5.1 Derivation of the Boltzmann equation

For the description of the motion of quantum mechanical particles interacting with inner and outer forces often the Boltzmann equation is applied. It is a semi quantum mechanical approach based on the following well known relations:

$$\begin{aligned}\vec{F} &= -\vec{\nabla} V \\ \vec{F} &= \frac{d\vec{p}}{dt} \\ \vec{p} &= \hbar \vec{k}\end{aligned} \tag{5.1}$$

The physical system is described by the distribution function

$$f(\vec{r}, \vec{k}, t) \tag{5.2}$$

which quantifies the number of electrons occupying a state $\vec{k}$ at time t at position $\vec{r}$. The function f describes the equilibrium as well.
The solution is:

$$\frac{df(\vec{r}, \vec{k}, t)}{dt} = \frac{\partial f}{\partial t} + \left\langle \vec{\nabla}_r f, \frac{d\vec{r}}{dt} \right\rangle + \left\langle \vec{\nabla}_k f, \frac{d\vec{k}}{dt} \right\rangle = \frac{\partial f}{\partial t} + \left\langle \vec{\nabla}_r f, \vec{v} \right\rangle + \frac{1}{\hbar} \left\langle \vec{\nabla}_k f, \vec{F} \right\rangle \tag{5.3}$$

Following the Liouville theorem (Phase space volume does not change), i.e.

$$\frac{df(\vec{r}, \vec{k}, t)}{dt} = 0 \tag{5.4}$$

we get

$$-\frac{\partial f}{\partial t} = \left\langle \vec{\nabla}_r f, \vec{v} \right\rangle + \frac{1}{\hbar} \left\langle \vec{\nabla}_k f, \vec{F} \right\rangle \tag{5.5}$$

The time evolution of the distribution function in each point in phase space $(\vec{r}, \vec{k})$ depends on the motion of the particles in real and in momentum space.
As well known from equilibrium thermodynamics we separate the forces into macroscopic external forces and into internal forces which drive the system back to equilibrium by scattering processes:

$$\vec{F} = \vec{F}_a + \vec{F}_i \tag{5.6}$$

Defining

$$-\left(\frac{\partial f}{\partial t}\right)_{field} = \left\langle \vec{\nabla}_r f, \vec{v} \right\rangle + \frac{1}{\hbar} \left\langle \vec{\nabla}_k f, \vec{F}_a \right\rangle \tag{5.7}$$

and

$$-\left(\frac{\partial f}{\partial t}\right)_{scat} = \frac{1}{\hbar} \left\langle \vec{\nabla}_k f, \vec{F}_i \right\rangle \tag{5.8}$$

we get

$$\left(\frac{\partial f}{\partial t}\right) = \left(\frac{\partial f}{\partial t}\right)_{scat} + \left(\frac{\partial f}{\partial t}\right)_{field} \tag{5.9}$$

In steady state $\left(\frac{\partial f}{\partial t}\right) = 0$ the changes in the distribution function due to the external forces are compensated by scattering of particles as a result of the internal forces (scattering at local defects which destroy the lattice periodicity).
The Boltzmann equation as a quasi classical description does not account for very fast processes in small areas (restrictions due to the uncertainty relation). In addition the forces must be small in comparison to the undisturbed system.
A general approach for solving the Boltzmann equation leads to an integro-differential equation which can not be solved exactly. In the following we will therefor focus on the most common approximation.