Institute for Mechanical Systems
Center of Mechanics
Prof. Dr. Sanjay Govindjee
Felix Hildebrand

Useful Definitions

Phase Average of the Microcanonical Ensemble

The microcanonical ensemble is characterized by a constant total energy E, i.e. for all replicas in the ensemble

$$H(\mathbf{q}, \mathbf{p}) = E. \tag{1}$$

As a result of this restriction, the representation of the ensemble in phase space is a $(2N-1)$-dimensional hypersurface. The ensemble average can be calculated from

$$\bar{F} = \frac{1}{\Omega(E)} \frac{\mathrm{d}}{\mathrm{d}E} \int_{V_E} F(\mathbf{q}, \mathbf{p}) \, \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{p}, \tag{2}$$

where V_E is the domain in phase space for which $H(\mathbf{q}, \mathbf{p}) \leq E$ holds for the system Hamiltonian and where

$$\Omega(E) = \frac{\mathrm{d}}{\mathrm{d}E} \int_{V_E} \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{p}, \tag{3}$$

is the so-called structure function or density of states of the system.

Weakly Coupled Systems

An (isolated) combination of two systems A and B is called *uncoupled* if its Hamiltonian is

$$H_{A+B}(\mathbf{q}_A, \mathbf{q}_B, \mathbf{p}_A, \mathbf{p}_B) = H_A(\mathbf{q}_A, \mathbf{p}_A) + H_B(\mathbf{q}_B, \mathbf{p}_B), \tag{4}$$

where H_{A+B} is the Hamiltonian of the entire system and H_A and H_B are the individual Hamiltonians of the isolated systems.

An (isolated) combination of two systems A and B is called *coupled* if its Hamiltonian has the form

$$H_{A+B}(\mathbf{q}_A, \mathbf{q}_B, \mathbf{p}_A, \mathbf{p}_B) = H_A(\mathbf{q}_A, \mathbf{p}_A) + H_B(\mathbf{q}_B, \mathbf{p}_B) + H_{AB}(\mathbf{q}_A, \mathbf{q}_B, \mathbf{p}_A, \mathbf{p}_B), \tag{5}$$

where H_{A+B} is the Hamiltonian of the entire system, H_A and H_B are the Hamiltonians of the isolated systems A and B and where $H_{AB} \neq 0$ contains all coupling terms.

A coupled (isolated) combination of two systems A and B with Hamiltonian

$$H_{A+B}(\mathbf{q}_A, \mathbf{q}_B, \mathbf{p}_A, \mathbf{p}_B) = H_A(\mathbf{q}_A, \mathbf{p}_A) + H_B(\mathbf{q}_B, \mathbf{p}_B) + H_{AB}(\mathbf{q}_A, \mathbf{q}_B, \mathbf{p}_A, \mathbf{p}_B) \tag{6}$$

is called *weakly coupled* if one can neglect the coupling term $H_{AB} \neq 0$ when calculating integrals over phase space.

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Problem 1 - Time and phase averages

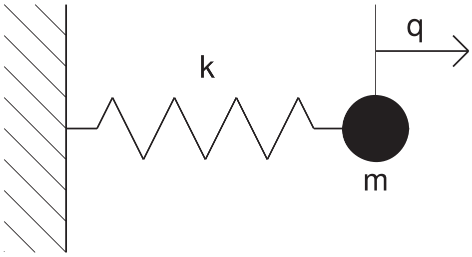

Figure 1: A one-dimensional harmonic oscillator.

Consider a one-dimensional oscillator (see Figure 1) with mass $m = 1$ and stiffness $k = 2$. The deviation from the undeformed configuration is described by q, the initial conditions of the system are $q(t = 0) = 1$ and $\dot{q}(t = 0) = 0$.

For the given system, calculate the time and phase averages of the displacement q, the potential energy $\frac{1}{2}kq^2$, the momentum $p = m\dot{q}$ and the kinetic energy $\frac{1}{2}m\dot{q}^2 = \frac{p^2}{2m}$

To to so, carry out the following steps:

a) Derive and solve the equations of motion for the system for the given boundary condition. Does this motion cover the whole constant-energy hypersurface?

b) Compute the time average of the desired phase functions.

c) Calculate the two-dimensional volume of the domain in phase space $V(E)$ for which $H(q, p) \leq E$ and take its derivative to determine the structure function $\Omega(E)$ according to (3).

d) Now determine the phase averages of the desired phase functions using (2) and verify its equality with the time averages.

The Mathematica file corresponding to this problem, *harmonicOscillator.nb*, can be downloaded from the course homepage.

ETH Zurich
Department of Mechanical and Process Engineering
Statistical Mechanics of Elasticity
Exercise 3 - Summer 2007

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Homework 1 - Time and phase averages

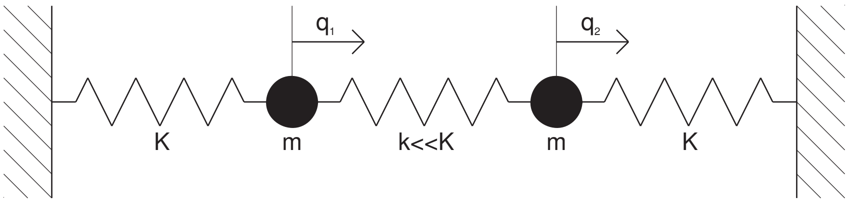

Figure 2: Two weakly coupled one-dimensional harmonic oscillators.

Now consider two harmonic oscillators with masses $m = 1$ and stiffnesses $K = 10$ that are weakly coupled by a spring of stiffness $k << K$. The positions of the oscillators are described by q_1 and q_2 where $q_i = 0$ refers to the undeformed state. The initial conditions of the system are given by $q_1(t = 0) = 1$, $q_2(t = 0) = 0$ and $p_i(t = 0) = 0$.

a) Calculate the four-dimensional volume of the domain in phase space $V(E)$ for which $H(\mathbf{q}, \mathbf{p}) \leq E$ and take its derivative to determine the structure function $\Omega(E)$. In carrying out the calculation, make sure that your integration boundaries are such that the total energy is smaller or equal to E and that all possible distributions of the energy to the two systems are considered. Assume the system is weakly coupled.

b) Now determine the phase averages of the square displacement of the first mass q_1^2, the square momentum of the second mass p_1^2, the kinetic energy of the system $\frac{p_1^2+p_2^2}{2m}$ and its potential energy $\frac{1}{2}K(q_1^2 + q_2^2) + \frac{1}{2}k(q_1 - q_2)^2$ using (2) for the cases (i) $k = 0$, (ii) $k = 0.1$ and (iii) $k = 1$. Again, weak coupling can be assumed.

c) Compare the computed phase averages with the time averages obtained in the last homework. How is the agreement related with the stiffness k? Identify the terms H_A, H_B and H_{AB} of the system Hamiltonian for all three values of k and relate your results to the agreements of time and phase averages.

Questions/Comments/Suggestions? Felix Hildebrand - CLA H23.1 - 044/632-7755 - felixhi@ethz.ch