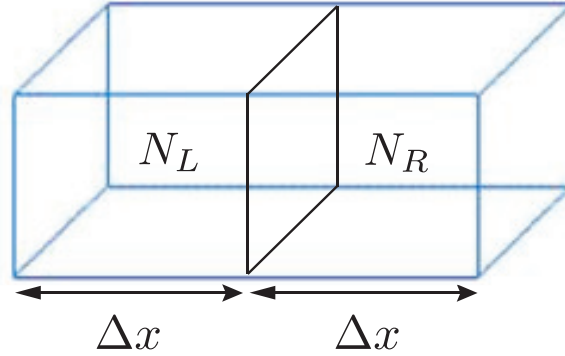


Physics 112: Classical Electromagnetism, Fall 2013

Diffusion

1 Diffusion

We will model the diffusion as a collection of molecules which are all jiggling around and bouncing into each other. We will denote the average distance a molecule travels before colliding with another molecule by Δx and the amount of time between collisions by Δt . Even though these are average quantities, in what follows, we will approximate the process as discrete: each molecule is approximated as moving a distance Δx in a time Δt before colliding with another molecule.



To simplify the discussion, we will first think about diffusion of the molecules in one direction (though they we will imagine they occupy all 3 dimensions). We assume that the molecules are moving on a random walk, so that in one time step (Δt) half will move to the left and half will move to the right.

We want to calculate the flux of molecules across the black-lined surface in the center of the above figure. Since these regions are so small, we will approximate the number of molecules in each region by the density of molecules (denoted by n) at the center of each region: $N_L = n(x - \Delta x/2)A\Delta x$ molecules and in the region to the right there are $N_R = n(x + \Delta x/2)A\Delta x$ molecules (where A is the cross-sectional area so that $A\Delta x$ is the volume of each region). We will choose the positive x -direction to the right so that a flux from left to right is positive; a flux from right to left is negative. Using this sign convention the number of particles that pass through the dashed surface in one time-step is

$$\Delta N_x = \frac{1}{2}(N_L - N_R) = -\frac{\Delta x A}{2} [n(x + \Delta x/2) - n(x - \Delta x/2)]. \quad (1)$$

The total flux of molecules along the x -direction is

$$\mathcal{F}_x = \frac{\Delta N_x}{A\Delta t} = -\frac{(\Delta x)^2}{2\Delta t} \frac{n(x + \Delta x/2) - n(x - \Delta x/2)}{\Delta x} \approx -\frac{(\Delta x)^2}{2\Delta t} \frac{dn}{dx} = D \frac{dn}{dx}, \quad (2)$$

where the constant of proportionality is $D \equiv (\Delta x)^2/(2\Delta t)$ — this is known as *the diffusion coefficient*.

Generalizing this to three dimensions is not hard (the spatial derivative becomes a gradient), and we see that

$$\vec{F} = -D\vec{\nabla}n, \quad (3)$$

which in words says that the flux of molecules is proportional to the negative of the number density (also known as concentration) gradient! This results just came from assuming that equal numbers of molecules will be diffusing in all directions.

Does it make sense? We know that if we drop a small amount of cream into a cup of coffee that we should see it spread out... at first there is a large gradient of cream— and the gradient points towards the maximum concentration of cream. In order for the cream to spread out it must flow from high concentration to low concentration— hence, it flows *down the gradient of the concentration*.

The relationship between the molecular flux and the concentration that we derived above,

$$\vec{F} = -D\vec{\nabla}n, \quad (4)$$

is known as ‘Ficks’ first law’.

A similar equation can be written down for *heat flow*:

$$\vec{Q} = -k\vec{\nabla}T, \quad (5)$$

where \vec{Q} is the heat-flux (flow of heat), T is the temperature and k is the material’s thermal conductivity. This equation is known as Fourier’s law. I hope that the fact that it is *identical* to Fick’s first law makes you think!¹

Now, we can go one step further by using the fact that, in many cases, the number of molecules is conserved (i.e., use mass conservation).

If the number of molecules is conserved then there is a relationship between the flux and the number density called the *continuity equation*:

$$\frac{\partial n}{\partial t} + \vec{\nabla} \cdot \vec{F} = 0. \quad (6)$$

This is an *extremely* important equation that appears all over the place in physics— we’ll see it in a few forms in our course— so *think about it for a moment!* Integrating this equation over some volume we have

$$\frac{dN}{dt} = \frac{d}{dt} \int n d\tau = \int \frac{\partial n}{\partial t} d\tau = - \oint \vec{F} \cdot d\vec{a}, \quad (7)$$

which in words this equation says: if the number of molecules in the volume is increasing or decreasing it is solely due to the flow of molecules across the surface of the volume \mathcal{V} . (*Note what happened to the time derivative above... does that make sense?*)

- Combine the continuity equation and Fick’s first law to show that

$$\frac{\partial n}{\partial t} = D\nabla^2 n. \quad (8)$$

¹In Fick’s case the collisions between molecules make their concentration at different locations change; in Fourier’s case, the collisions redistribute kinetic energy among the molecules so that the concentration of kinetic energy is different at different locations. It seems reasonable to suppose that in the case of heat, just as in the case of collisions, an equal amount of heat is redistributed in all directions (i.e., just like the position of the molecules themselves, heat is distributed in a random walk).

In words it says that the time-rate of change of the concentration of a substance is proportional to the Laplacian of the concentration. This is a very important equation— known as the *diffusion equation*— and we’ll return to it again a few times later in the course.

A very similar treatment (including the first law of thermodynamics— which is really just a restatement of the conservation of energy) can be applied to Fourier’s law in order to derive the *heat equation*:

$$\frac{\partial T}{\partial t} = k \nabla^2 T. \quad (9)$$

What do these equations say? As long as the concentration of molecules is distributed in such a way that $\nabla^2 n \neq 0$, the concentration will change in time.

- What does this equation predict will be the end state when I drop a bit of cream into my coffee?
- What was essential in the above discussion in order for us to finally write down the diffusion equation? Articulate the essential steps as you see them.
- In this equation, what is the ‘physical significance’ of the Laplacian of the concentration? In what ways would we be able to interpret electrostatics as a diffusion-like process?