IV.4.3 Relaxation-time approximation

It may happen that the inter-particle interactions entering the collision integral of the Boltzmann equation are only imperfectly known, so that the approximation methods presented in the previous section IV.4.2 cannot be used. In order to still be able to derive qualitative behaviors in that situation, it is customary to perform a rather drastic approximation of the collision term, based on the physical significance of the latter, whose role is to let the distribution $\bar{\mathsf{f}}(t,\vec{r},\vec{p})$ relax to a local equilibrium distribution $\bar{\mathsf{f}}^{(0)}$, given by expression (IV.38), with local density, temperature and average particle velocity which are specific to the conditions imposed on the system.

In the so-called *relaxation-time approximation*, it is assumed that the approach to the local equilibrium distribution is exponential, with a characteristic time scale $\tau_{\rm r}(\vec{r},\vec{p})$. In that case, the Boltzmann equation is approximated by the linear partial differential equation

$$\boxed{\frac{\partial\bar{\mathsf{f}}(t,\vec{r},\vec{p})}{\partial t}+\vec{v}\cdot\vec{\nabla}_{\vec{r}}\bar{\mathsf{f}}(t,\vec{r},\vec{p})+\vec{F}\cdot\vec{\nabla}_{\vec{p}}\bar{\mathsf{f}}(t,\vec{r},\vec{p})=-\frac{\bar{\mathsf{f}}(t,\vec{r},\vec{p})-\bar{\mathsf{f}}^{(0)}(t,\vec{r},\vec{p})}{\tau_{\rm r}(\vec{r},\vec{p})}.}\qquad\text{(IV.40)}$$

This approximation thus leaves the integral aspect of the collision term, amounting to a "first linearization" of the Boltzmann equation.

Remarks:

∗ The *relaxation time* $\tau_{\rm r}$ models the typical duration for reaching local equilibrium (see § IV.4.1 b). In Eq. (IV.40) it is introduced as a free parameter. It should nevertheless naturally be larger than the *mean free time*, i.e. the average "free-flight" time between two successive scatterings of a given particle, since one expects that equilibration requires several collisions. On the other hand, it should remain (much) smaller than "external" time scales imposed by macroscopic conditions on the systems.

∗ $\tau_{\rm r}$ is often assumed to be uniform over the whole system—which is to a large extent justified as long as the spatial density does not vary too much—, yet still momentum dependent.

∗ When $\tau_{\rm r}$ is also assumed to be independent of $\vec{p}$—which is far less obvious—, the approximation is sometimes referred to as the Bhatnagar[(as)]–Gross[(at)]–Krook[(au)] (BGK) approximation [40].

∗ The approximation (IV.40) may be seen as a truncation prescription of the BBGKY hierarchy (III.14), irrespective of the Boltzmann equation.

If the departure from equilibrium remains always small, then the true solution $\bar{\mathsf{f}}(t,\vec{r},\vec{p})$ to the Boltzmann equation never deviates much from a local equilibrium distribution $\bar{\mathsf{f}}^{(0)}(t,\vec{r},\vec{p})$. One may then write

$$\bar{\mathsf{f}}(t,\vec{r},\vec{p})=\bar{\mathsf{f}}^{(0)}(t,\vec{r},\vec{p})+\bar{\mathsf{f}}^{(1)}(t,\vec{r},\vec{p})\quad\text{with}\quad\left|\bar{\mathsf{f}}^{(1)}(t,\vec{r},\vec{p})\right|\ll\bar{\mathsf{f}}^{(0)}(t,\vec{r},\vec{p})\quad\forall\,t,\vec{r},\vec{p}.\qquad\text{(IV.41)}$$

The right-hand side of the simplified equation (IV.40) is then simply $-\bar{\mathsf{f}}^{(1)}(t,\vec{r},\vec{p})/\tau_{\rm r}(\vec{p})$, while on the left-hand side one will account for the assumption $|\bar{\mathsf{f}}^{(1)}|\ll\bar{\mathsf{f}}^{(0)}$ by linearizing the various terms with respect to the small perturbation $\bar{\mathsf{f}}^{(1)}$. This constitutes the "second linearization" of the Boltzmann equation, and will be illustrated on a few examples in the following section.

IV.5 Computation of transport coefficients

In this section, we show how the Boltzmann equation allows the computation of transport coefficients in a system which is slightly out of equilibrium, working within the relaxation-time approximation introduced in Sec. IV.4.3.

[(as)] P. L. Bhatnagar, 1912–1976 [(at)] E. P. Gross, 1926–1991 [(au)] M. Krook, 1913–1985

IV.5.1 Electrical conductivity

As first example, consider a gas of charged particles of mass m, in the presence of a constant and uniform electric field $\vec{\mathscr{E}}$. These particles diffuse among a system of particles of a different species, which we shall not consider explicitly. As a result of the various possible types of (elastic) two-to-two collisions between the different particle species, the single-particle distribution $\bar{\mathsf{f}}(t,\vec{r},\vec{p})$ obeys the Boltzmann equation (IV.15), with the external force $\vec{F} = q\vec{\mathscr{E}}$ in the drift term, where q is the electric charge of the particles under study.

We shall assume that we are in a regime where the Boltzmann equation can be approximated by Eq. (IV.40) while the single-particle distribution can be written in the form (IV.41). For reasons which will be made clearer below, we search for a stationary particle distribution. Given the uniformity and stationarity of the electric field, it is consistent to consider a local equilibrium distribution $\bar{\mathsf{f}}^{(0)}$ involving time- and position-independent local quantities n, T, $\vec{\mathsf{v}}$. $\bar{\mathsf{f}}^{(0)}$ then only depends on momentum:

$$\bar{\mathsf{f}}^{(0)}(\vec{p}) = n\left(\frac{2\pi\hbar^2}{mk_BT}\right)^{3/2} \mathrm{e}^{-(\vec{p}-m\vec{\mathsf{v}})^2/2mk_BT}.$$

Assuming that the average velocity $\vec{\mathsf{v}}$ of the moving charges vanishes—which is only a matter of choosing the proper reference frame, since it is uniform across the system—, this local equilibrium distribution reduces to

$$\bar{\mathsf{f}}^{(0)}(\vec{p}) = n\left(\frac{2\pi\hbar^2}{mk_BT}\right)^{3/2} \mathrm{e}^{-\vec{p}^{\,2}/2mk_BT} \qquad \text{(IV.42)}$$

i.e. actually to the Maxwell–Boltzmann distribution (IV.35). Given the homogeneity of the system, the relaxation time τ_{r} can be taken to be independent of position.

Inserting $\bar{\mathsf{f}}(\vec{r},\vec{p}) = \bar{\mathsf{f}}^{(0)}(\vec{p}) + \bar{\mathsf{f}}^{(1)}(\vec{r},\vec{p})$ in Eq. (IV.40), the leading remaining term on the left-hand side is that involving $\vec{\nabla}_{\vec{p}}\bar{\mathsf{f}}^{(0)}(\vec{p})$: there is no term involving either the time or space derivative of $\bar{\mathsf{f}}^{(0)}$—since $\bar{\mathsf{f}}^{(0)}$ does not depend on either—, and the terms involving gradients of $\bar{\mathsf{f}}^{(1)}$ are of subleading order—physically, the corresponding time scales [cf. Eq. (III.16)] are much larger than $\tau_{\mathrm{r}}(\vec{p})$, since many more collisions are needed for smoothing out large-scale inhomogeneities than small-scale ones. All in all, Eqs. (IV.40) and (IV.41) thus give to leading order

$$q\vec{\mathscr{E}}\cdot\vec{\nabla}_{\vec{p}}\bar{\mathsf{f}}^{(0)}(\vec{p}) = -\frac{\bar{\mathsf{f}}^{(1)}(\vec{r},\vec{p})}{\tau_{\mathrm{r}}(\vec{p})}.$$

from where one reads off $\bar{\mathsf{f}}^{(1)}$ at once:

$$\bar{\mathsf{f}}^{(1)}(\vec{p}) = \frac{q}{mk_BT}\tau_{\mathrm{r}}(\vec{p})\,\bar{\mathsf{f}}^{(0)}(\vec{p})\,\vec{p}\cdot\vec{\mathscr{E}} \qquad \text{(IV.43)}$$

In particular, $\bar{\mathsf{f}}^{(1)}$ is independent of $\vec{r}$.

Now, the electric current (density) is the sum over all carriers of their electric charge multiplied by their velocity

$$\vec{J}_{\mathrm{el.}}(t,\vec{r}) = \int_{\vec{p}} q\vec{v}\,\bar{\mathsf{f}}(t,\vec{r},\vec{p}) = \frac{q}{m}\int_{\vec{p}}\vec{p}\,\bar{\mathsf{f}}(t,\vec{r},\vec{p}).$$

Here the current is stationary and uniform, and one can replace $\bar{\mathsf{f}}$ by $\bar{\mathsf{f}}^{(0)} + \bar{\mathsf{f}}^{(1)}$, with Eqs. (IV.42) and (IV.43). The integral of the term involving the local equilibrium distribution $\bar{\mathsf{f}}^{(0)}$ vanishes by symmetry.(49) There thus only remains the contribution of $\bar{\mathsf{f}}^{(1)}$, which gives for the i-th component of $\vec{J}_{\mathrm{el.}}$

$$J^i_{\mathrm{el.}} = \frac{q}{m}\int_{\vec{p}} p^i\,\bar{\mathsf{f}}^{(1)}(\vec{p}) = \sum_{j=1}^{3}\frac{q^2}{m^2k_BT}\int_{\vec{p}}\bar{\mathsf{f}}^{(0)}(\vec{p})\,\tau_{\mathrm{r}}(\vec{p})\,p^ip^j\mathscr{E}^j.$$

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(49) Had we allowed for a non-vanishing average velocity $\vec{\mathsf{v}}$, the $\bar{\mathsf{f}}^{(0)}$-term would have given a contribution $nq\vec{\mathsf{v}}$ to $\vec{J}_{\mathrm{el.}}$.

This is the i-th component of the relation

$$\vec{J}_{\rm el.} = \boldsymbol{\sigma}_{\rm el.} \cdot \vec{\mathscr{E}}, \tag{IV.44a}$$

where the electrical-conductivity tensor $\boldsymbol{\sigma}_{\rm el.}$ has the components

$$\sigma^{ij}_{\rm el.} \equiv \frac{q^2}{m^2 k_B T} \int_{\vec{p}} \bar{\mathsf{f}}^{(0)}(\vec{p})\, \tau_{\rm r}(\vec{p})\, p^i p^j. \tag{IV.44b}$$

If the relaxation time $\tau_{\rm r}(\vec{p})$ only depends on the modulus $|\vec{p}|$ of momentum, not on its orientation, then the product $\bar{\mathsf{f}}^{(0)}(\vec{p})\, \tau_{\rm r}(\vec{p})$ is an even function of the (Cartesian) components p^i. The integrand in Eq. (IV.44b) is then odd in p^i (or p^j) when $i \neq j$, so that the non-diagonal elements of the tensor vanish. In turn, all three diagonal elements are equal, i.e. the tensor is proportional to the identity. Assuming that the relaxation time is independent of momentum (BGK approximation), one obtains

$$\sigma^{ii}_{\rm el.} = \frac{q^2 \tau_{\rm r}}{m^2 k_B T} \int_{\vec{p}} (p^i)^2\, \bar{\mathsf{f}}^{(0)}(\vec{p}) = \frac{q^2 \tau_{\rm r}}{m^2 k_B T}\, n m k_B T = \frac{n q^2 \tau_{\rm r}}{m}.$$

All in all, one thus finds Ohm's law [cf. Eq. (I.40b)]

$$\vec{J}_{\rm el.} = \sigma_{\rm el.} \vec{\mathscr{E}} \quad \text{with} \quad \sigma_{\rm el.} = \frac{n q^2 \tau_{\rm r}}{m}. \tag{IV.45}$$

Taking into account the dependence of the relaxation time on momentum gives a similar expression, with a different—yet in principle computable—expression of the electrical conductivity $\sigma_{\rm el.}$, or more generally of the electrical-conductivity tensor $\boldsymbol{\sigma}_{\rm el.}$ if $\tau_{\rm r}(\vec{p})$ depends on the direction of $\vec{p}$.

Remarks:

∗ Our interest in the electrical conductivity, which as recalled in the first remark on page 13 is defined in the stationary regime, justifies a posteriori the restriction to time-independent solutions.

∗ In writing down the local equilibrium distribution $\bar{\mathsf{f}}^{(0)}$ as uniform, we ignored the electrostatic potential which gives rise to the electric field $\vec{\mathscr{E}}$. The reason is again our interest in the electrical conductivity $\sigma_{\rm el.}$, which is defined as the coefficient between $\vec{\mathscr{E}}$ and the electric current $\vec{J}_{\rm el.}$ in the absence of a gradient in the number of charge carriers, i.e. for a uniform particle number density—the reader should compare with § I.2.3 c.

∗ The electrical conductivity (IV.45) computed within the relaxation-time approximation is proportional to the relaxation time $\tau_{\rm r}$. Since the latter is supposedly governed by collisions, it should be roughly proportional to the mean-free time between two successive scatterings, or equivalently to the mean-free path $\ell_{\rm mfp}$. In this picture, a larger $\ell_{\rm mfp}$ results in a more efficient transport of charge carriers, which seems rather coherent with the longer way traveled by the moving charges in each step.

IV.5.2 Diffusion coefficient and heat conductivity

As second application of the ideas of Sec. IV.4.3, consider a Lorentz gas—i.e. a gas of light particles colliding on much heavier ones—, submitted to time-independent gradients in temperature and in chemical potential (or density)—which are imposed through the heavy, motionless collision partners.

The evolution equation of the single-particle distribution $\bar{\mathsf{f}}(t,\vec{r},\vec{p})$ is again approximated as Eq. (IV.40), here without external force. As local equilibrium distribution, we take

$$\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p}) = n(\vec{r}) \left(\frac{2\pi\hbar^2}{m k_B T(\vec{r})}\right)^{3/2} {\rm e}^{-\vec{p}^{\,2}/2mk_BT(\vec{r})},$$

where the local density $n(\vec{r})$ and temperature $T(\vec{r})$ are those imposed by the heavy partners. Instead of this "canonical" form of the Maxwell–Boltzmann velocity distribution, it will be more convenient to replace it by the "grand-canonical" expression(50)

$$\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p}) = \exp\!\left[-\frac{\vec{p}^{\,2}/2m - \mu(\vec{r})}{k_B T(\vec{r})}\right], \tag{IV.46}$$

with the local chemical potential $\mu(\vec{r})$ instead of the number density. This will enable us to make more easily contact with the formalism of non-equilibrium thermodynamics in the entropy representation of Chapter I.

Looking for stationary solutions $\bar{\mathsf{f}}(\vec{r},\vec{p}) = \bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p}) + \bar{\mathsf{f}}^{(1)}(\vec{r},\vec{p})$ with $|\bar{\mathsf{f}}^{(1)}| \ll \bar{\mathsf{f}}^{(0)}$, Eq. (IV.40) reads to leading order

$$\frac{\partial \bar{\mathsf{f}}^{(1)}(\vec{r},\vec{p})}{\partial t} + \vec{v}\cdot\vec{\nabla}_{\vec{r}}\,\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p}) = -\frac{\bar{\mathsf{f}}^{(1)}(\vec{r},\vec{p})}{\tau_{\rm r}(\vec{r},\vec{p})},$$

i.e.

$$\bar{\mathsf{f}}^{(1)}(\vec{r},\vec{p}) = -\frac{\tau_{\rm r}(\vec{r},\vec{p})}{m}\,\vec{p}\cdot\vec{\nabla}_{\vec{r}}\,\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p}). \tag{IV.47}$$

IV.5.2 a Fluxes

With the help of the leading and subleading contributions (IV.46), (IV.47) to the single-particle distribution, we can first easily compute the fluxes of particle number and energy.

$$\vec{\mathcal{J}}_N(t,\vec{r}) = \int_{\vec{p}} \bar{\mathsf{f}}(t,\vec{r},\vec{p})\,\vec{v} = \frac{1}{m}\int_{\vec{p}} \bar{\mathsf{f}}(t,\vec{r},\vec{p})\,\vec{p},$$

$$\vec{\mathcal{J}}_E(t,\vec{r}) = \int_{\vec{p}} \bar{\mathsf{f}}(t,\vec{r},\vec{p})\frac{\vec{p}^{\,2}}{2m}\,\vec{v} = \frac{1}{m}\int_{\vec{p}} \bar{\mathsf{f}}(t,\vec{r},\vec{p})\frac{\vec{p}^{\,2}}{2m}\,\vec{p}.$$

The local equilibrium distribution $\bar{\mathsf{f}}^{(0)}$ does not contribute for parity reasons—the integrands are odd in $\vec{p}$ and integrated over all momentum space.

To handle the contribution of $\bar{\mathsf{f}}^{(1)}$, we first use the chain rule to rewrite the gradient of $\bar{\mathsf{f}}^{(0)}$ with respect to position as

$$\vec{\nabla}_{\vec{r}}\,\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p}) = -\frac{1}{k_B}\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p})\left\{\frac{\vec{p}^{\,2}}{2m}\vec{\nabla}_{\vec{r}}\!\left[\frac{1}{T(\vec{r})}\right] + \vec{\nabla}_{\vec{r}}\!\left[-\frac{\mu(\vec{r})}{T(\vec{r})}\right]\right\}.$$

As in Sec. IV.5.1, inserting $\bar{\mathsf{f}}^{(1)}$, given by Eq. (IV.47), computed with this gradient in the flux densities $\vec{\mathcal{J}}_N$, $\vec{\mathcal{J}}_E$ leads to linear relations between the latter and the gradients $\vec{\nabla}_{\vec{r}}(1/T)$, $\vec{\nabla}_{\vec{r}}(-\mu/T)$, where the coefficients are in the general case tensors of rank 2. If the relaxation time $\tau_{\rm r}$ does not depend on the orientation of $\vec{p}$, as we assume from now on, the tensors are all diagonal and proportional to the unit tensor. The integrand of the diagonal coefficients of any of these tensors involves $(p^i)^2$, which has to be averaged—with a weight involving $\bar{\mathsf{f}}^{(0)}$, τ_r and various powers of $\vec{p}^{\,2}$—over all directions. Such an average is simply $\frac{1}{3}$ of the corresponding average of $\vec{p}^{\,2}$, so that one eventually obtains

$$\vec{\mathcal{J}}_N(\vec{r}) = \frac{1}{3m^2k_B}\int_{\vec{p}} \tau_{\rm r}(\vec{r},\vec{p})\,\vec{p}^{\,2}\,\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p})\left\{\frac{\vec{p}^{\,2}}{2m}\vec{\nabla}_{\vec{r}}\!\left[\frac{1}{T(\vec{r})}\right] + \vec{\nabla}_{\vec{r}}\!\left[-\frac{\mu(\vec{r})}{T(\vec{r})}\right]\right\}, \tag{IV.48a}$$

$$\vec{\mathcal{J}}_E(\vec{r}) = \frac{1}{6m^3k_B}\int_{\vec{p}} \tau_{\rm r}(\vec{r},\vec{p})\,\vec{p}^{\,4}\,\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p})\left\{\frac{\vec{p}^{\,2}}{2m}\vec{\nabla}_{\vec{r}}\!\left[\frac{1}{T(\vec{r})}\right] + \vec{\nabla}_{\vec{r}}\!\left[-\frac{\mu(\vec{r})}{T(\vec{r})}\right]\right\}. \tag{IV.48b}$$

Note that since T and μ only depend on position, not on momentum, we may drop the $\vec{r}$ subscripts from the $\vec{\nabla}$ operators without ambiguity.

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(50) A simple mnemonic is to remember that it corresponds to the phase-space occupancy, as given by the Boltzmann factor, for a macrostate at temperature T and chemical potential μ.

IV.5.2 b Kinetic and transport coefficients

In the language of Chapter I, the relations (IV.48) express the fluxes $\vec{\mathcal{J}}_N$, $\vec{\mathcal{J}}_E$ as functions of the affinities $\vec{\nabla}(1/T)$ and $\vec{\nabla}(-\mu/T)$. Using the notation of Eq. (I.31), we may write these relations in the form

$$\vec{\mathcal{J}}_N = L_{NN}\vec{\nabla}\left(-\frac{\mu}{T}\right) + L_{NE}\vec{\nabla}\left(\frac{1}{T}\right),$$
$$\vec{\mathcal{J}}_E = L_{EN}\vec{\nabla}\left(-\frac{\mu}{T}\right) + L_{EE}\vec{\nabla}\left(\frac{1}{T}\right),$$

with position-dependent kinetic coefficients L_{NN}, L_{NE}, L_{EN} and L_{EE} that can be directly read off Eqs. (IV.48):

$$\begin{cases} L_{NN}(\vec{r}) = \dfrac{1}{3m^2k_B}\displaystyle\int_{\vec{p}} \tau_{\rm r}(\vec{r},\vec{p})\,\vec{p}^{\,2}\,\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p}), \\ L_{EN}(\vec{r}) = L_{NE}(\vec{r}) = \dfrac{1}{6m^3k_B}\displaystyle\int_{\vec{p}} \tau_{\rm r}(\vec{r},\vec{p})\,\vec{p}^{\,4}\,\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p}), \\ L_{EE}(\vec{r}) = \dfrac{1}{12m^4k_B}\displaystyle\int_{\vec{p}} \tau_{\rm r}(\vec{r},\vec{p})\,\vec{p}^{\,6}\,\bar{\mathsf{f}}^{(0)}(\vec{r},\vec{p}). \end{cases} \tag{IV.49}$$

In particular, we see that the Onsager reciprocal relation $L_{EN} = L_{NE}$ is fulfilled.

If we assume that the relaxation time is independent of position and momentum, $\tau_{\rm r}(\vec{r},\vec{p}) = \tau_{\rm r}$, the integrals can be performed with the help of formula (A.1c) with $a = 1/2mk_BT(\vec{r})$ and $2n = 4$, 6 and 8, and lead to

$$\begin{cases} L_{NN}(\vec{r}) = \dfrac{n(\vec{r})\tau_{\rm r}T(\vec{r})}{m}, \\ L_{EN}(\vec{r}) = L_{NE}(\vec{r}) = \dfrac{5}{2}\dfrac{n(\vec{r})\tau_{\rm r}T(\vec{r})}{m}k_BT(\vec{r}), \\ L_{EE}(\vec{r}) = \dfrac{35}{4}\dfrac{n(\vec{r})\tau_{\rm r}T(\vec{r})}{m}\big[k_BT(\vec{r})\big]^2. \end{cases}$$

From these kinetic coefficients, one deduces expressions for various transport coefficients using relations which were derived in Sec. I.2.3.

Thus, the diffusion coefficient of the particles of the Lorentz gas is related through Eq. (I.38c) to the kinetic coefficient L_{NN}

$$D = \frac{1}{T}\left(\frac{\partial\mu}{\partial n}\right)_T L_{NN} = \frac{\tau_{\rm r}k_BT}{m},$$

where the second identity holds when the relaxation time is independent of position and momentum. In turn, inserting the above expressions of the kinetic coefficients in the heat conductivity (I.54) yields

$$\kappa = \frac{L_{NN}L_{EE} - L_{NE}L_{EN}}{T^2\,L_{NN}} = \frac{5}{2}\frac{nk_B\tau_{\rm r}}{m}k_BT.$$

For both transport coefficients, we now have expressions in terms of microscopic quantities.