



Photronics Center, Laboratory for Photoacoustics,  
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# L1 – Transport Processes in Physics

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As a result of a non-equilibrium **state**, any physical system tends to **return** to **equilibrium**.

This **return process** is followed by some kind of **transport** of **particles, heat, charges, etc.**

Transport processes are usually called **rate processes** due to their **time-dependence nature**.

In physics, we are dealing with **mass and energy** transport in terms of **particle** and **heat** transfer, respectively.



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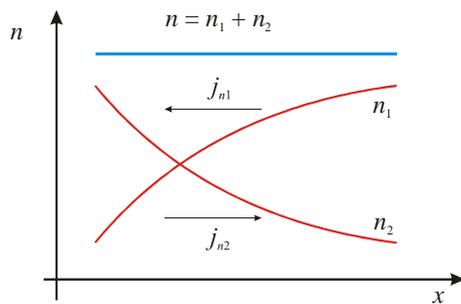


Particle transfer is usually explained in terms of **diffusion** and heat transfer is usually explained in terms of **thermal conductivity**.

Constitutive equations (fluxes) for both of them are first established **empirically**:

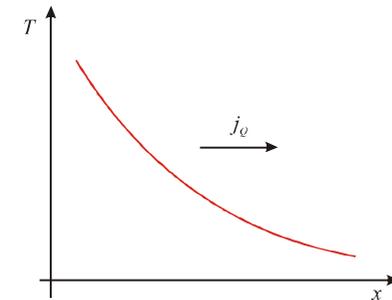
**diffusion**

**thermal conductivity**



$$j_{n_i} = -D \frac{\partial n_i}{\partial x}$$

$$j_Q = -k \frac{\partial T}{\partial x}$$

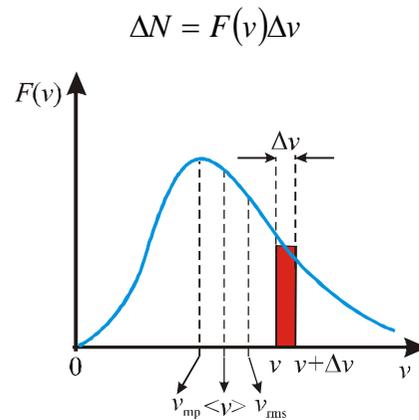


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## Transport Processes Molecular-Kinetic Explanation



In physics, **Maxwell distribution**  $F(v)$  is a particular **probability distribution** first defined and used for describing **particle speeds**  $v$  in ideal gases.

The term "particle" in this context refers to **gaseous particles** (atoms and molecules) and the **system of particles** is assumed to have reached **thermodynamic equilibrium**.

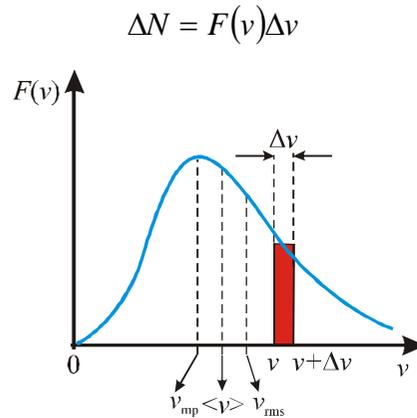


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## Transport Processes Molecular-Kinetic Explanation



In thermodynamic equilibrium there are **no net macroscopic flows** of mass or energy, either **within** a system or **between** systems; macroscopic equilibrium exists.

In a **macroscopic equilibrium**, almost or perfectly exactly balanced **microscopic exchanges occur**; this is the physical explanation **of the notion** of macroscopic equilibrium.

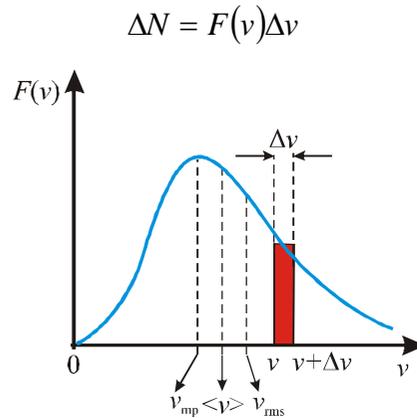


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## Transport Processes Molecular-Kinetic Explanation



A system in thermodynamic equilibrium has a **spatially uniform intensive properties** (temperature, pressure, density,...). All of them may be driven to **local spatial inhomogeneity** (non-equilibrium).

In non-equilibrium there are **net flows** of mass or energy, either **within** a system or **between** systems; transport processes occurs.

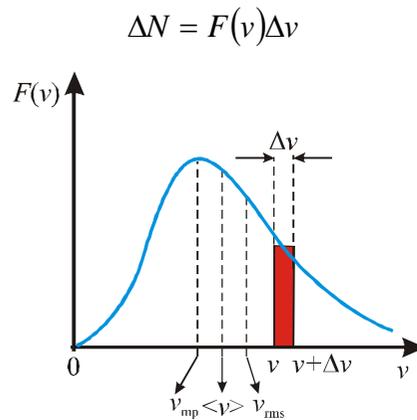


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## Transport Processes Molecular-Kinetic Explanation



The Maxwell distribution is a result of the **kinetic theory of gases** which provides a simplified explanation of many fundamental **gaseous properties** in the terms of **particle movement** (*pressure and diffusion*).

Diffusion is **particle transfer process** based on the net movement of particles as a result of their **random motion**. Diffusion also can explain **heat transfer** as well.

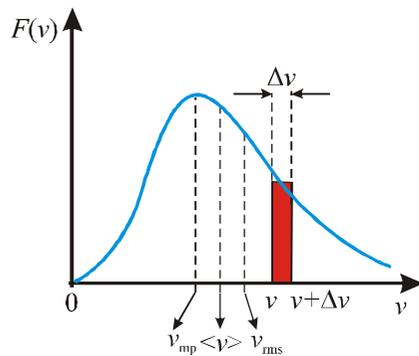


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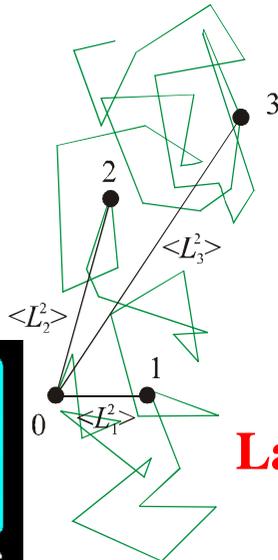
## Transport Processes Molecular-Kinetic Explanation



By particle “random motion” we mean that **any molecule** can move in **any direction** with **equal probability**.

Particle “migration” represents the **essence** of the diffusion process.

$$\langle L^2 \rangle \sim t$$

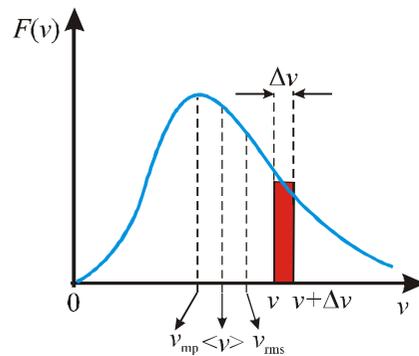


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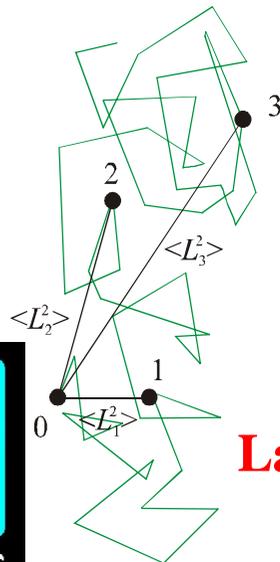
## Transport Processes Molecular-Kinetic Explanation



Einstein found that the **mean-square displacement** can be expressed in terms of the **observation time**, **properties** of the gas and **the size** of the particles.

$$\langle L^2 \rangle \sim t \rightarrow \langle L^2 \rangle = Dt$$

$\langle L^2 \rangle$  – mean-square displacement  
 $t$  – observation time  
 $D$  – diffusion coefficient



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## Transport Processes Molecular-Kinetic Explanation

Particle migration is a kind of transport process in which particle moves from one point in a system to another carrying, in the same time, its physical properties, too. For this kind of transport it is customary to define a **particle flux** by determining the rate at which the corresponding physical quantity of particle appears **to move across** an imaginary unit surface in the system because of the **decrease** in the conserved quantity on one side of the surface and the corresponding **increase** on the other.



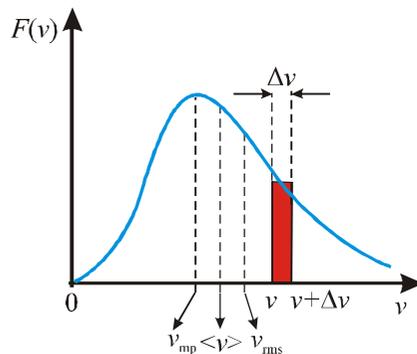
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## Transport Processes Molecular-Kinetic Explanation

In a gas, **particle flux** is easy to specify because **physical properties** carried by gas molecules crossing an imaginary unit surface in a unit time may be **readily determined** in terms of the **velocities and concentrations** of the molecules.



$$\Delta N_i = F(v) \Delta v_i \rightarrow N_i = F(v) v_i$$

$$\Delta n_i \rightarrow n_i, \quad \sum_i n_i = n,$$



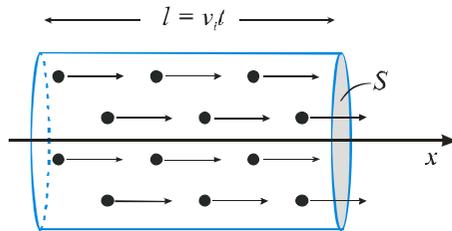
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## Transport Processes Molecular-Kinetic Explanation

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$$N_i = \frac{1}{6} n_i V = \frac{1}{6} n_i S l = \frac{1}{6} n_i S v_i t \quad j_i = \frac{N_i}{S t} = \frac{1}{6} n_i v_i,$$

$$j = \sum_i j_i = \frac{1}{6} \sum_i n_i v_i \cdot \frac{n}{n} = \frac{1}{6} \frac{\sum_i n_i v_i}{n} \cdot n$$

$$j = \frac{1}{6} \langle v \rangle n$$



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## Transport Processes Molecular-Kinetic Explanation

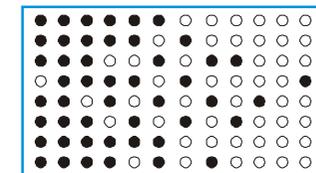
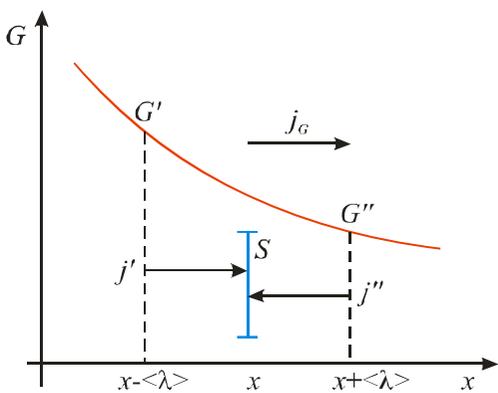
Changes of **physical properties**  $G$  carried by gas molecules crossing an imaginary unit surface  $S$  in a unit time are determined by **general transport equation**  $j_G$ :

$$(j' = j'' = j)$$

$$j_G = j'G' - j''G'' = j(G' - G'') = \frac{1}{6} \langle v \rangle n (G' - G'')$$

$$G' - G'' = -\frac{\partial G}{\partial x} 2 \langle \lambda \rangle,$$

$$j_G = -\frac{1}{3} n \langle v \rangle \langle \lambda \rangle \frac{\partial G}{\partial x}.$$

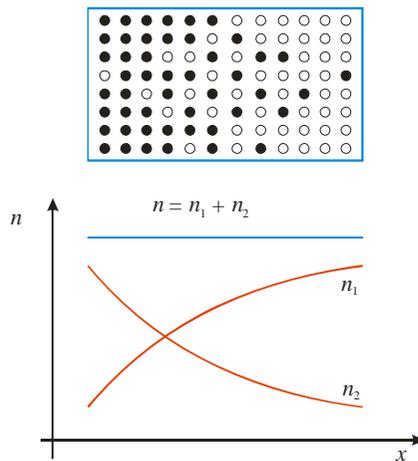


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## Transport Processes Molecular-Kinetic Explanation

Transport processes in gases are often of great **practical importance**. The **concentration changes** of fuel in air will affect the **performances** of gasoline engine.



$$G = n_1 / n,$$

$$j_G = -\frac{1}{3} n \langle v \rangle \langle \lambda \rangle \frac{\partial G}{\partial x} = -\frac{1}{3} n \langle v \rangle \langle \lambda \rangle \frac{\partial \left( \frac{n_1}{n} \right)}{\partial x}.$$

$$j_{n_1} = -\frac{1}{3} \langle v \rangle \langle \lambda \rangle \frac{\partial n_1}{\partial x}.$$



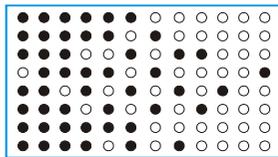
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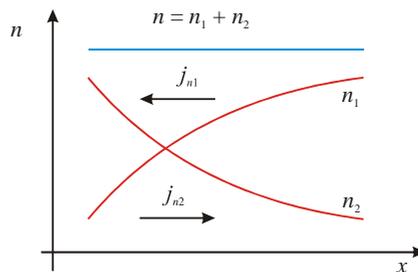
## Transport Processes Molecular-Kinetic Explanation

Transport processes in gases are often of great **practical importance**. The **concentration changes** of fuel in air will affect the **performances** of gasoline engine.



$$j_{n_1} = -\frac{1}{3} \langle v \rangle \langle \lambda \rangle \frac{\partial n_1}{\partial x} = -D \frac{\partial n_1}{\partial x}.$$

$$D = \frac{1}{3} \langle v \rangle \langle \lambda \rangle$$



$$j_n = -D \frac{\partial n}{\partial x}$$

Fick's first law of diffusion



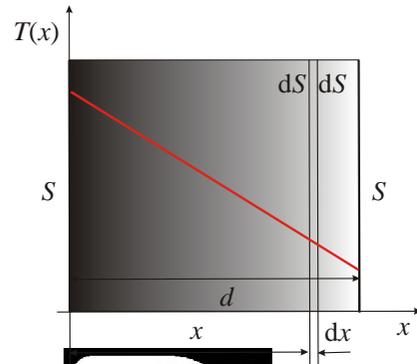
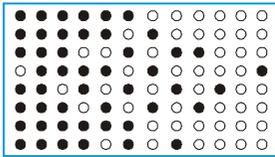
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## Transport Processes Molecular-Kinetic Explanation

Heat conduction in a gas will determine the rate of heating of a space vehicle entering the atmosphere of the Earth as well as the amount of isolator surface required for cooling.



$$G = Q = \frac{3}{2} kT,$$

$$j_G = -\frac{1}{3} n \langle v \rangle \langle \lambda \rangle \frac{\partial G}{\partial x} = -\frac{1}{3} n \langle v \rangle \langle \lambda \rangle \frac{\partial \left( \frac{3}{2} kT \right)}{\partial x}.$$

$$j_{n_1} = -\frac{1}{3} n \langle v \rangle \langle \lambda \rangle \frac{3}{2} k \frac{\partial T}{\partial x}.$$

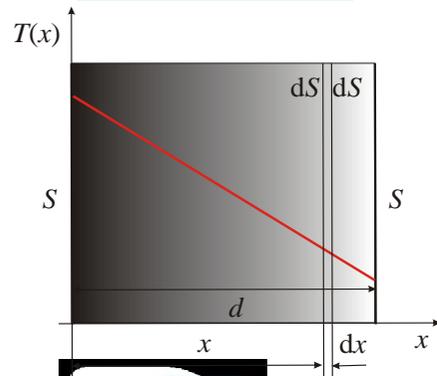
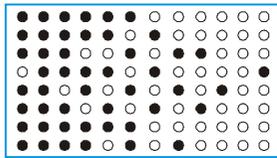
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## Transport Processes Molecular-Kinetic Explanation

In an undeformed solid, the **internal energy** of the solid is changed only by the addition of **heat** and where **no work** is done, the **internal energy flux** is simply called **heat flux**.



$$j_{n_1} = -\frac{1}{3} n \langle v \rangle \langle \lambda \rangle \frac{3}{2} k \frac{\partial T}{\partial x}, \quad n = N_A / V, \quad \frac{3}{2} k \frac{N_A}{V} = c_V \rho$$

$$j_Q = -\frac{1}{3} \langle v \rangle \langle \lambda \rangle \rho c_V \frac{\partial T}{\partial x},$$

$$k = \frac{1}{3} \langle v \rangle \langle \lambda \rangle \rho c_V.$$

$$j_Q = -k \frac{\partial T}{\partial x}$$

Fourier's law of heat conduction



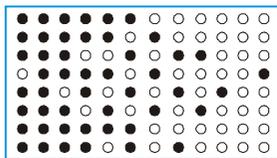
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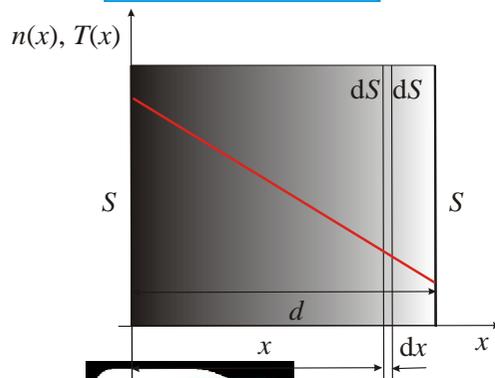
## Transport Processes Molecular-Kinetic Explanation

How diffusion causes the **concentration** and **temperature** to **change with time**?



$$\frac{\partial n}{\partial t} = \frac{1}{\partial x} [j_n(x) - j_n(x + dx)] = -\frac{\partial j_n}{\partial x},$$

$$j_n = -D \frac{\partial n}{\partial x},$$



$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2}$$

Fick's second law of diffusion



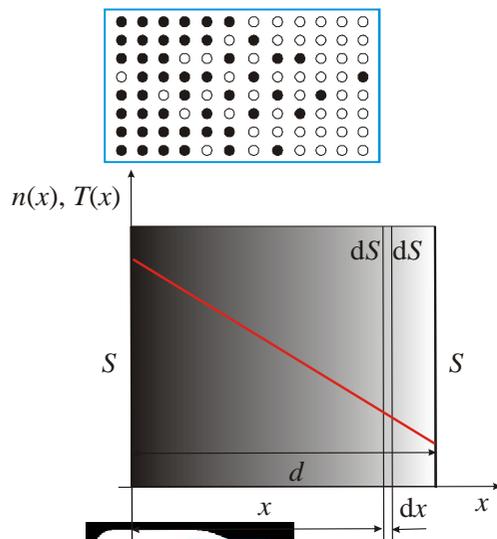
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## Transport Processes Molecular-Kinetic Explanation

How diffusion causes the **concentration** and **temperature** to **change with time**?



$$e = U / V = \rho c_V T, \quad \frac{\partial e}{\partial t} = -\frac{\partial j_Q}{\partial x}, \quad \boxed{j_Q = -k \frac{\partial T}{\partial x}},$$

$$\rho c_V \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2}, \quad \boxed{D_T = \frac{k}{\rho c_V}}$$

$$\boxed{\frac{\partial T}{\partial t} = D_T \frac{\partial^2 T}{\partial x^2}} \quad \text{Heat equation}$$



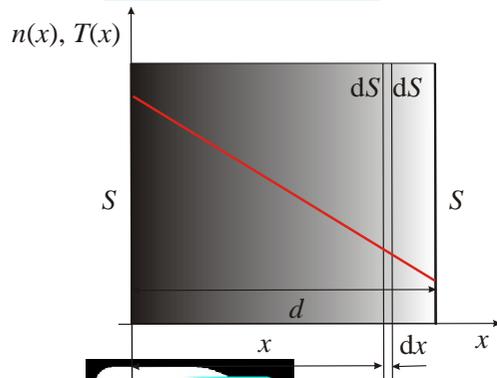
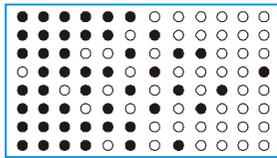
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## Transport Processes Molecular-Kinetic Explanation

Fundamental transport equations that describes the distribution of particles and heat in a given region over time



$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2}$$

Fick's second law of diffusion

$$[D] = [D_T] = [\langle v \rangle][\langle \lambda \rangle] = \frac{\text{m}^2}{\text{s}}$$

$$\frac{\partial T}{\partial t} = D_T \frac{\partial^2 T}{\partial x^2}$$

Heat equation



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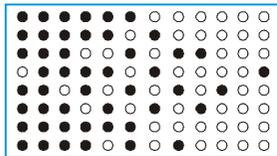




## Transport Processes Molecular-Kinetic Explanation

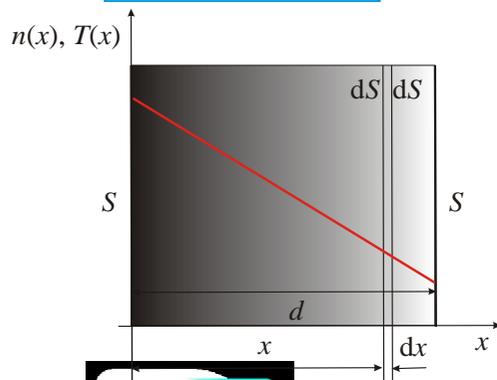
Fundamental transport equations in the case of **surface** and **volume** absorbers (light/matter interaction).

### Fick's second law of diffusion



$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2}$$

$$\frac{\partial n}{\partial t} - D \frac{\partial^2 n}{\partial x^2} = \frac{\beta I}{\varepsilon} e^{-\beta x} - \frac{n}{\tau}$$



### Heat equation

$$\frac{\partial T}{\partial t} = D_T \frac{\partial^2 T}{\partial x^2}$$

$$D_T \frac{\partial^2 T}{\partial x^2} - \frac{\partial T}{\partial t} = -\frac{H}{\rho c}$$



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