Tutorial sheet 9

The exercise marked with a star is homework.

Discussion topic: BBGKY hierarchy; single-particle kinetic equations

23. Collisionless evolution of the single-particle phase space density

Let $f_1(t,\vec{r},\vec{p})$ denote the single-particle phase space density of a system of non-interacting particles with mass m evolving in the absence of long-range interactions deriving from a vector potential. Consider the particles which are at time t in an infinitesimal volume element $d^3\vec{r}\,d^3\vec{p}$ around the point $(\vec{r},\vec{p})$.

Where are these particles at the instant $t+dt$? Show that the volume element $d^3\vec{r}'\,d^3\vec{p}'$ which they then occupy equals (to leading order in dt) $d^3\vec{r}\,d^3\vec{p}$. Derive the partial differential equation governing the evolution of f_1.

24. Two-particle phase space density in a classical ideal gas

The purpose of this exercise is to show that even in a classical ideal gas of identical particles, (small) correlations between particles arise when their total number N is fixed.

i. Canonical equilibrium

Consider first the case of a classical gas of N non-interacting identical particles, each of which is described by a Hamilton function h, so that the total Hamilton function reads

$$H_N = h(1) + h(2) + \cdots + h(N),$$

where for the sake of brevity the positions and momenta of the particles have been denoted by the particle label. At thermodynamic equilibrium, the canonical partition function for this gas is

$$Z_N(\beta,\mathcal{V}) = \frac{\left[Z_1(\beta,\mathcal{V})\right]^N}{N!},$$

with Z_1 the partition function for a single particle—which need not be specified hereafter.

a) Compute first the single-particle phase space density $f_1(\vec{r}_1,\vec{p}_1)$.

b) Write down the two-particle phase space density $f_2(\vec{r}_1,\vec{p}_1,\vec{r}_2,\vec{p}_2)$. How does it compare to the product of the single-particle densities for particles 1 and 2?

ii. Grand canonical equilibrium

The number of particles in the gas is now allowed to vary, so that the proper description at thermodynamic equilibrium takes place in the grand canonical ensemble, involving the "chemical" Lagrange multiplier $\alpha = \beta\mu$.

a) Recall the expression of the grand canonical partition function $Z(\beta,\mathcal{V},\alpha)$ in terms of the canonical partition functions Z_N and α, then in terms of Z_1 and α.

b) Derive the single-particle phase space density $f_1(\vec{r}_1,\vec{p}_1)$.

Hint: Consider first the contribution to f_1 coming from the case when the gas consists of N particles, then carefully sum over all possible values of N.

c) Compute the two-particle phase space density $f_2(\vec{r}_1,\vec{p}_1,\vec{r}_2,\vec{p}_2)$ and rewrite it as function of the single-particle densities for particles 1 and 2. Compare with the result in the canonical approach.

*25. 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 $\mathbf{X}(t) \equiv \big(\{q_a(t)\}, \{p_a(t)\}\big)$ in Γ.

To each trajectory $\mathbf{X}(t)$, one may associate a "time-reversed trajectory" $\mathbf{X}^t(t) \equiv \big(\{q_a^t(t)\}, \{p_a^t(t)\}\big)$ such that
$$q_a^t(t) = q_a(-t), \qquad p_a^t(t) = -p_a(-t) \quad \forall a. \tag{1}$$
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
$$H\big(t, \{q_a\}, \{p_a\}\big) = H\big(-t, \{q_a\}, \{-p_a\}\big). \tag{2}$$
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
$$H\big(\{q_a\}, \{p_a\}, \vec{A}\big) = H\big(\{q_a\}, \{-p_a\}, -\vec{A}\big).$$

ii. Liouville equation

Let us now consider a probability density $\rho(t, \{q_a\}, \{p_a\})$ 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
$$\rho^t(t, \{q_a\}, \{p_a\}) = \rho(-t, \{q_a\}, \{-p_a\}). \tag{3}$$

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?

Merry Christmas and Happy New Year!