ETH Zurich | Institute for Mechanical Systems
Department of Mechanical and Process Engineering | Center of Mechanics
Statistical Mechanics of Elasticity | **Prof. Dr. Sanjay Govindjee**
Exercise 2 - Summer 2007 | Felix Hildebrand

Useful Definitions

Time Averages

The time average of a phase function $F(\mathbf{q},\mathbf{p})$ is obtained from

$$\hat{F} = \lim_{t\to\infty} \frac{1}{t}\int_0^t F(\mathbf{q}(\tau),\mathbf{p}(\tau))\,\mathrm{d}\tau, \tag{1}$$

where $\mathbf{q}$,$\mathbf{p}$ are shorthand for q_i and p_i and similarly $\mathrm{d}\mathbf{q} = \mathrm{d}q_1\mathrm{d}q_2...$ and $\mathrm{d}\mathbf{p} = \mathrm{d}q_1\mathrm{d}q_2...$, $i \in \{1,...,N\}$, where N is the number of total degrees of freedom of the given system.

Phase Averages

The phase average of a phase function $F(\mathbf{q},\mathbf{p})$ is obtained from

$$\bar{F} = \int_\Gamma F(\mathbf{q},\mathbf{p})\rho(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{p}, \tag{2}$$

where Γ refers to the associated phase space and where $\rho(\mathbf{q},\mathbf{p})$ is the distribution function of the given system with the properties

$$\rho(\mathbf{q},\mathbf{p}) \geq 0, \qquad \int_\Gamma \rho(\mathbf{q},\mathbf{p})\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{p} = 1. \tag{3}$$

Ergodicity

For an ergodic system, the values of time and phase averages coincide independent of the considered phase function $F(\mathbf{q},\mathbf{p})$, yielding

$$\hat{F} = \bar{F} \qquad \forall \qquad F(\mathbf{q},\mathbf{p}). \tag{4}$$

Conservation of the distribution function ρ along a trajectory

The distribution function $\rho(\mathbf{q},\mathbf{p})$ of a Hamiltonian system is conserved along trajectories $\mathbf{y}(t)$,

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = 0 \qquad \text{on } \mathbf{y} \qquad \forall t. \tag{5}$$

Although this holds for time-dependent distribution functions as well, we are specifically interested in equilibrium situations. We define equilibrium by

$$\frac{\partial\rho}{\partial t} = 0 \tag{6}$$

and will thus assume only systems with time-independent distribution functions such that ρ is locally constant. A family of distribution functions satisfying both (6) and (5) is $\rho(\mathbf{q},\mathbf{p}) = \rho(H(\mathbf{q},\mathbf{p}))$.

Conservation of the Hamiltonian H along a trajectory

For general Hamitonian systems, the variation of the Hamiltonian along a trajectory $\mathbf{y}(t)$ is equal to its local variation, i.e.

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial t} \qquad \text{on } \mathbf{y} \qquad \forall t. \tag{7}$$

For isolated systems, the Hamiltonian is time-independent, hence

$$\frac{\mathrm{d}H}{\mathrm{d}t} = 0 \qquad \text{on } \mathbf{y} \qquad \forall t. \tag{8}$$

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Metrical Decomposability of $S(E)$

A constant energy hypersurface $S(E)$ is said to be *metrically decomposable* if it can be divided into (at least) two open sets S_1 and S_2 with $S_1 \cap S_2 = \emptyset$ and $\overline{S_1 \cup S_2} = S(E)$ such that any trajectory starting in S_1 will stay there $\forall t$ and any trajectory starting in S_2 will stay there $\forall t$. If $S(E)$ is not *metrically decomposable* it is said to be *metrically undecomposable*.

Homework 1 - Undecomposability and time averages

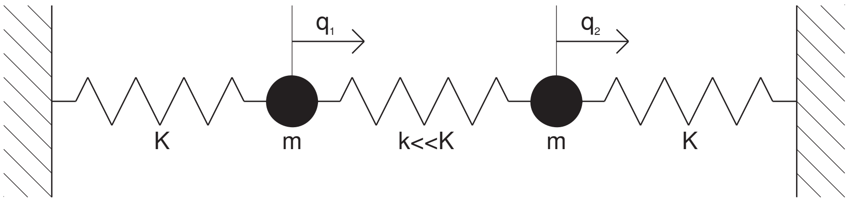

Figure 1: Two weakly coupled one-dimensional harmonic oscillators.

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 solely described by the positions, the initial momenta are zero, i.e. $p_i(t = 0) = 0$.

a) Derive the equations of motion for the system for $k = k_1 = 0$, $k = k_2 = 0.1$ and $k = k_3 = 1$ for initial conditions $q_1(t = 0) = 1$ and $q_2(t = 0) = 0$.

b) Calculate the period T of the (combined) system. Generate two (seperate) plots of $q_1(t)$ and $q_2(t)$ as well as two (seperate) three-dimensional plots of ($q_1(t)$,$p_1(t)$,t) and ($q_2(t)$,$p_2(t)$,t) for $0 \leq t \leq T$.

c) Describe the constant energy surface $S(E)$ of the system for a given energy E in the phase space spanned by (q_1, q_2, p_1, p_2). For which of the values of k used in a) is the trajectory covering all of $S(E)$?

d) For values of $k \neq 0$, the system is metrically undecomposable. However, there are two sets S_1 and S_2, $S_1, S_2 \subset S(E)$, for which trajectories starting in each one of them will stay there forever. What are these sets? Plot two trajectories starting in both sets for $0 \leq t \leq T$ as in b). How are these related to the eigenmodes of the system (see a))? Why does this comply with the definition of undecomposability given above?

e) Choosing an initial condition such that $E = (k + K)/2$ and $(q_1(t = 0), q_2(t = 0), p_1(t = 0), p_2(t = 0)) \notin S_1 \cup S_2$ from c), compute the time 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 $\frac{1}{2}K(q_1^2 + q_2^2) + \frac{1}{2}k(q_2 - q_1)^2$ using (1) for both k_2 and k_3. Recall that the solution in a) assumed zero initial momenta. Does the integration of the time avergage have to be carried out for $t \to \infty$?

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