6.1 Basics using some examples

Thermodynamic equilibrium implies no time dependencies and no net (current) flows. What a boring world! In contrast, transport explicitly describes current flow and kinetics explicitly takes into account changes with time. Still there may be no net current flow or no net changes with time if e.g. several currents compensate each other or e.g. two chemical reactions with opposite reaction directions compensate each other. Such states with transport and/or kinetic processes which have no explicit time dependencies are in "steady state". Often time dependencies show up in disguise, e.g. the absorption of light in material is described by the Lambert law

$$\frac{dI}{dx} = -\alpha I = \frac{dI}{dt}\frac{dt}{dx} = \frac{dI}{dt}\frac{1}{c} \quad \text{so} \quad \frac{dI}{dt} = -\alpha cI = -kI \quad ; \tag{6.1}$$

here α is the absorption coefficient, c is the velocity of light in the investigated material, and $k = \alpha c$ is called a kinetic coefficient. Introducing the penetration depth of light $l = 1/\alpha$ and (relaxation) time variable $\tau = 1/k$ the solutions of the above linear differential equations of first order with constant coefficients are

$$I(x) = I_0 \exp\left(-\alpha x\right) = I_0 \exp\left(-\frac{x}{l}\right) \quad \text{and} \quad I(t) = I_0 \exp\left(-k t\right) = I_0 \exp\left(-\frac{t}{\tau}\right) \quad . \tag{6.2}$$

So while light is penetrating into the material, i.e. photons are penetrating into the material, the light intensity/ photon density is exponentially decreasing, reducing the intensity by a constant fraction vs. time or vs. depth, respectively. If our material is a semiconductor the photons generate electron hole pairs; this process is close to a chemical reaction and k could be interpreted as a kinetic reaction coefficient. This simple example already illustrates some typical features:

- Often transport and kinetic phenomena are tightly connected.
- Transport and kinetics are typically described by constant scaling factors.
- Combining such scaling factors generates an effective constant which describes the total effect of transport and kinetics.

A second typical example is the diffusion length $L=\sqrt{D\,\tau}$ where D is the diffusion constant representing a scaling factor for a transport process (diffusion) and τ is the life time of minority carriers representing a scaling factor for a reaction of electrons with holes. This reaction is called recombination and leads to a reduction of minority carriers with a functionality $\exp\left(\pm x/L\right)$ (exponential functions are extremely common in transport and kinetics!). Time dependencies do not always lead to an exponential decay in concentration I(t). Often oscillations in time are found. The most prominent examples show up in quantum mechanics, e.g. for free electrons one finds for the energy $E=\hbar\omega=\frac{p^2}{2\,m}$. Here $p=\hbar\,k$ and k is the wave vector (don't mix up with a kinetic coefficient). The solution is

$$\psi(x,t) = \psi_0 \exp(ikx) \exp(-i\omega t) = I_0 \psi_0 \exp(ikx - i\omega t)$$
 (6.3)

This solution (wave function of a free electron) shows an oscillation in time and in space and is called a plane wave. So oscillatory solutions show up when the kinetic coefficients are imaginary. Reactions and transport phenomena in solid state physics are typically difficult to describe, especially when quantum mechanics is needed. Therefore in what follows we will discuss typical and general concepts of transport and kinetics using examples of classical physics and chemistry.