Freie Universität Berlin
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Statistical Physics and Thermodynamics (SS 2017)

Problem sheet 4

Hand in: Friday, May 19 during the lecture

http://www.physik.fu-berlin.de/en/einrichtungen/ag/ag-netz/lehre/

1 Phase space and 1D harmonic oscillator (17 points)

Consider a 1D harmonic oscillator with mass m, position q in a potential $V(q) = kq^2/2$.

a) Write down the Lagrange function $L(q, \dot{q}) = T - V$, where T is the kinetic energy and V the potential energy, and derive the equation of motion for q from it using the Euler-Lagrange equation. **(2 points)**

b) For the 1D harmonic oscillator, explicitly calculate the Legendre transformation

$$\mathcal{H}(q, p) = p \cdot \dot{q}(q, p) - L(q, \dot{q}(q, p)), \tag{1}$$

where the canonical momentum is defined by $p = \partial L/\partial \dot{q}$. **(2 points)**

c) Calculate Hamilton's equations of motion for $\mathcal{H}$, and solve them to obtain the phase space trajectory $(q(t), p(t))$ with initial conditions $q(0) = q_0$, $p(0) = p_0$. **(2 points)**

d) Use your result from c) to calculate $\mathcal{H}(q(t), p(t))$ and $L(q(t), \dot{q}(t))$ along a solution of the equations of motion. Are they conserved along a trajectory? **(2 points)**

e) Sketch a solution from c) with initial energy $E = \mathcal{H}(q_0, p_0)$ in phase space, i.e. in the (q, p)-plane. Is the resulting curve closed? What geometric shape does the trajectory have? At which points does it intersect the q- and p-axes? **(3 points)**

f) Assume the oscillator starts at rest with energy E. Calculate the running averages of kinetic and potential energy, i.e.

$$\bar{E}_{\text{kin}}(t) = \frac{1}{t}\int_0^t T(t')\,\mathrm{d}t', \qquad \bar{E}_{\text{pot}}(t) = \frac{1}{t}\int_0^t V(t')\,\mathrm{d}t' \tag{2}$$

and express them in terms of E. What are the limits for $t \to 0$, $t \to \infty$? **(3 points)**

g) Now we move from individual trajectories in phase space to probability distributions. Consider a uniform probability distribution in phase space for all states with energy E, i.e.

$$\rho(q, p) = \frac{1}{\omega(E)} \cdot \delta\left(E - \mathcal{H}(q, p)\right), \tag{3}$$

where the normalization constant $\omega(E)$ is called the density of states and $\delta(x)$ is the Dirac-delta distribution. Calculate $\omega(E)$. Is it proportional to the contour length of the curve in the (q, p) plane that corresponds to all states with energy E? **(3 points)**

2 Conservation of probability (3 points)

Consider a particle moving in phase space according to Hamilton's equations of motion for a Hamiltonian $\mathcal{H}$. The phase space trajectory of the particle is $(Q(t), P(t)) \in \mathbb{R}^2$, and the corresponding probability density is given by

$$\rho(q,p,t) = \delta(q - Q(t)) \cdot \delta(p - P(t)), \tag{4}$$

with δ the Dirac-delta distribution.

Verify the conservation of probability in a rectangle $[-q_0, q_0] \times [-p_0, p_0]$ in phase space by explicitly calculating both sides of the equation

$$-\frac{\mathrm{d}}{\mathrm{d}t} \int_{-q_0}^{q_0} \mathrm{d}q \int_{-p_0}^{p_0} \mathrm{d}p \, \rho(q,p,t) = \int_{-q_0}^{q_0} \mathrm{d}q \int_{-p_0}^{p_0} \mathrm{d}p \, \vec{\nabla} \cdot (\vec{v}(q,p)\rho(q,p,t)) \tag{5}$$

to show that they are equal. Here,

$$\vec{v}(q,p) = \begin{pmatrix} \dot{q}(q,p) \\ \dot{p}(q,p) \end{pmatrix} = \begin{pmatrix} \partial\mathcal{H}(q,p)/\partial p \\ -\partial\mathcal{H}(q,p)/\partial q \end{pmatrix} \tag{6}$$

is the phase space velocity field and

$$\vec{\nabla} = \begin{pmatrix} \partial/\partial q \\ \partial/\partial p \end{pmatrix} \tag{7}$$

is the gradient in phase space. At which point in the calculation do you need to use that $(Q(t), P(t))$ obeys Hamilton's equations of motion?

Hint: Use the Heaviside step function

$$\Theta(x) = \begin{cases} 0 & \text{if } x < 0, \\ 1 & \text{if } x \geq 0, \end{cases} \tag{8}$$

and note that its derivative is the delta distribution, $\partial\Theta(x)/\partial x = \delta(x)$.