Theoretical Statistical Physics

Solution to Exercise Sheet 7

1 Dynamics of a Hamiltonian system (4 points)

Consider the motion of a particle in two dimensions in a harmonic potential. In terms of the coordinate vector $q = (q_1, q_2)$, and in suitably chosen length and time units, the Newtonian equations of motion are

$$\ddot{q}_1 = -q_1, \qquad \ddot{q}_2 = -\omega^2 q_2, \tag{1}$$

where $\omega > 0$.

a) Formulate the potential and the Hamiltonian $H(p, q)$ for which (1) arise as the Hamiltonian equations of motion. Interpret ω.

b) Determine the energy shell $\mathcal{E}$ in phase space for an energy $E > 0$, and its geometric shape. Determine also the projection P of the energy shell onto position space; how can one describe P geometrically? Is the region R, in which the motion in coordinate space really takes place, all of P or a proper subset of P? How can one describe R geometrically?

c) Describe the motion in P for $\omega = 3/2$ and $\omega = \sqrt{2}$ qualitatively.

d) Are there constants of motion besides the Hamiltonian? Is the system ergodic for any of the two values of ω given in c)?

a) Hamilton's equations read

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \qquad i \in \{1, 2\}. \tag{2}$$

For $\omega^2 = k/m$, where m denotes the mass of the particle and k determines the slope of the potential in q_2-direction (it may be thought of as a spring constant), we write the potential as

$$V(q) = \frac{m}{2} q_1^2 + \frac{k}{2} q_2^2. \tag{3}$$

Then the Hamiltonian takes the form

$$H(p, q) = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{m}{2} q_1^2 + \frac{k}{2} q_2^2. \tag{4}$$

Inserting (4) into Hamilton's equations yields

$$\dot{q}_1 = \frac{p_1}{m}, \qquad \dot{q}_2 = \frac{p_2}{m}, \qquad \dot{p}_1 = -m\, q_1, \qquad \dot{p}_2 = -k\, q_2. \tag{5}$$

By differentiating the first two equations w.r.t. time and inserting the second two, we recover the Newtonian equations of motion (1).

ω is the angular frequency of the oscillatory motion of the particle in q_2-direction.

b) The energy shell $\mathcal{E}$ at energy E is the subset of phase space Γ defined by

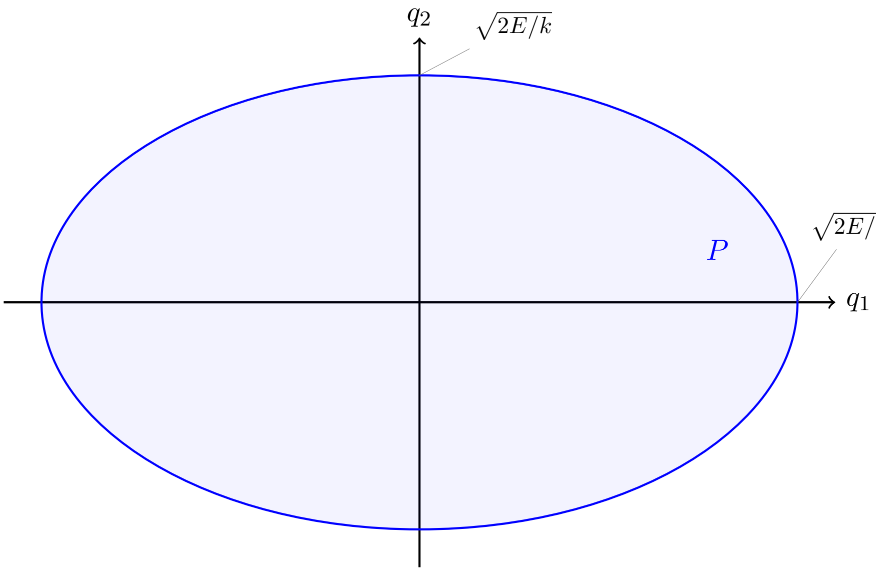
$$\mathcal{E} = \left\{ x = (p, q) \in \Gamma \,\middle|\, H(p, q) = E \right\}. \tag{6}$$

Inserting (4), we get

$$\frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{m}{2}\,q_1^2 + \frac{k}{2}\,q_2^2 = E, \tag{7}$$

which defines the three-dimensional surface of a four-dimensional ellipsoid with semi-principal axes of length $\sqrt{2mE}$, $\sqrt{2mE}$, $\sqrt{2E/m}$, and $\sqrt{2E/k}$ in dimensions p_1, p_2, q_1, and q_2, respectively.

Projected onto two-dimensional position space, the shadow of this ellipsoid gives the area enclosed by an ellipse with semi-principal axes $\sqrt{2E/m}$, and $\sqrt{2E/k}$.



Solving Newton's equations of motion (1) with initial conditions $q_i(0) = q_{i,0}$ and $p_i(0) = p_{i,0}$, we find

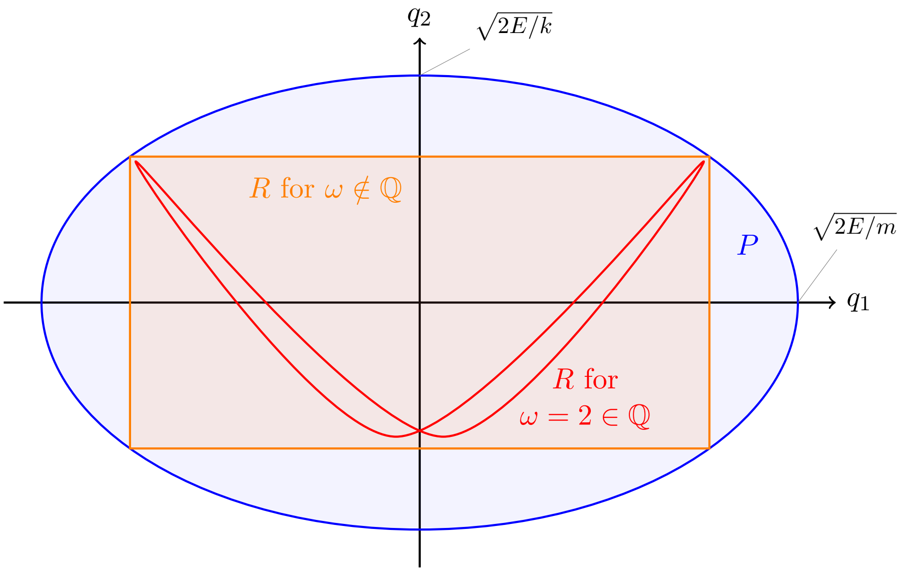
$$\begin{aligned} q_1(t) &= q_{1,0}\cos(t) + \frac{p_{1,0}}{m}\,\sin(t), \\ q_2(t) &= q_{2,0}\cos(\omega t) + \frac{p_{2,0}}{m\omega}\,\sin(\omega t), \end{aligned} \qquad \text{with } p_i = m\dot{q}_i. \tag{8}$$

Since the motion in q_1- and q_2-direction decouples, $R \subset P$ can at most be a rectangle inscribed into the region P. The lengths of the sides of this rectangle are determined by the energies E_1 and E_2 available in dimensions q_1 and q_2, which are conserved over time and determined by the initial conditions.

However, there is still an intersting distinction to make on whether or not R is dense (after an infinite time) within the rectangle it can at most inscribe in P. This depends on two factors:

1. The initial conditions we impose. Consider for instance $q_{1,0} = 1$, $p_{1,0} = 0$, $q_{2,0} = 0$, $p_{2,0} = 0$. In this case, $q_2(t) = 0$ for all times and q_1 oscillates according to $q_1(t) = \cos(t)$. The trajectory never leaves the q_1-axis and hence the region R in which the motion actually takes place is just $R = \{(q_1, 0) \mid q_1 \in [-1, 1]\}$.
2. The ratio between the frequencies $\omega_1 = 1$ and $\omega_2 = \omega$. If one ignores such pathological cases as in 1., then two possibilities remain. For $\omega_2/\omega_1 = \omega \in \mathbb{Q}$, i.e. when ω is rational, there is a finite time t_c after which the trajectory closes. This may be seen as follows. Let $\omega = \frac{m}{n} > 0$ with $m, n \in \mathbb{N}$. Then for $t_c = 2\pi n$, we have $q_1(t) = q_1(t + t_c)$ and $q_2(t) = q_2(t + t_c)$ due to the 2π-periodicity of sine and cosine. An orbit that closes after a finite time can never become dense in the P-inscribed rectangle.

   On the other hand, if $\omega \notin \mathbb{Q}$ is irrational, the orbit never closes. After an infinite time, the orbit will then trace out the full rectangle of accessible states.



c) As explained in b), for $\omega = 3/2$, the orbit will close after a time $t_c = 4\pi$ (Lissajous curve), while for $\omega = \sqrt{2}$ the trajectory never closes, instead becoming dense in $R \subset P$ for $t \to \infty$ (provided we don't consider pathological initial conditions).

d) Since there are no coupling terms in the Hamiltonian, we may write $H(p_1, p_2, q_1, q_2) = H_1(p_1, q_1) + H_2(p_2, q_2)$, i.e. the particle describes two uncoupled harmonic oscillators, one in each dimension. Energy is conserved under Hamiltonian time-evolution and H_1 and H_2 both satisfy Hamilton's equations (2). Thus, they are conserved individually. Their values depend on the initial conditions,

$$H_1 = \frac{{p_{1,0}}^2}{2m} + \frac{m}{2}\, q_{1,0}^2, \qquad H_2 = \frac{{p_{2,0}}^2}{2m} + \frac{k}{2}\, q_{2,0}^2, \qquad \forall\, t. \tag{9}$$

The fact that H_1 and H_2 are conserved individually explains why motion is restricted to the rectangle $q_{i,\min} \leq q_i \leq q_{i,\max}$, $i \in \{1, 2\}$ whose corners touch the edge of P.
Furthermore, if $\omega = 1$, the potential becomes isotropic, i.e. it attains rotational symmetry under $SO(2)$ acting on (q_1, q_2). By Noether's theorem, we expect an additional conserved quantity, namely the angular momentum L. In two dimensions, L is the scalar quantity

$$L = q_1\, p_2 - q_2\, p_1. \tag{10}$$

Using (8), this is easily shown to be conserved,

$$\begin{aligned} L &= \Big(q_{1,0}\, \cos(t) + \frac{p_{1,0}}{m}\, \sin(t)\Big)\Big(-m\, q_{2,0}\, \sin(t) + p_{2,0}\, \cos(t)\Big) \\ &\quad - \Big(q_{2,0}\, \cos(t) + \frac{p_{2,0}}{m}\, \sin(t)\Big)\Big(-m\, q_{1,0}\, \sin(t) + p_{1,0}\, \cos(t)\Big) \\ &= \big(q_{1,0}\, p_{2,0} - q_{2,0}\, p_{1,0}\big). \end{aligned} \tag{11}$$

Ergodicity requires time and ensemble averages of any observable to be equal. Since $R \subset P$ for all values of ω both rational and irrational, it is obvious that the system is not ergodic. Averaging over time corresponds to averaging over the restricted set $R \subset P$, which cannot be equal to the average over the ensemble of initial conditions sampling all of P.

2 Time evolution of the Gibbs entropy (3 points)

Assume that an ensemble of initial conditions at constant energy E is given by a distribution $x = (q, p) \mapsto w_0(x)$ on phase space Γ, and that w_t is the distribution obtained from it by

Hamiltonian time evolution. Determine how the entropy

$$\sigma(w_t) = -k_\mathrm{B} \int_\Gamma w_t(x) \ln w_t(x) \, \mathrm{d}\mu_m(x) \tag{12}$$

changes with time. (Here $\mathrm{d}\mu_m(x) = \delta(E - H(x)) \, \mathrm{d}^{6N}x$ is the unnormalized microcanonical measure.[1])

The time derivative of $\sigma(w_t)$ is

$$\frac{\mathrm{d}\sigma}{\mathrm{d}t} = -k_\mathrm{B} \int_\Gamma \frac{\mathrm{d}w_t}{\mathrm{d}t} (1 + \ln w_t) \, \mathrm{d}\mu_m(x). \tag{13}$$

Liouville's continuity equation (which follows directly from Hamilton's equations)

$$\frac{\mathrm{d}w_t}{\mathrm{d}t} = 0, \tag{14}$$

describes the incompressible flow of phase-space probability density and identifies w_t as the conserved current associated via Noether's theorem with conservation of energy under Hamiltonian time evolution. Thus, the Gibbs entropy is constant,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}t} = 0. \tag{15}$$

3 Ideal paramagnet (3 points)

Using the results derived in the lectures and the Gibbs fundamental relation, calculate the thermodynamic equation of state for the ideal paramagnet of independent spins, and solve it approximately in the limits $h\,m \ll k_\mathrm{B}\,T$ and $h\,m \gg k_\mathrm{B}\,T$, where h denotes the external field and m the magnetic moment of a single spin.

The energy of an ideal paramagnet consisting of N uncoupled Ising spins in the configuration $s = (s_1, \dots, s_N) \in \mathcal{S}_N = \{\pm 1\}^N$, each of gyromagnetic factor $m > 0$ and subject to the external field h is $H(s) = -hm \sum_{j=1}^N s_j$. A given energy shell corresponds to a fixed number $N_\downarrow$ of down spins $s_j = -1$, and the microcanonical partition function is the number of such configurations,

$$Z_m = \binom{N}{N_\downarrow} = \frac{N!}{N_\downarrow!(N - N_\downarrow)!}. \tag{16}$$

Since the spins are uncoupled, all possible configurations that conform to a given macrostate are equally likely to occur, justifying the use of the microcanonical ensemble.

The entropy $S = k_\mathrm{B} \ln(Z_m)$ is maximized in the microcanonical ensemble. $N_\downarrow = \frac{N}{2}$ maximizes the binomial coefficient, so we insert $N_\downarrow = \frac{N-k}{2}$, where $k \ll N$ parametrizes fluctuations, and use Stirling's approximation for large factorials to write S as

$$\begin{aligned} S(E,h) &= k_\mathrm{B}\Big(\ln(N!) - \ln(N_\downarrow!) - \ln[(N - N_\downarrow)!]\Big) \\ &\approx k_\mathrm{B}\Big(N\ln(N) - \cancel{N} - \tfrac{N-k}{2}\ln\big(\tfrac{N-k}{2}\big) + \cancel{\tfrac{N-k}{2}} - \tfrac{N+k}{2}\ln\big(\tfrac{N+k}{2}\big) + \cancel{\tfrac{N+k}{2}}\Big) \\ &= k_\mathrm{B}\Big(N\ln(2N) - \cancel{N\ln(2)} - \tfrac{N-k}{2}\ln(N-k) + \cancel{\tfrac{N-k}{2}\ln(2)} - \tfrac{N+k}{2}\ln(N+k) + \cancel{\tfrac{N+k}{2}\ln(2)}\Big) \\ &= Nk_\mathrm{B}\ln(2) - \tfrac{Nk_\mathrm{B}}{2}\Big[\big(1 - \tfrac{k}{N}\big)\ln\big(1 - \tfrac{k}{N}\big) + \big(1 + \tfrac{k}{N}\big)\ln\big(1 + \tfrac{k}{N}\big)\Big] \\ &= Nk_\mathrm{B}\ln(2) - \tfrac{Nk_\mathrm{B}}{2}\Big[\big(1 + \tfrac{E}{Nmh}\big)\ln\big(1 + \tfrac{E}{Nmh}\big) + \big(1 - \tfrac{E}{Nmh}\big)\ln\big(1 - \tfrac{E}{Nmh}\big)\Big], \end{aligned} \tag{17}$$

[1] We can fix the units, i.e. make $\mathrm{d}\mu_m(x)$ dimensionless, correct the counting of states for systems of identical particles, and thus avoid the Gibbs paradox by including the factor $\frac{1}{h^{3N}N!}$.

where $E = -kmh$ is the deviation in energy from Nmh.

The Gibbs fundamental relation for a magnetic system exhibiting total magnetization M and subject to the magnetic field h reads

$$\mathrm{d}S(E,h) = \frac{1}{T}\,\mathrm{d}E + \frac{M}{T}\,\mathrm{d}h. \tag{18}$$

Therefore,

$$\frac{1}{T} = \frac{\partial S}{\partial E}\bigg|_h = -\frac{k_\mathrm{B}}{mh}\,\operatorname{arctanh}\left(\frac{E}{Nmh}\right) \tag{19}$$

$$\frac{M}{T} = \frac{\partial S}{\partial h}\bigg|_E = \frac{k_\mathrm{B}E}{mh^2}\,\operatorname{arctanh}\left(\frac{E}{Nmh}\right) \tag{20}$$

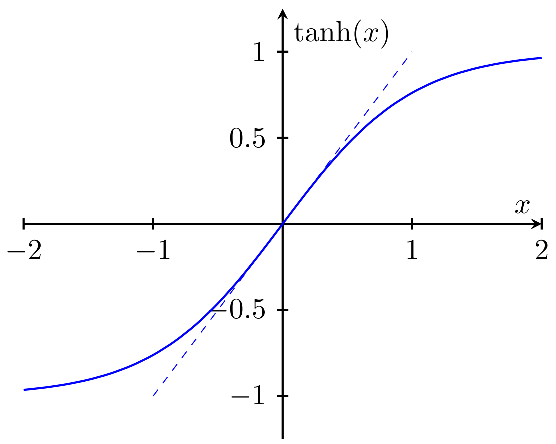
Solving (19) for E gives

$$E = -Nmh\tanh\left(\frac{mh}{k_\mathrm{B}T}\right). \tag{21}$$

Inserting (21) into (20) yields the magnetization

$$M(h,T) = Nm\tanh\left(\frac{mh}{k_\mathrm{B}T}\right). \tag{22}$$

The plot below shows that $\tanh(x) \to \pm 1$ for $x \to \pm\infty$ while $\tanh(x) \approx x$ for $|x| \ll 1$.



The asymptotic behavior of the magnetization at low and high temperatures is thus

$$M \approx \begin{cases} \frac{Nm^2h}{k_\mathrm{B}T} & \text{for } mh \ll k_\mathrm{B}T, \qquad \text{(Curie's law)} \\ Nm & \text{for } mh \gg k_\mathrm{B}T. \end{cases} \tag{23}$$

An intuitive interpretation of this result is that for low temperatures, all spins align to give a large magnetization, whereas for high temperatures, thermal fluctuations disturb spin alignment, resulting in a low magnetization that tends to zero as $mh/k_\mathrm{B}T \to 0$.