

## Tutorial sheet 4

### Discussion topics:

- Classical Liouville operators
- BBGKY hierarchy; single-particle kinetic equations

### 9. Liouville operator in classical mechanics

The lecture introduced the Liouville operator  $\mathcal{L}$ , acting on functions on the  $N$ -particle phase space  $\Gamma$  with canonical variables  $(\{q_i\}, \{p_i\})$ . Let  $d^{6N}\mathcal{V} \propto \prod_i dq_i dp_i$  denote a uniform measure on  $\Gamma$ , as e.g. that used in the lecture.

#### i. Hermiticity of $\mathcal{L}$

Consider two functions  $g(\{q_i\}, \{p_i\})$ ,  $h(\{q_i\}, \{p_i\})$  which vanish sufficiently rapidly at infinity; let  $g^*$ ,  $h^*$  denote the complex conjugate functions. Show that

$$\int_{\Gamma} g^*(\{q_i\}, \{p_i\}) \mathcal{L} h(\{q_i\}, \{p_i\}) d^{6N}\mathcal{V} = \int_{\Gamma} (\mathcal{L} g)^*(\{q_i\}, \{p_i\}) h(\{q_i\}, \{p_i\}) d^{6N}\mathcal{V}.$$

Recognizing in the integral of  $g^*h$  over  $\Gamma$  an inner product, which can be denoted as  $\langle g, h \rangle$ , the identity can be recast as  $\langle g, \mathcal{L}h \rangle = \langle \mathcal{L}g, h \rangle$ , which expresses the property that the Liouville operator is Hermitian<sup>1</sup> for this inner product.

#### ii. Unitarity of $e^{\pm i\mathcal{L}}$

Show that the operator  $e^{i\mathcal{L}}$  acting on phase-space functions is unitary.

### 10. 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  $f_1$ .

### 11. 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

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

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

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

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

<sup>1</sup>... according to the physicists' denomination; mathematicians may prefer "self-adjoint".

- 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  $\alpha$ , then in terms of  $Z_1$  and  $\alpha$ .
- 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.