Non-equilibrium physics WS 20/21 – Exercise Sheet 4:

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1 Discussion:

i) How is a microscopic state characterized in classical mechanics? What is the significance of the *phase-space distribution*? Illustrate these at the example of the harmonic oscillator.

- Microscopic state of N particles in classical system is described by the $6N$-dimensional phase-space : $\{x_i, p_i\} = (x_1, ..., x_{3N}, p_1, ..., p_{3N})$, where an observable is a function $O(\{x_i\}, \{p_i\}, t)$.
- The *phase-space distribution* $f(\{x_i, p_i\}, t)$ represent the probability to find the system in a certain microscopic state where particles positions and momentums are given by $\{x_i, p_i\}$.
- The evolution of each member of the statistical ensemble is described by Classical EOM, giving a trajectory in the phase space.

2 In-class problems:

2.1 Evolution of phase-space density

We first consider a statistical ensemble of free particles, with Hamiltonian $H(\{x_i\}, \{p_i\}) = \sum_i \frac{p_i^2}{2m}$ and initial phase-space distribution $f(t_0, \{x_i\}, \{p_i\}) = f_0(\{x_i\}, \{p_i\})$ at initial time $t_0 = 0$.

i) Write down the Liouville equation for the time evolution of the phase-space distribution and construct the formal solution in terms of the Liouville operator.

- The Liouville equation is given by

$$\frac{\partial}{\partial t} f(t_0, \{x_i\}, \{p_i\}) + \Big\{ f(t_0, \{x_i\}, \{p_i\}), H \Big\} = 0 \,, \tag{1}$$

where the Poisson bracket is defined

$$\Big\{ f(t_0, \{x_i\}, \{p_i\}), H \Big\} = \sum_i \left(\frac{\partial f}{\partial x_i}\frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial x_i}\frac{\partial f}{\partial p_i} \right) \,. \tag{2}$$

We define the Liouville operator

$$i\mathcal{L} \equiv \sum_i \left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial x_i} - \frac{\partial H}{\partial x_i}\frac{\partial}{\partial p_i} \right) = \{\bullet, H\} \,. \tag{3}$$

- The formal solution to the Liouville equation is written

$$f(t_0, \{x_i\}, \{p_i\}) \;\;=\;\; e^{-i\mathcal{L}t} f_0(, \{x_i\}, \{p_i\}) \,. \tag{4}$$

ii) Calculate the the action of the Liouville operator $\mathcal{L}f$ and $\mathcal{L}^2 f$ on the phase-space distribution f. Deduce from this result the form $\mathcal{L}^n f$.

- The action of the Liouville operator is written

$$
\begin{aligned}
i\mathcal{L}f &= \sum_i \left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial x_i} - \frac{\partial H}{\partial x_i}\frac{\partial}{\partial p_i} \right) f \, , && (5)\\
&= \sum_i \frac{p_i}{m}\frac{\partial}{\partial x_i} f \, , && (6)\\
&= \frac{\vec{p}}{m}\cdot\vec{\nabla} f \, . && (7)
\end{aligned}
$$

For second order we have

$$
\begin{aligned}
(i\mathcal{L})^2 f &= \sum_i \left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial x_i} - \frac{\partial H}{\partial x_i}\frac{\partial}{\partial p_i} \right) \frac{\vec{p}}{m}\cdot\vec{\nabla} f \, , && (8)\\
&= \left(\frac{\vec{p}}{m}\cdot\vec{\nabla} \right)^2 f \, , && (9)
\end{aligned}
$$

where $\vec{p} = \{p_i\}$ and $\vec{\nabla} = \{\frac{\partial}{\partial x_i}\}$. We can deduce the general form

$$
(i\mathcal{L})^n f = \left(\frac{\vec{p}}{m}\cdot\vec{\nabla} \right)^n f \, . \qquad (10)
$$

iii) Construct the explicit solution to the solution Liouville equation.
$\left(\text{Hint: } e^{a\partial/\partial_x} f(x) = \sum_{n=0}^{\infty} \frac{a^n}{n!} f^{(n)}(x) = f(x+a)\right)$

- The explicit solution is

$$
\begin{aligned}
f(t_0, \{x_i\}, \{p_i\}) &= e^{-i\mathcal{L}t} f_0(\{x_i\}, \{p_i\}) \, , && (11)\\
&= \sum_n \frac{(-i\mathcal{L}t)^n}{n!} f_0 \, , && (12)\\
&= \sum_n \frac{1}{n!} \left(-t\frac{\vec{p}}{m}\cdot\vec{\nabla} \right)^n f_0 \, , && (13)\\
&= f_0\left(\left\{ x_i - \frac{p_i}{m} t \right\}, \{p_i\} \right) \, . && (14)
\end{aligned}
$$

Next consider a statistical ensemble of classical harmonic oscillators, with Hamiltonian $H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$ and initial phase-space distribution $f(t_0, x, p) = f_0(x, p)$ at initial time $t_0 = 0$.

iv) Write down Hamilton's equations of motion for $\dot{x}, \dot{p}$ and solve them for general initial conditions $x(0) = x_0$ and $p(0) = p_0$.

- Hamilton's equations are given by

$$
\begin{aligned}
\dot{x} &= \frac{\partial H}{\partial p} = \frac{p}{m} \, , && (15)\\
\dot{p} &= -\frac{\partial H}{\partial x} = -m\omega^2 x \, , && (16)
\end{aligned}
$$

which admit the solution

$$\ddot{x} = -\omega^2 x \Rightarrow x(t) = c_1 \cos(\omega t) + c_2 \sin(\omega t) \ , \quad p(t) = m\omega(c_2 \cos(\omega t) - c_1 \sin(\omega t)) \ . \tag{17}$$

Using the initial conditions we find

$$c_1 = x_0 \ , \qquad c_2 = \frac{p_0}{m\omega} \ . \tag{18}$$

- The classical trajectories are

$$x_{cl}(t) = x_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) \ , \quad p_{cl}(t) = p_0 \cos(\omega t) - m\omega x_0 \sin(\omega t) \ . \tag{19}$$

v) Exploit your result in iv) to compute the time evolution of the phase-space distribution $f(t, x, p)$

- The phase-space distribution follows the classical trajectories

$$f(t, x, p) = \int dx_0 dp_0 \ f_0(x_0, p_0) \delta(x - x_{cl}(t|x_0, p_0)) \delta(p - p_{cl}(t|x_0, p_0)) \ , \tag{20}$$

Now solving the δ constraints

$$x = x_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin(\omega t) \ , \tag{21}$$

$$p = -m\omega x_0 \sin(\omega t) + p_0 \cos(\omega t) \ , \tag{22}$$

for x_0 and p_0

$$x_0 = x \cos(\omega t) - \frac{p}{m\omega} \sin(\omega t) \ , \tag{23}$$

$$p_0 = m\omega x \sin(\omega t) + p \cos(\omega t) \ , \tag{24}$$

so using $det(...) = 1$, we can re-write the constraints in terms of x_0 and p_0

$$f(t, x, p) = \int dx_0 dp_0 \ f_0(x_0, p_0) \delta\Big(x_0 - (x \cos(\omega t) - \frac{p}{m\omega} \sin(\omega t))\Big) \delta\Big(p_0 - (m\omega x \sin(\omega t) + p \cos(\omega t))\Big) \ , \tag{25}$$

which directly gives the solution

$$f(t, x, p) = f_0(x \cos(\omega t) - \frac{p}{m\omega} \sin(\omega t), m\omega x \sin(\omega t) + p \cos(\omega t)) \ , \tag{26}$$

3 Homework problems:

3.1 Entropy production in non-relativistic hydrodynamics

i) Show that the entropy production rate $\sigma_S = \sum_i (J_i - J_i^{eq})F_i$ for a Newtonian fluid is given by

$$\sigma_S = \kappa T^2 \left(\vec{\nabla}\frac{1}{T}\right)^2 + \frac{\zeta}{T}(\vec{\nabla}\vec{v})^2 + \frac{2\eta}{T}\sum_{\alpha\beta}(\sigma^{\alpha\beta})^2$$

- As entropy production is frame independent, we compute in the local rest-frame defined as the frame comoving with the fluid at point $\vec{r}_0$ where the fluid velocity at time t_0 is $\vec{v}_0$, the position is given by $\vec{r}' = \vec{r} - \vec{v}_0(t-t_0)$ and velocity $\vec{v}' = \vec{v} - \vec{v}_0$. The relevant affinities are given by

$$\vec{\nabla}\,\vec{Y}_E\Big|_{LRF} = \vec{\nabla}\frac{1}{T}\,, \qquad \vec{\nabla}\,\vec{Y}_P\Big|_{LRF} = -\vec{\nabla}\,\frac{\vec{v}'}{T}\Big|_{t_0,\vec{r}_0} = -\vec{\nabla}\,\frac{\vec{v}-\vec{v}_0}{T}\Big|_{t_0,\vec{r}_0} = -\frac{1}{T}\vec{\nabla}\vec{v}\,, \tag{27}$$

The fluxes are given by

$$\vec{J}_E\Big|_{LRF} = -\kappa\vec{\nabla}T\,, \qquad \vec{J}_N\Big|_{LRF} = 0\,, \qquad J_P^{\alpha\beta}\Big|_{LRF} = \pi^{\alpha\beta}\,, \tag{28}$$

$$\vec{J}_E^{\rm eq}\Big|_{LRF} = -\kappa\vec{\nabla}T\,, \qquad \vec{J}_N^{\rm eq}\Big|_{LRF} = 0\,, \qquad J_P^{\alpha\beta\ {\rm eq}}\Big|_{LRF} = P\delta^{\alpha\beta}\,, \tag{29}$$

with

$$\pi^{\alpha\beta} = (P - \zeta(\vec{\nabla}.\vec{v}))\delta^{\alpha\beta} - 2\eta\sigma^{\alpha\beta}\,, \qquad \sigma^{\alpha\beta} = \frac{1}{2}\left(\frac{\partial v^\alpha}{\partial x_\beta} + \frac{\partial v^\beta}{\partial x_\alpha}\right) - \frac{1}{3}(\vec{\nabla}\vec{v})\delta^{\alpha\beta} \tag{30}$$

- The entropy production rate in local rest frame is written

$$\sigma_S = \sum_i (J_i - J_i^{eq})F_i\,, \tag{31}$$

$$= \left(-\kappa\vec{\nabla}T\right)\cdot\vec{\nabla}\frac{1}{T} - \sum_{\alpha\beta}\left(-\zeta(\vec{\nabla}.\vec{v})\delta^{\alpha\beta} - 2\eta\sigma^{\alpha\beta}\right)\vec{\nabla}^\alpha\frac{\vec{v}'^\beta}{T}\,, \tag{32}$$

$$= \left(\kappa T^2\vec{\nabla}\frac{1}{T}\right)\cdot\vec{\nabla}\frac{1}{T} + \sum_{\alpha\beta}\left(\zeta(\vec{\nabla}.\vec{v})\delta^{\alpha\beta} + 2\eta\sigma^{\alpha\beta}\right)\left(\frac{1}{T}\vec{\nabla}^\alpha\vec{v}^\beta\right)\,,$$

$$= \kappa T^2\left(\vec{\nabla}\frac{1}{T}\right)^2 + \frac{\zeta}{T}(\vec{\nabla}\vec{v})^2 + \frac{2\eta}{T}\sum_{\alpha\beta}(\sigma^{\alpha\beta})^2\,, \tag{33}$$

where we used $\sum_{\alpha\beta}\sigma_{\alpha\beta}\delta_{\alpha\beta} = 0$.

ii) Determine the entropy current J_S in the local rest-frame, according to the general relation

$$J_S|_{LRF} = \sum_i Y_i J_i\,.$$

(Hint: Which intensive quantities Y_i and fluxes J_i are non-zero in the LRF?)

- In the local rest-frame

$$\vec{J}_E\Big|_{LRF} = \vec{J}_U\,, \qquad \vec{J}_N\Big|_{LRF} = 0\,, \qquad J_P^{\alpha\beta}\Big|_{LRF} = \pi^{\alpha\beta}\,, \tag{34}$$

$$\vec{Y}_E\Big|_{LRF} = \frac{1}{T}\,, \qquad \vec{Y}_P\Big|_{LRF} = -\frac{\vec{v}'}{T}\Big|_{t_0,\vec{r}_0} = -\frac{\vec{v}-\vec{v}_0}{T}\Big|_{t_0,\vec{r}_0} = 0\,, \tag{35}$$

(36)

- The entropy current is given by

$$J_S^\alpha|_{LRF} = -\frac{\kappa}{T}\vec{\nabla}^\alpha T \,, \tag{37}$$

iii) Since the entropy density is frame independent, the entropy current in an arbitrary frame is given by

$$\vec{J}_S = \vec{J}_S\Big|_{LRF} + s\vec{v} \,.$$

Based on this result, along with the results of i) and ii), write down the explicit form of the entropy balance equation for a Newtonian fluid.

- We have

$$\vec{\nabla}\cdot\vec{J}_S\Big|_{LRF} = -\kappa\vec{\nabla}\left(\frac{\vec{\nabla}T}{T}\right) \,. \tag{38}$$

- Entropy balance equation is written

$$\frac{\partial s}{\partial t} + \vec{\nabla}\cdot\vec{J}_s = \sigma_s \,, \tag{39}$$

$$\frac{\partial s}{\partial t} + \vec{\nabla}\cdot\left(s\vec{v} - \kappa\left(\frac{\vec{\nabla}T}{T}\right)\right) = \frac{1}{T}\left[\frac{\kappa}{T}\left(\vec{\nabla}T\right)^2 + \zeta(\vec{\nabla}\vec{v})^2 + 2\eta\sum_{\alpha\beta}(\sigma^{\alpha\beta})^2\right] \,, \tag{40}$$

3.2 Evolution of expectation values in classical & quantum theories

Consider a classical system described by a Hamiltonian $H(x,p) = \frac{p^2}{2m} + V(x)$ and its quantum mechanical analogue, where the phase-space variables x, p are replaced by operators $\hat{x}$ and $\hat{p}$. Note that quantum mechanically $[\hat{x},\hat{p}] = i\hbar$ which implies the useful identity $[\hat{p}, V(\hat{x})] = -i\hbar V'(\hat{x})$ that you can use without proof.

i) Determine the classical and quantum evolution equations for the observables

$$\left\langle \frac{1}{2}x^2 \right\rangle, \qquad \left\langle \frac{1}{2}p^2 \right\rangle \quad \text{and} \quad \langle xp + px \rangle \,.$$

$\Big($Hints: Commutators can be simplified according to $[AB, C] = A[B, C] + [A, C]B$. $\Big)$

- The classical evolution equation can be inferred from the Liouville equation as follows

$$\frac{\partial}{\partial t}\left\langle \frac{1}{2}x^2 \right\rangle = -\left\{\frac{1}{2}x^2, H\right\} = -\left\langle \frac{xp}{m} \right\rangle \,, \tag{41}$$

$$\frac{\partial}{\partial t}\left\langle \frac{1}{2}p^2 \right\rangle = -\left\{\frac{1}{2}p^2, H\right\} = \langle pV'(x)\rangle \,, \tag{42}$$

$$\frac{\partial}{\partial t}\langle xp + px\rangle = -\Big\{2xp, H\Big\} = \left\langle 2xV'(x) - 2\frac{p^2}{m} \right\rangle \,. \tag{43}$$

- Let us compute the following commutators

$$\left[\hat{x}^2, \hat{p}\right] = \hat{x}[\hat{x},\hat{p}] + [\hat{x},\hat{p}]\hat{x} = 2i\hbar\hat{x} \,, \tag{44}$$

$$\left[\hat{p}^2, \hat{x}\right] = \hat{p}[\hat{p},\hat{x}] + [\hat{p},\hat{x}]\hat{p} = -2i\hbar\hat{p} \,, \tag{45}$$

$$\left[\hat{p}^2, V(\hat{x})\right] = \hat{p}[\hat{p},V(\hat{x})] + [\hat{p},V(\hat{x})]\hat{p} = -i\hbar\left(V'(\hat{x})\hat{p} + \hat{p}V'(\hat{x})\right) \,, \tag{46}$$

- For a quantum system we can use the Heisenberg picture to write

$$\begin{aligned}
\frac{\partial}{\partial t}\left\langle \frac{1}{2}\hat{x}^2 \right\rangle &= -\frac{i}{\hbar}\left[H, \frac{1}{2}\hat{x}^2\right] = -\frac{i}{\hbar}\frac{1}{4m}\left(\hat{p}\left[\hat{p}, \hat{x}^2\right] + \left[\hat{p}, \hat{x}^2\right]\hat{p}\right) = -\left\langle \frac{\hat{x}\hat{p} + \hat{p}\hat{x}}{2m} \right\rangle , \quad (47)\\
\frac{\partial}{\partial t}\left\langle \frac{1}{2}\hat{p}^2 \right\rangle &= -\frac{i}{\hbar}\left[H, \frac{1}{2}\hat{p}^2\right] = \frac{1}{2}\left\langle V'(\hat{x})\hat{p} + \hat{p}V'(\hat{x})\right\rangle , \quad (48)\\
\frac{\partial}{\partial t}\left(\hat{x}\hat{p} + \hat{p}\hat{x}\right) &= \frac{\partial}{\partial t}\left(2\hat{x}\hat{p} - i\hbar\right) = \frac{2i}{\hbar}\left(\hat{x}\left[\hat{p}, H\right] + \frac{1}{2m}\left[\hat{x}, \hat{p}^2\right]\hat{p}\right) = \left\langle 2\hat{x}V'(\hat{x}) - 2\frac{\hat{p}^2}{m}\right\rangle . \quad (49)
\end{aligned}$$

ii) Specialize now on the case of a harmonic oscillator $V(x) = \frac{1}{2}m\omega^2 x^2$ and solve the coupled set of evolution equations for $\langle E_{pot}\rangle = \langle \frac{1}{2}m\omega^2 x^2\rangle$, $\langle E_{kin}\rangle = \langle \frac{p^2}{2m}\rangle$ and $\langle xp + px\rangle$. How do the results compare between the classical and quantum theory?
$\Big($Hint: Energy conservation$\Big)$

- The classical evolution equation for the energies are given by

$$\begin{aligned}
\frac{\partial}{\partial t}\langle E_{pot}\rangle &= -\omega^2\langle xp\rangle , \quad (50)\\
\frac{\partial}{\partial t}\langle E_{kin}\rangle &= \frac{1}{m}\langle pV'(x)\rangle = \omega^2\langle xp\rangle , \quad (51)\\
\frac{\partial}{\partial t}\langle xp + px\rangle &= 2\left\langle m\omega^2 x^2 - \frac{p^2}{m}\right\rangle = 4\left(\langle E_{pot}\rangle - \langle E_{kin}\rangle\right) , \quad (52)\\
\frac{\partial^2}{\partial t^2}\langle xp\rangle &= -4\omega^2\langle xp\rangle , \quad (53)
\end{aligned}$$

as the total energy is constant

$$\langle xp\rangle = c_1\cos(2\omega t) + c_2\sin(2\omega t) . \quad (54)$$

- The energies are written

$$\begin{aligned}
\langle E_{pot}\rangle &= \frac{\omega}{2}(c_1\cos(2\omega t) - c_2\sin(2\omega t)) + c_0 , \quad (55)\\
\langle E_{kin}\rangle &= -\frac{\omega}{2}(c_1\cos(2\omega t) - c_2\sin(2\omega t)) + c_0' , \quad (56)
\end{aligned}$$

- For a quantum system we can use the Heisenberg picture to write

$$\begin{aligned}
\frac{\partial}{\partial t}\langle E_{pot}\rangle &= -\omega^2\left\langle \frac{\hat{x}\hat{p} + \hat{p}\hat{x}}{2}\right\rangle , \quad (57)\\
\frac{\partial}{\partial t}\langle E_{kin}\rangle &= \omega^2\left\langle \frac{\hat{x}\hat{p} + \hat{p}\hat{x}}{2}\right\rangle , \quad (58)\\
\frac{\partial}{\partial t}\left(\hat{x}\hat{p} + \hat{p}\hat{x}\right) &= \left\langle 2m\omega^2\hat{x}^2 - 2\frac{\hat{p}^2}{m}\right\rangle = 4\left(\langle E_{pot}\rangle - \langle E_{kin}\rangle\right) . \quad (59)
\end{aligned}$$

Leading to the same solution as in the classical case

$$\begin{aligned}
\langle E_{pot}\rangle &= \frac{\omega}{2}(c_1\cos(2\omega t) - c_2\sin(2\omega t)) + c_0 , \quad (60)\\
\langle E_{kin}\rangle &= -\frac{\omega}{2}(c_1\cos(2\omega t) - c_2\sin(2\omega t)) + c_0' . \quad (61)
\end{aligned}$$