Tutorial sheet 5

Discussion topic: Boltzmann kinetic equation: assumptions, formulation. Which change(s) should be made to include inelastic scatterings or decays?

12. Time reversal in classical statistical mechanics

Consider a system of classical particles, characterized by their positions and momenta, which span the phase space Γ. The system evolution is described by a trajectory $\mathbf{X}(t) \equiv \big(\{q_i(t)\},\{p_i(t)\}\big)$ in Γ.

To each trajectory $\mathbf{X}(t)$, one may associate a "time-reversed trajectory" $\mathbf{X}^t(t) \equiv \big(\{q_i^t(t)\},\{p_i^t(t)\}\big)$ such that

$$q_i^t(t) = q_i(-t), \qquad p_i^t(t) = -p_i(-t) \quad \forall i. \tag{1}$$

That is, the system goes through the same microscopic states, yet in reverse chronological order.

The system is said to be invariant under time reversal if for every solution $\mathbf{X}(t)$ of its (Hamilton) equations of motion, the time-reversed trajectory defined by Eq. (1) is also a solution of the equations of motion.

i. Hamilton equations

a) Show that for a system of neutral particles—i.e. in particular in the absence of a vector potential—a necessary and sufficient condition for time-reversal symmetry is that the Hamilton function of the system obey the property

$$H\big(t,\{q_i\},\{p_i\}\big) = H\big(-t,\{q_i\},\{-p_i\}\big). \tag{2}$$

From now on we shall consider time-independent Hamilton functions only.

b) Show that for charged particles in the presence of an external vector potential $\vec{A}$ resp. magnetic field $\vec{B} = \vec{\nabla}\times\vec{A}$, the condition becomes

$$H\big(\{q_i\},\{p_i\},\vec{A}\big) = H\big(\{q_i\},\{-p_i\},-\vec{A}\big).$$

ii. Liouville equation

Let us now consider a probability density $\rho\big(t,\{q_i\},\{p_i\}\big)$ on the phase space Γ, so as to describe an evolving macroscopic state (macrostate). Similar to Eq. (1), we associate with ρ a "time-reversed macrostate" defined as

$$\rho^t\big(t,\{q_i\},\{p_i\}\big) = \rho\big(-t,\{q_i\},\{-p_i\}\big). \tag{3}$$

a) Show that if a system is invariant under time reversal, then the corresponding Liouville equation possesses the same symmetry, i.e. for every solution ρ of the Liouville equation the time-reversed density ρ^t solves the Liouville equation as well.

b) (*Loschmidt paradox*) If a system possesses time-reversal symmetry, can it evolve towards some universal "equilibrium (macro)state" which is independent of the actual initial condition?

13. Lorentz gas

In various physical situations—for instance the motion of neutrons in a nuclear reactor or of electrons in a non-degenerate semi-conductor—one can describe the diffusion of (light) particles inside a medium made of more massive constituents as resulting from collisions on *fixed* scattering centers. The diffusing particles are then referred to as a *Lorentz gas*. The evolution of the corresponding (coarse-grained) single-particle phase-space density is governed by a simplified version of the Boltzmann kinetic equation, which will be derived hereafter.

Throughout this problem, it is assumed that no external vector potential is present, so that the linear and canonical momenta $\vec{p}$ of particles are identical. Furthermore, one neglects the collisions between the particles of the Lorentz gas.

i. Conservation laws

One assumes that the collisions between the particles and the scattering centers are instantaneous and local, as well as elastic and invariant under space parity and time reversal.
Write down the relevant conservation laws. Explain why the collision of a particle on a scattering center amounts to a change $\vec{p} \to \vec{p}'$ of its momentum, with $|\vec{p}| = |\vec{p}'|$. The corresponding differential cross-section will be denoted as $\sigma(\vec{p} \to \vec{p}')$. What can you say about reference frames?

ii. Kinetic equation

Let $\bar{\mathsf{f}}(t,\vec{r},\vec{p})$ be the (dimensionless) single-particle phase-space density of the particles of the Lorentz gas. As in the case of the Boltzmann equation, the dynamics of $\bar{\mathsf{f}}$ obeys an equation of the type

$$\frac{\partial \bar{\mathsf{f}}}{\partial t} + \vec{v}\cdot\vec{\nabla}_{\vec{r}}\bar{\mathsf{f}} + \vec{F}\cdot\vec{\nabla}_{\vec{p}}\bar{\mathsf{f}} = \left(\frac{\partial \bar{\mathsf{f}}}{\partial t}\right)_{\text{coll.}}, \qquad \left(\frac{\partial \bar{\mathsf{f}}}{\partial t}\right)_{\text{coll.}} \equiv \left(\frac{\partial \bar{\mathsf{f}}}{\partial t}\right)_{\text{gain}} - \left(\frac{\partial \bar{\mathsf{f}}}{\partial t}\right)_{\text{loss}}, \tag{4}$$

where $\vec{v}$ is the particle velocity, while the collision integral is conveniently expressed as the difference between a gain and a loss term, which we now want to compute.

a) Loss term. Consider a scattering center at position $\vec{r}$. What is the flux density of particles with a momentum between $\vec{p}$ and $\vec{p}+\mathrm{d}^3\vec{p}$ falling on this scattering center? Show that the number of collisions of the type $\vec{p} \to \vec{p}'$, where $\vec{p}$, $\vec{p}'$ are known up to infinitesimal uncertainties $\mathrm{d}^3\vec{p}$, $\mathrm{d}^3\vec{p}'$, in a time interval $\mathrm{d}t$ is given by

$$\bar{\mathsf{f}}(t,\vec{r},\vec{p})\,\frac{\mathrm{d}^3\vec{p}}{(2\pi\hbar)^3}\big|\vec{v}\big|\,\sigma(\vec{p}\to\vec{p}')\,\mathrm{d}^2\Omega'\,\mathrm{d}t,$$

where Ω' is the solid angle associated with the direction of $\vec{p}'$.
Deduce that the loss term is given by

$$\left(\frac{\partial \bar{\mathsf{f}}}{\partial t}\right)_{\text{loss}} = n_{\mathrm{d}}(\vec{r})\,\big|\vec{v}\big|\,\bar{\mathsf{f}}(t,\vec{r},\vec{p})\int\sigma(\vec{p}\to\vec{p}')\,\mathrm{d}^2\Omega',$$

with n_{d} the density of scattering centers. What is the integral equal to?

b) Gain term. The gain term corresponds to collisions of the type $\vec{p}' \to \vec{p}$, where the initial and final momenta are known up to infinitesimal uncertainties. Show that between t and $t+\mathrm{d}t$, there are

$$\bar{\mathsf{f}}(t,\vec{r},\vec{p}')\,\frac{\mathrm{d}^3\vec{p}'}{(2\pi\hbar)^3}\big|\vec{v}'\big|\,\sigma(\vec{p}'\to\vec{p})\,\mathrm{d}^2\Omega\,\mathrm{d}t,$$

such collisions on a single scattering center at position $\vec{r}$, where Ω is the solid angle associated with the direction of $\vec{p}$. Let Ω' be the solid angle associated with $\vec{p}'$. Justify the identity

$$\big|\vec{v}'\big|\,\mathrm{d}^3\vec{p}'\,\mathrm{d}^2\Omega = \big|\vec{v}\big|\,\mathrm{d}^3\vec{p}\;\mathrm{d}^2\Omega'.$$

Show that the gain term can be written as

$$\left(\frac{\partial \bar{\mathsf{f}}}{\partial t}\right)_{\text{gain}} = n_{\mathrm{d}}(\vec{r})\,\big|\vec{v}\big|\int\bar{\mathsf{f}}(t,\vec{r},\vec{p}')\,\sigma(\vec{p}\to\vec{p}')\,\mathrm{d}^2\Omega',$$

and thus the collision integral as

$$\left(\frac{\partial \bar{\mathsf{f}}}{\partial t}\right)_{\text{coll.}} = n_{\mathrm{d}}(\vec{r})\,\big|\vec{v}\big|\int\big[\bar{\mathsf{f}}(t,\vec{r},\vec{p}') - \bar{\mathsf{f}}(t,\vec{r},\vec{p})\big]\,\sigma(\vec{p}\to\vec{p}')\,\mathrm{d}^2\Omega'. \tag{5}$$