

Physical Principles in Biology
Biology 3550
Spring 2025

Lecture 18:

Thermal Motion of Molecules

Wednesday, 19 February 2025

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Announcements

■ Quiz 3:

- Friday, 21 February
- 25 min, second half of class.
- A ruler might come in handy!

■ Problem set 3:

- Due 11:59 PM, Wednesday, 26 February.
- Download problems from Canvas.
- Upload work to Gradescope and, optionally, Canvas (spreadsheet)!
- Work must be typed!

■ Discussion/Problem-solving Session:

- Wednesday, 3:00 P.M. - CSC 13

■ Instructor Office hours:

- Wednesdays, 11:00 AM - ASB 306
- Other times by appointment

Kinetic Energy

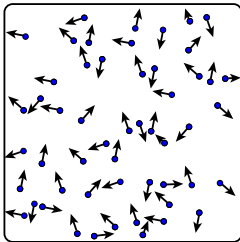
- A object of mass, m , moving with velocity, v , in the x -direction has kinetic energy in that direction of:

$$E_{k,x} = mv_x^2/2$$

- What does this mean?
 - The energy required to accelerate the mass, m , from rest to velocity, v_x .
 - Also the energy released during the deceleration of the mass from velocity, v_x , to rest.
 - Kinetic energy does not depend on the rate of acceleration or deceleration, only the final velocity.

Kinetic Energy of Molecules

- Temperature is the measure of kinetic energy of molecules.
- How do we measure temperature?
- Pressure of a gas is due to the collision of molecules against container walls.



$$PV = nRT$$

P = pressure, V = volume, n = number of moles, T = temperature,
 R = gas constant.

Clicker Question #1

$$PV = nRT$$

What are the units of the gas constant?

A) pascal \cdot L \cdot K⁻¹mol⁻¹

B) kg \cdot m²s⁻²K⁻¹mol⁻¹

C) m³bar \cdot K⁻¹mol⁻¹

D) JK⁻¹mol⁻¹

E) L \cdot atm \cdot K⁻¹mol⁻¹

All of the above!

Units of the Gas Constant

- From the ideal gas law:

$$R = \frac{PV}{nT}$$

- In SI basic units:

Pressure, force per unit area: $\text{kg} \cdot \text{m} \cdot \text{s}^{-2} \div \text{m}^2 = \text{kg} \cdot \text{m}^{-1} \text{s}^{-2} = \text{Pa}$

Volume: m^3

$$\text{Gas constant: } \frac{\text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-2} \times \text{m}^3}{\text{K} \cdot \text{mol}} = \text{kg} \cdot \text{m}^2 \text{s}^{-2} \text{K}^{-1} \text{mol}^{-1}$$

- Joule (unit of energy) = $\text{Nm} = \text{kg} \cdot \text{m}^2 \text{s}^{-2}$
- The gas constant expressed in energy units:

$$R \approx 8.314 \text{ J K}^{-1} \text{mol}^{-1} \approx 1.987 \text{ cal} \cdot \text{K}^{-1} \text{mol}^{-1}$$

- The kinetic energy of a molecule at temperature T is proportional to RT .

Kinetic Energy of Molecules

- The Boltzmann constant, k , the “gas constant per molecule”:

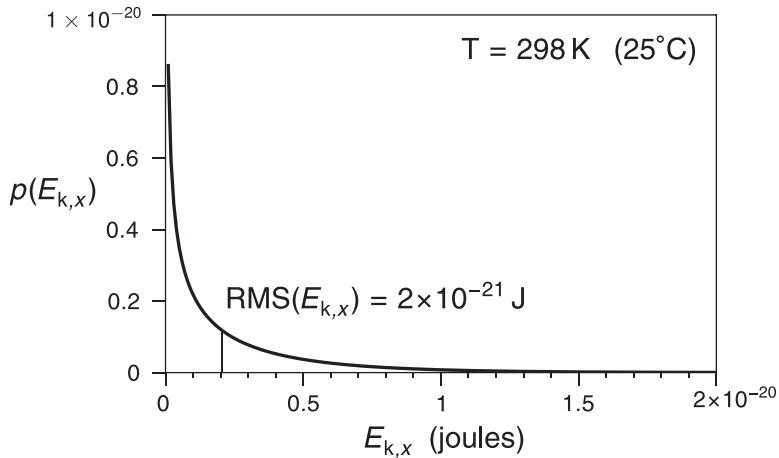
$$\begin{aligned}k &= R/N_A = 8.314 \text{ JK}^{-1}\text{mol}^{-1} \div 6.02 \times 10^{23} \text{ molecule/mol} \\&= 1.38 \times 10^{-23} \text{ JK}^{-1}\end{aligned}$$

- Molecules at a given temperature do not have unique velocities or kinetic energies.
- Molecules have a broad distribution of energies, with RMS average translational kinetic energy in each direction (x , y or z):

$$\text{RMS}(E_{k,x}) = kT/2$$

- Translational kinetic energy does *not* depend on mass or structure.
- In context of molecular motion, “ $E_{k,x}$ ” will imply RMS value.

Distribution of Molecular Kinetic Energies



$$p(E_{k,x}) = \frac{1}{\sqrt{\pi E_{k,x} kT}} e^{-E_{k,x}/(kT)}$$

Clicker Question #2

How fast does a small molecule move at room temperature
(between collisions)?

A) 10^{-4} m/s

B) 10^{-2} m/s

C) 1 m/s

D) 10^2 m/s

E) 10^4 m/s

All answers count for now.

Velocities of Molecules

- Kinetic energy of a molecule, in x -direction: $\text{RMS}(E_{k,x}) = kT/2$
- Kinetic energy of any object: $E_{k,x} = mv_x^2/2$
- Solving for v :

$$mv_x^2/2 = kT/2$$

$$v_x^2 = kT/m$$

$$v_x = \sqrt{kT/m}$$

(also an RMS value)

- Velocity increases with \sqrt{T} and decreases with \sqrt{m} .
- Energy does not depend on molecular mass, but velocity does.

Velocity of an N₂ Molecule at Room Temperature

■ Mass

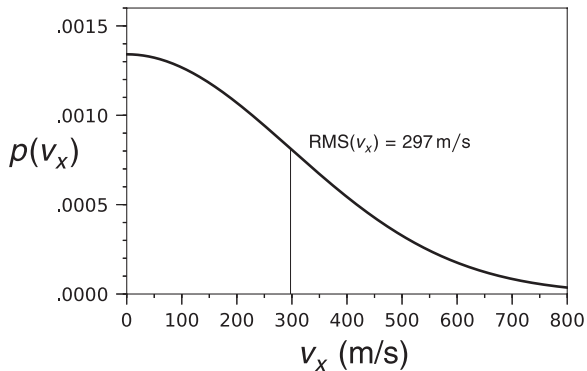
$$\begin{aligned} m &= 28 \text{ g/mol} \div 6.02 \times 10^{23} \text{ molecules/mol} \\ &= 4.65 \times 10^{-23} \text{ g} = 4.65 \times 10^{-26} \text{ kg} \end{aligned}$$

■ Temperature = 25°C = 298 K

■ Velocity:

$$\begin{aligned} \text{RMS}(v_x) &= \sqrt{kT/m} \\ &= \sqrt{1.38 \times 10^{-23} \text{ kg} \cdot \text{m}^2\text{s}^{-2}\text{K}^{-1} \times 298 \text{ K} / 4.65 \times 10^{-26} \text{ kg}} \\ &\approx 300 \text{ m/s} \quad (1,000 \text{ km/hr}) \end{aligned}$$

Distribution of N₂ Velocities in a Gas at 298 K



- The Maxwell-Boltzmann distribution

$$p(v_x) = \sqrt{\frac{m}{2\pi kT}} e^{-mv_x^2/(2kT)}$$

(assumes ideal gas behavior)

Diffusion of Bromophenol Blue Revisited

■ From diffusion experiment: $D = 2 \times 10^{-10} \text{ m}^2/\text{s}$

■ Definition of the diffusion coefficient: $D = \frac{\delta_x^2}{2\tau}$.

■ δ_x/τ = velocity, which we can calculate now!

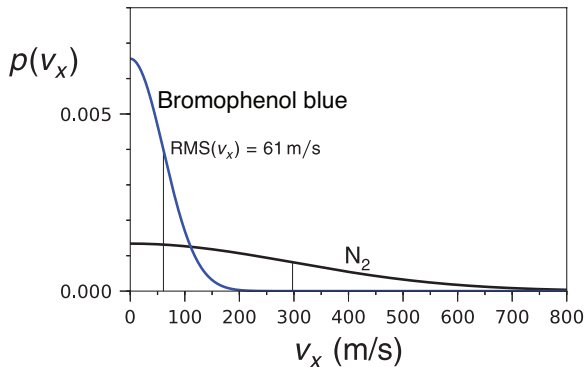
- $v_x = \sqrt{kT/m}$

- Molar mass = 670 g/mol

Molecular mass = $1.11 \times 10^{-24} \text{ kg}$

$$\begin{aligned} v_x &= \sqrt{1.38 \times 10^{-23} \text{ kg} \cdot \text{m}^2\text{s}^{-2}\text{K}^{-1} \times 298 \text{ K} / 1.1 \times 10^{-24} \text{ kg}} \\ &= 61 \text{ m/s} \end{aligned}$$

Distribution of Velocities at 298 K



- Average (RMS) kinetic energies of molecules are the same.
- Based on ideal gas behavior.
- Distribution is similar in liquids.

Diffusion of Bromophenol Blue Revisited

- $D = \delta_x^2 / (2\tau) = 2 \times 10^{-10} \text{ m}^2/\text{s}$

- Express D in terms of velocity:

$$D = v_x \delta_x / 2$$

- $v_x = \delta_x / \tau = 61 \text{ m/s}$

- Solve for δ_x

$$\begin{aligned}\delta_x &= 2D / v_x = 2 \times 2 \times 10^{-10} \text{ m}^2/\text{s} \div 61 \text{ m/s} \\ &= 6.5 \times 10^{-12} \text{ m}\end{aligned}$$

Diffusion of Bromophenol Blue Revisited

- From the previous slide

$$\delta_x = v_x \cdot \tau = 6.5 \times 10^{-12} \text{ m}$$

- Solve for τ

$$v_x = \delta_x / \tau$$

$$\begin{aligned}\tau &= \delta_x / v_x = 6.5 \times 10^{-12} \text{ m} \div 61 \text{ m/s} \\ &= 10^{-13} \text{ s} = 0.1 \text{ ps}\end{aligned}$$

- VERY short distances and times!

Clicker Question #3

A “typical” protein molecule in water: $D = 1 \times 10^{-11} \text{ m}^2/\text{s}$ and $v_x = 6 \text{ m/s}$

What is the RMS step length, δ_x , as the molecule diffuses via a random walk?

A) $1 \times 10^{-13} \text{ m}$

B) $3 \times 10^{-13} \text{ m}$

C) $1 \times 10^{-12} \text{ m}$

D) $3 \times 10^{-12} \text{ m}$

E) $1 \times 10^{-11} \text{ m}$

$$D = \frac{\delta_x^2}{2\tau}$$

$$\delta_x = \frac{2D}{v_x} = \frac{2 \times 1 \times 10^{-11} \text{ m}^2/\text{s}}{6 \text{ m/s}} = 3.3 \times 10^{-12} \text{ m}$$

Clicker Question #4

A “typical” protein molecule in water: $D = 1 \times 10^{-11} \text{ m}^2/\text{s}$ and $v_x = 6 \text{ m/s}$.

What is the RMS average time between direction changes, τ , as the molecule diffuses via a random walk?

A) $5 \times 10^{-14} \text{ s}$

B) $5 \times 10^{-13} \text{ s}$

C) $5 \times 10^{-12} \text{ s}$

D) $5 \times 10^{-11} \text{ s}$

E) $5 \times 10^{-10} \text{ m}$

$$D = \frac{\delta_x^2}{2\tau}$$

$$\tau = \frac{\delta_x}{v_x} = \frac{3.3 \times 10^{-12} \text{ m}}{6 \text{ m/s}} = 5.5 \times 10^{-13} \text{ s}$$

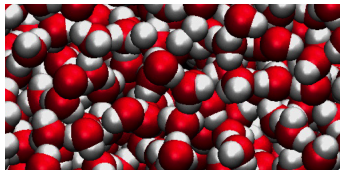
A Small Molecule Versus a Big One

	Bromophenol blue	Protein
Molar mass	670 g/mol	60,000 g/mol
Velocity	60 m/s	6 m/s
D	$2 \times 10^{-10} \text{ m}^2/\text{s}$	$1 \times 10^{-11} \text{ m}^2/\text{s}$
δ_x	$6 \times 10^{-12} \text{ m}$	$3 \times 10^{-12} \text{ m}$
τ	$1 \times 10^{-13} \text{ s}$	$5 \times 10^{-13} \text{ s}$

- How do we think about the numbers on a molecular scale?
- Have to think about liquids.

The Nature of Liquids

- Molecules are very densely packed
- Motions of molecules are limited by the “energy barriers” surrounding them.
- Other molecules in a solution are similarly constrained.
- Molecules move only very short distances before they change direction.
- The larger the molecule is, the less freedom it has and the more slowly it moves.



From a simulation of liquid water.

