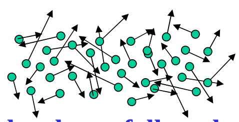
Georgia Tech College of Engineering
School of Aerospace Engineering

Introductory Gas Kinetic Theory

- Approach to understanding gas properties - both equilibrium and nonequilibrium (rates) by examining
  - translational **motions** of molecules and
  - their interactions or **collisions**
- In most systems of interest, there are large number of molecules present
  - SATP ~3×10^{19} molec/cm^3 or in V=(10μm)^3 we have 30×10^9 molecules >> human population
  - each molecule in constant state of motion and with different velocities



  - **too many molecules to follow them all individually ⇒use statistical approach**

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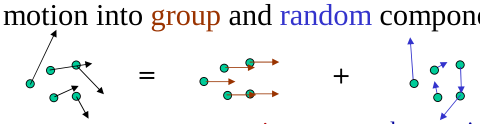
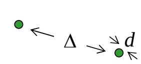
Random (Statistical) Motion

- Break motion into group and random components



- Random motion is free motion of molecules, until a "collision" with another molecule or surface
  - free motion means molecule moves in straight line between collisions
  - significant time spent in free/straight-line motion; this is why gas is different from liquid/solid
  - why? – related to large spacing between molec. d~3Å=3×10^{-8} cm; Δ_{avg}~$n^{-1/3}$ @SATP=3×10^{-7} cm



$$\frac{\Delta}{d} \sim O(10)$$

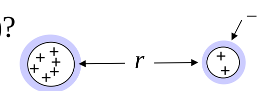
will show later $\lambda >> \Delta >> d$

Summary: Gas Kinetic Theory

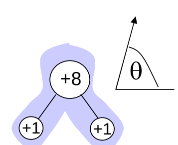
- Examines properties of statistical motion of all molecules, not trying to follow each one
  - valid only for large numbers of molecules
- Assumes molecules spend most of their time moving in straight lines between collisions
  - but molecules do interact
  - need models to describe molecular interactions

Molecular Models

- How do molecules interact ("collide")?
  - through force fields
    - attractive: electrostatic + ↔ – (, gravity, …)
    - repulsive: electrostatic + ↔ + (,Pauli exclusion,…)



- Simplifications to force models
  1) often assume only elastic collisions, no internal energy changes
  2) assume **spherically symmetric** force fields
     - only function of separation (r), not θ, ϕ
     - not strictly true, e.g., polar molec. like H_2O (but rotations tend to avg. out directionality)



Intermolecular Potentials

- Model **short range attractive** intermolecular forces of **neutral** molecules with electrostatic potentials

$$V_{attr}(r) = -\sum_{\alpha=1}^{\infty} \frac{B_\alpha}{r^\alpha}$$

$$F = -\frac{dV}{dr} = \sum_{\alpha=1}^{\infty} \alpha \frac{B_\alpha}{r^{\alpha+1}}$$

- α=1 monopole-monopole (Coulomb)
- α=2 monopole-dipole (e^- - H_2O)
- α=3 dipole-dipole (H_2O – H_2O)
- α=4 dipole-quadrupole
- α=6 dipole-induced dipole
  induced dipole - induced dipole
- α→∞ hard-sphere (no attraction)

- Also **repulsive terms**
  - e.g., when electron fields overlap
  - can also use power laws

Intermolecular Potentials

- Examples, Lennard-Jones 12-6 and 9-6 potentials

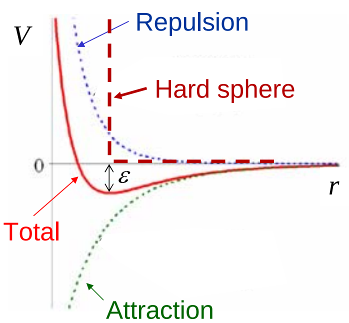
$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

LJ "diameter"

$$V(r) = \varepsilon\left[2\left(\frac{\sigma}{r}\right)^{9} - 3\left(\frac{\sigma}{r}\right)^{6}\right]$$

"well-depth"

separation distance



- Simplest model
  - elastic, **rigid hard sphere** or **billiard ball** model
  - gives useful results