): $Q = m \cdot C \cdot \Delta T$

Specific heat or heat capacity *C*

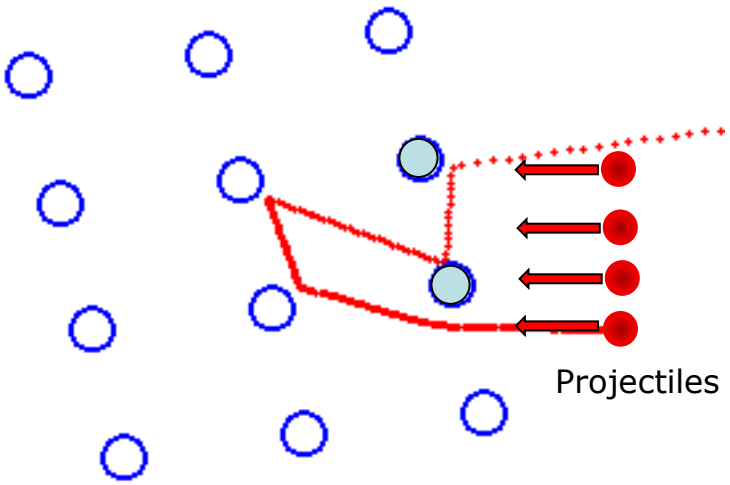
Heat energy ***Q*** required to raise temperature of ***m=1*** gram of a material by $\Delta T = 1^0C$
→ *material characteristic (T)*

of H_2O: $C_{water} \approx (4.17 - 4.22)\ J/(g \cdot °C)$
$C_{water\ ice} \approx 2.10\ J/(g \cdot °C)$

Energy Dissipation (Randomization)

Multiple Scattering @ Fixed Lattice

Lattice_Scattering.avi



Worst-case scenario: A solid lattice of heavy bound atoms or ions is hit by fast projectiles from the right. (In liquid or gas phases, there are no stationary particles.)

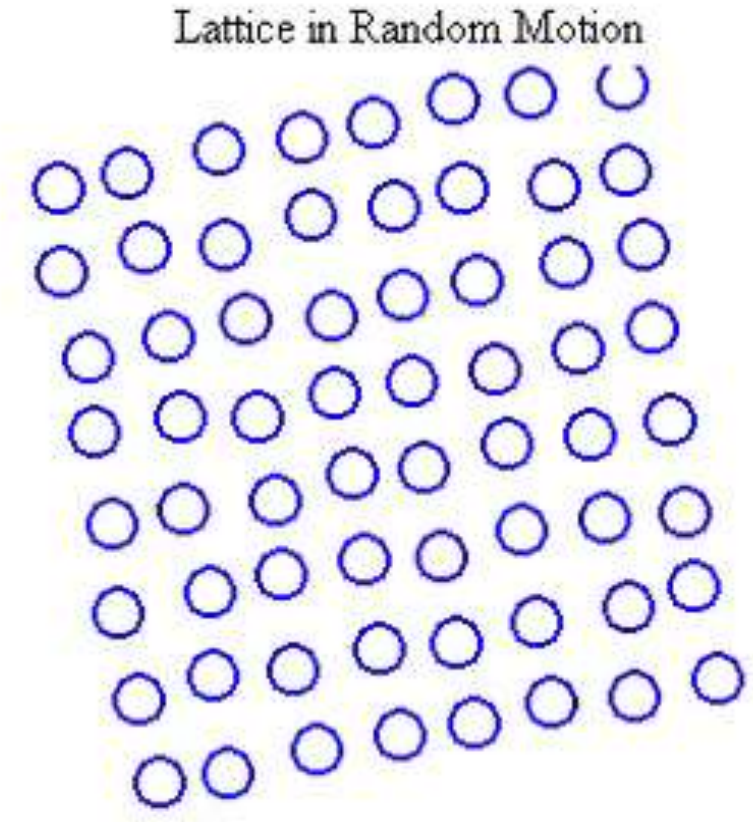
A number "projectile" particles enter the system at various initial conditions: positions from the right with identical momenta (e.g., kicked by racket).

Momentum and energy transfer from incoming particle depends very strongly on how and where the first lattice particle is hit.

The result is a random pattern of projectile deflections, momenta and energies. The particles hit by the projectiles are also accelerated and deflected to various extents. They themselves become projectiles and collide with other gas particles. In this fashion, the energy of the projectile is dissipated over all particles in the system.

Collisions with unbound, moving **gas** particles are "much more" random than collisions with a periodic solid-sate lattice structure. More complex structures arise naturally (spontaneously) via collisions between particles.

Thermal Motion in Solids



The individual constituents (atoms or ions) of an excited lattice have on average the same thermal energy. If one increases this average energy by introducing energy from the surroundings, the displacements of the particles increase.

→ ***Thermal Fluctuations***

At higher excitations, the structure begins to disappear, the lattice is "melting", becomes a liquid and, eventually, a gas.

→ max fluctuations

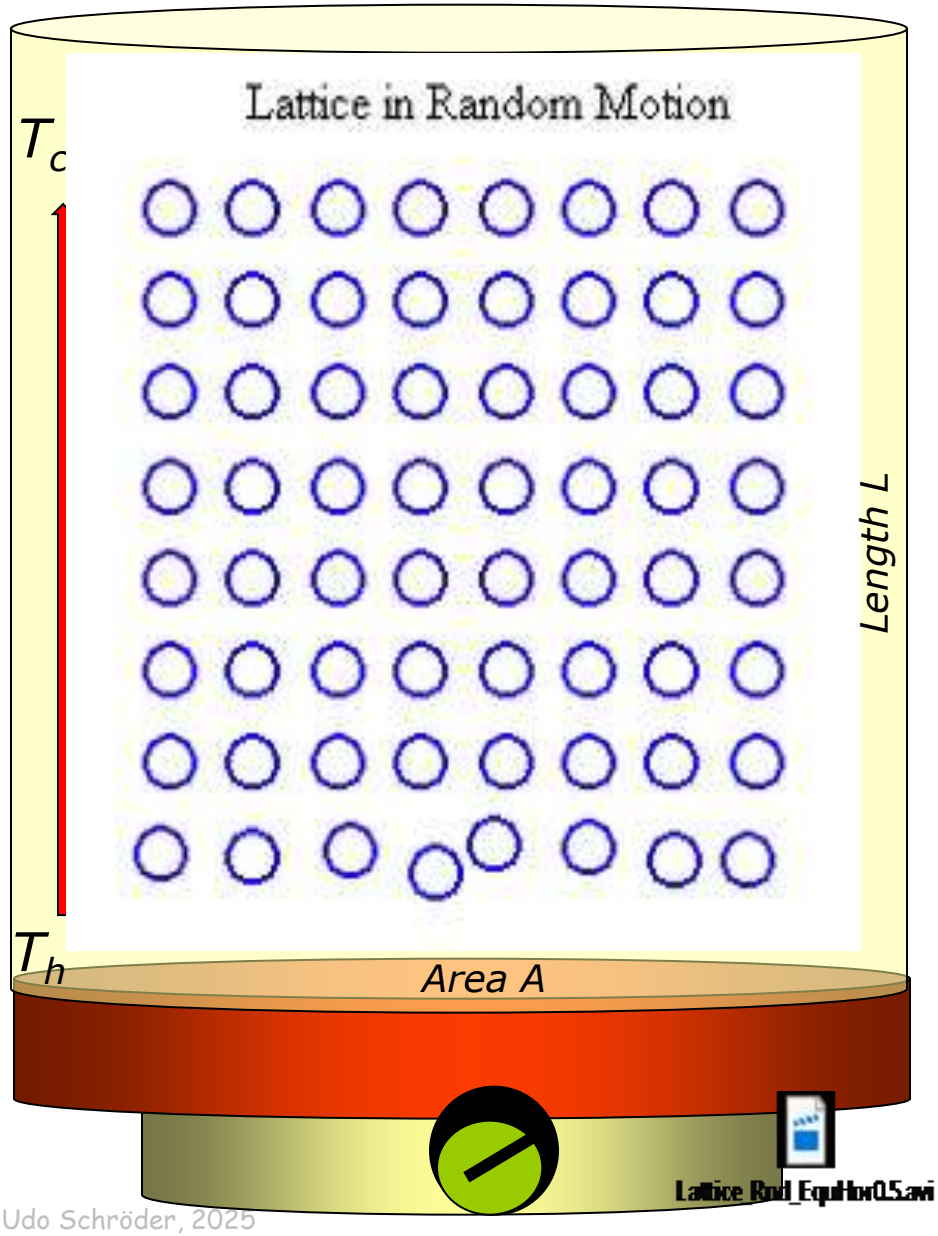
The average kinetic energy of each particle is known as "temperature *T*" (units of k_B)

$\boldsymbol{k_B}$=*1.380649×10⁻²³ J/K*

$$\langle \varepsilon \rangle = (1/2) \cdot k_B T \quad \textit{per particle}$$

per degree of freedom

Conduction of Thermal Energy in Solids



External energy and/or density disturbances propagate through its volume *V*, e.g., its solid lattice.

$$\frac{dq}{dt} = -\kappa A \frac{(T_c - T_h)}{L} \rightarrow \text{conductivity } \kappa$$

$$3D: \quad \vec{j}_q = \frac{d\vec{q}}{A \cdot dt} = -\kappa \cdot \vec{\nabla} T$$

Energy flow: hot → cold

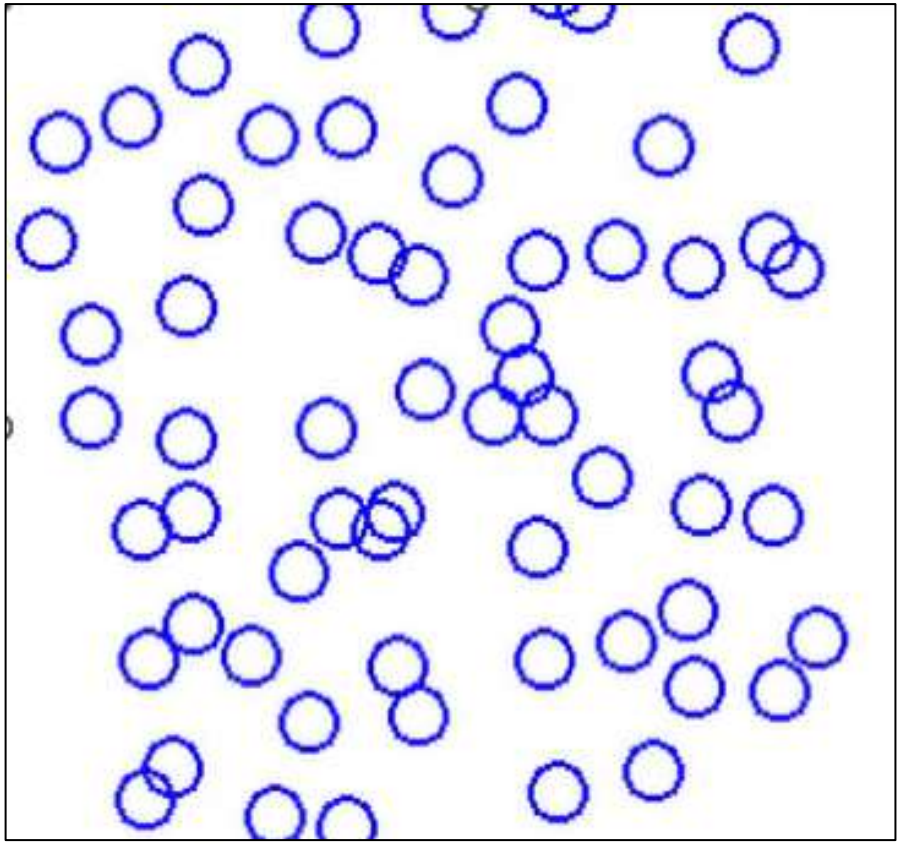
System expands in spatial dimensions

$$dV = V \cdot (1 + \alpha \cdot dT)$$

$$\rightarrow \alpha = \text{volume expansion coeff}$$

Systems at any temperature emit thermal radiation (IR photons), which can be absorbed (possibly re-emitted) by objects in the environment.
Stefan-Boltzmann Law

Thermal Motion in Liquids/Solutions



$$\langle \varepsilon \rangle = (1/2) \cdot k_B T \quad \textit{per particle}$$
$$\textit{per degree of freedom}$$

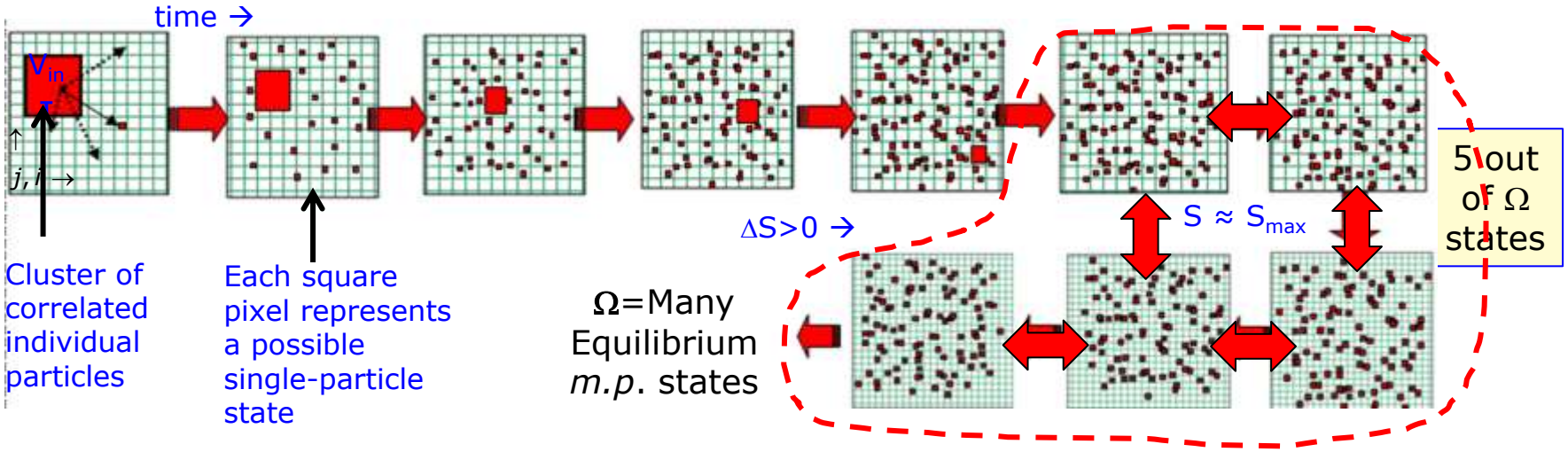
A finite crystal lattice (crystal) is in contact with a thermal heat bath at T. If ***T*** is raised above a characteristic threshold (atom-atom binding energy = latent heat of melting/fusion= ΔH_{fus}), lattice bonds can break sequentially. Atoms with sufficient energy at and near the surface are freed and released to the surroundings, shrinking the remaining crystal bulk. This process of melting proceeds spontaneously until the crystal has melted entirely.

Main difference between liquids and gases is the strength of particle interactions, a function of mean distance between particles, density.

At higher excitations, the structure begins to disappear, the lattice is "melting", becomes a liquid and, eventually, a gas..

Spontaneous Dissolution/Evaporation of Cluster

Cluster of correlated particles in a hot container (Heat Bath) → Transitions to multi-particle (*m.p.*) states are spontaneous and irreversible.



Natural direction of spontaneous process: Number Ω of visited multi-particle states increases in time, from simple to complex.

➔ Essentially irreversible.

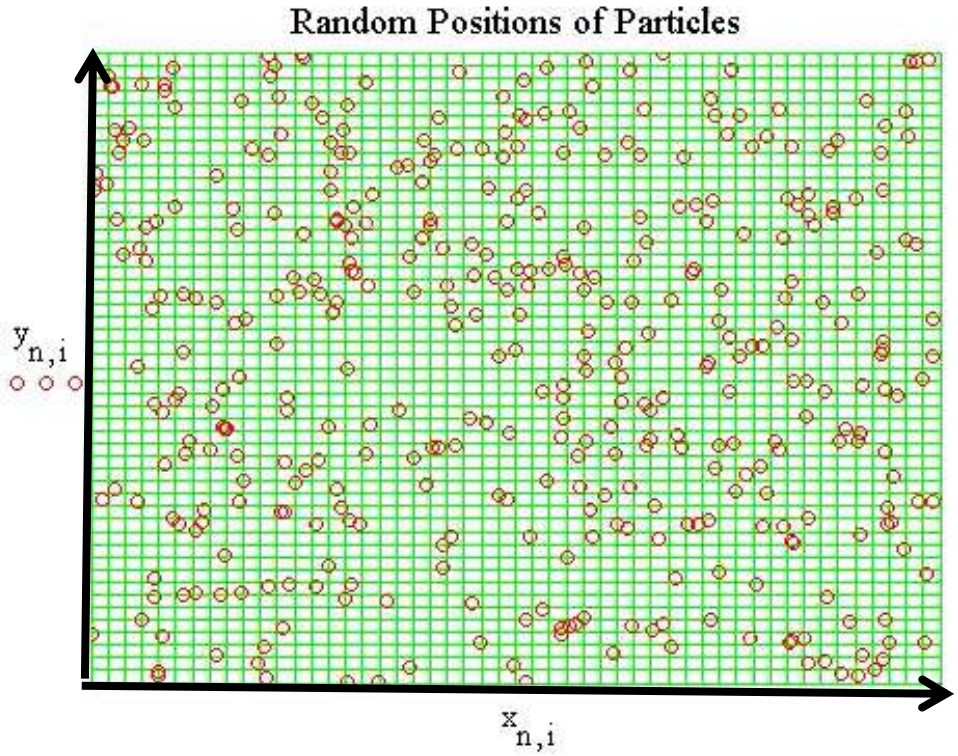
2. Law of TD: Entropy increases in spontaneous processes

$$\#\ visited\ m.p.\ states\ (configs) = \Omega = \Omega(disorder, complexity)$$

$$Entropy\ \ S := k_B \cdot Ln\ \Omega = -k_B \cdot \sum_{i,j} p_{ij}\ Ln\ p_{ij}$$ = State Function

$$S/k_B := Ln\ \Omega \ \rightarrow\ \Omega(S) = \exp\{S/k_B\}\ \ increases\ w.\ complexity$$

Random (Thermal) Motion in Space



Example: Motion in two dimensions of 300 non-interacting (ideal-gas) particles.

All particles move in random directions because of multiple collisions, which actually occur but are not explicitly visualized here.

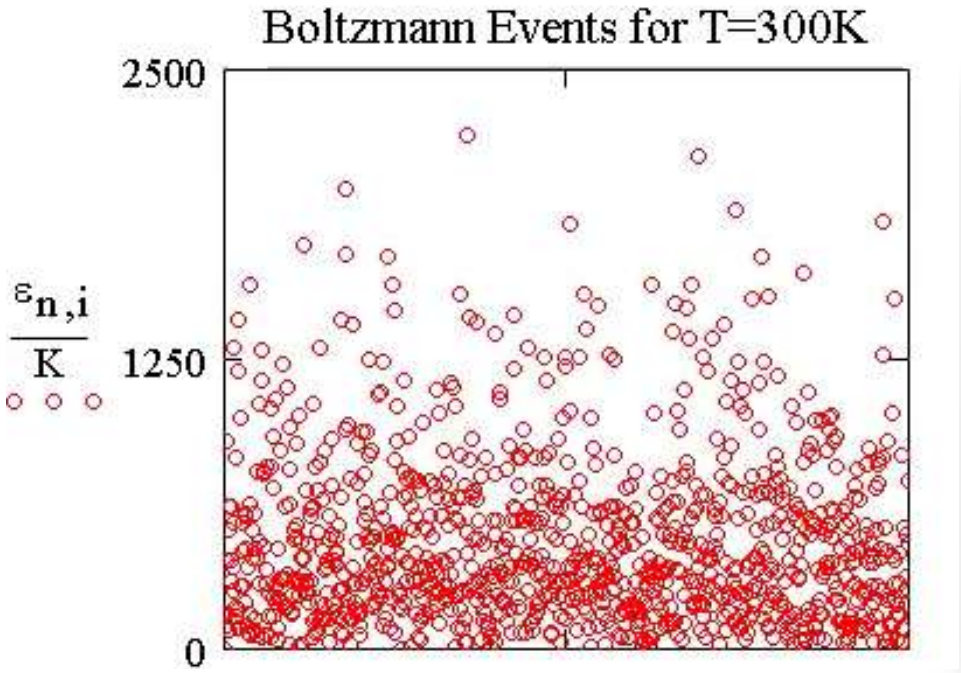
Every particle visits every one of the energetically equivalent cells.

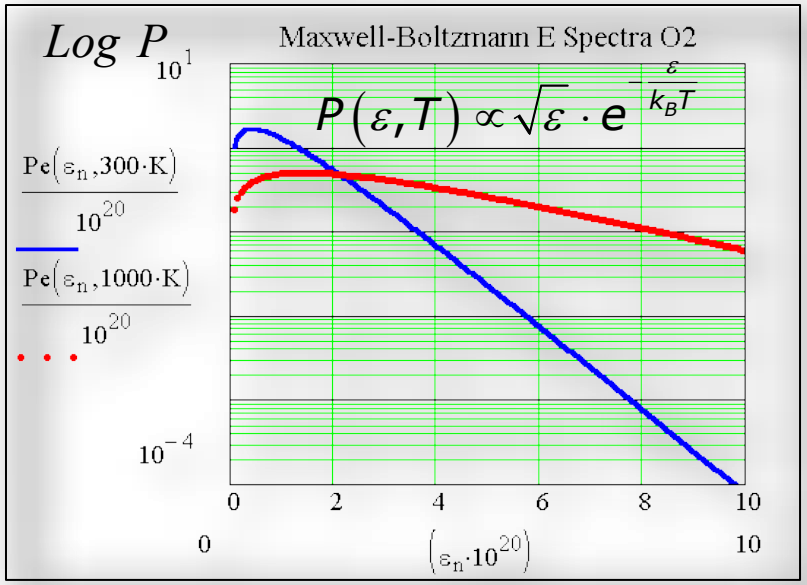
Contrast: Collective motion.

Particles in a gas move in different directions and at different speeds, colliding with one another often. Eventually, their positions at any given time are random. All available (accessible) space is visited by all particles, in due time.→ Ergodic Theorem

Rnd_Positions.avi

Gases in Randomized State (Thermal Equilibrium)



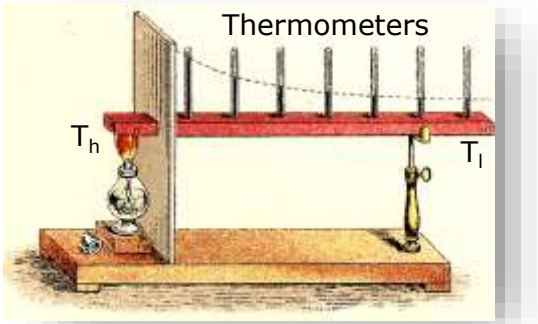


N Gas particles collide continuously. Multiple collisions lead to different momentum and energy transfers with random probabilities. The result is a characteristically fluctuating ("thermal") "Maxwell-Boltzmann" kinetic-energy spectrum → temperature of the gas.

$$Kin.\ Energy\ E = N \cdot (3/2) k_B \cdot T$$

(In the ***ideal gas*** model, particles are structureless point particles, only kinetic energy is considered explicitly. No potential energy since no interactions are)

Transfer of Randomized Energy: Heat Flow



Heat conduction, flow through area A = current density= flux

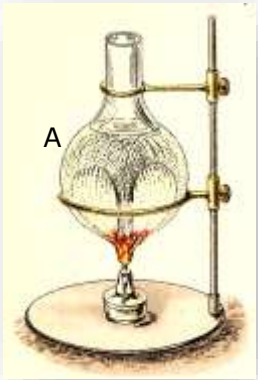
$$j_q = (dQ/dt) / A$$

$$\textit{Fourier's Law}: \vec{j}_q = -\kappa \cdot \vec{\nabla} T(\vec{r}) = -\kappa \cdot \left(\frac{\partial T}{\partial x}\vec{i} + \frac{\partial T}{\partial y}\vec{j} + \frac{\partial T}{\partial z}\vec{k} \right)$$

Thermal conductivity κ (W/mK)

Heat flow directed by T gradient

https://www.schoolmykids.com/learn/interactive-periodic-table/thermal-conductivity-of-all-the-elements



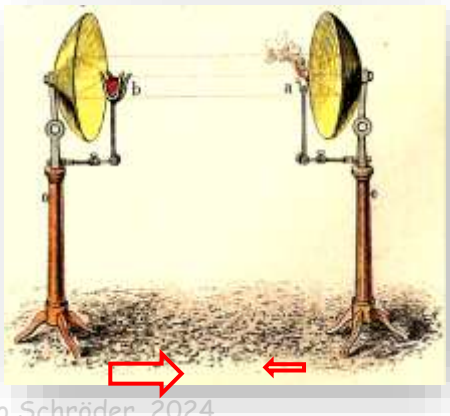
Heat convection: Heat transfer via particles (mass flow)

Newton's Law of cooling $dQ/dt = -h \cdot A \cdot (T - T_{ambient})$

Heat transfer coefficient h (W/m^2K); *area* A

Heat flow directed by T gradient

Heat transport relation: *convection* $\leftrightarrow$ *conduction*



Heat radiation: Heat transfer via elm. photons

Stefan – Boltzmann Law

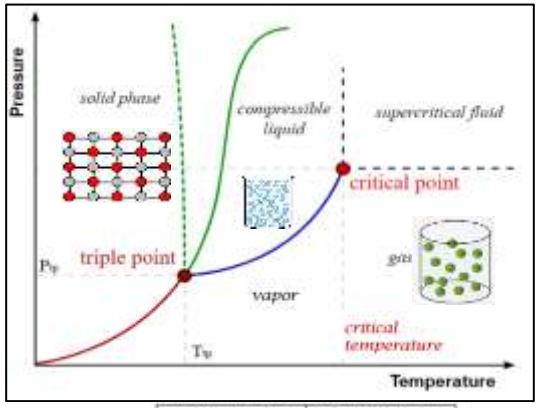
Radiated thermal flux $j_Q = \varepsilon \cdot \sigma_{SB} \cdot T^4$ *isotropic*

Emissivity ε (*often set* $\varepsilon \approx 1$)

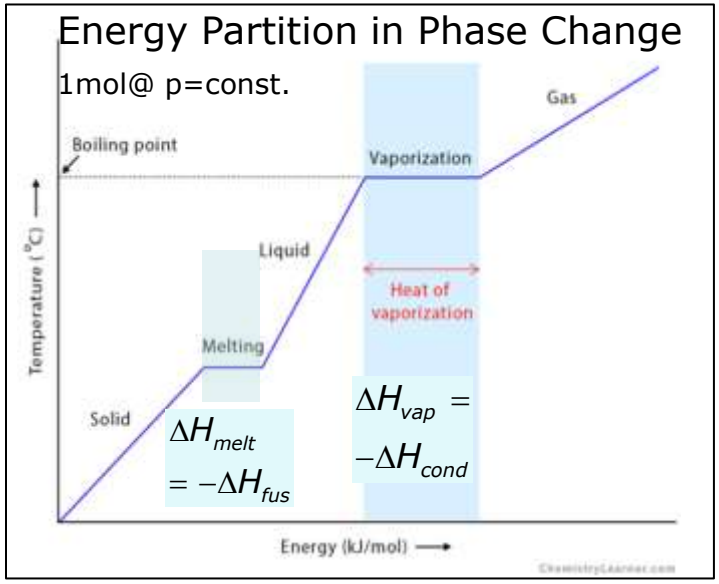
Stefan – Boltzmann constant $\sigma_{SB} = 5.6703 \cdot 10^{-8}\, W/m^2K^4$

Energy Repartition in Physical Configuration (Phase) Changes

Phase Diagram H_2O



Material	Formula	Critical pressure P_c psia	Critical pressure P_c bar (abs)	Critical temperature T_c °F	Critical temperature T_c °C	$k = C_p/C_v$
Water	H_2O	3206	221	705	374	1.32



Internal structural energy : 1*mole substance*

extensive (additive) state function energy U

Enthalpy = *Structural Energy* +

$+ p - V$ *work to access space*

$\rightarrow \quad H = U + P \cdot V$

Process @ $p = const \rightarrow \Delta H\big|_p = \Delta U + p \cdot dV$

$H =$ "*extensive*" *state function*

Reference "*zero*" *energy* H^0 @ *standard state*

$T = 25^0 C$, $P = 1 bar \leftarrow$ *large databases*

$H^0 = 0$ *for pure elemental substances*

Phase changes $\rightarrow \Delta H \neq 0$

latent heat transfer $\rightarrow$

ΔU *to change internal structure*

@ *phase transition* : $\Delta T = 0$

@ $1 bar$, $T = 100^0 C$ ($\neq$ *the standard state*)

$H_2O(\ell) \rightarrow H_2O(g) \rightarrow \Delta H_{vap} = +40.7\, kJ/mol$

$H_2O(g) \rightarrow H_2O(\ell) \rightarrow \Delta H_{cond} = -40.7\, kJ/mol$

	ft lb	kWh	hph	Btu	Calorie	Joule
ft lb	1	3.766×10^{-7}	5.050×10^{-7}	1.285×10^{-3}	0.324	1.356
kWh	2.655×10^{6}	1	1.341	3.413×10^{3}	8.606×10^{5}	3.6×10^{6}
hph	1.98×10^{6}	0.745	1	2.545×10^{3}	6.416×10^{5}	2.684×10^{6}
Btu	778.16	2.930×10^{-4}	3.930×10^{-4}	1	252	1.055×10^{3}
Calorie	3.086	1.162×10^{-6}	1.558×10^{-6}	3.97×10^{-3}	1	4.184
Joule	0.737	2.773×10^{-7}	3.725×10^{-7}	9.484×10^{-4}	0.2390	1

End
Work/Energy/Power I