Statistische Mechanik - WS 2020/21 Prof. Dr. O. Philipsen Universität Frankfurt
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Sheet 2

Hand in via OLAT until Tuesday the 17th of November 18:00.

4) Ergodicity *(4+2=6 Points)*

(i) Consider a particle of mass m in one dimension, subject to the potential

$$V(x) = \theta(x_1 - x)\kappa(x - x_1)^2 + \theta(x - x_2)\lambda(x - x_2)^2 + \\ \theta(x - x_1)\theta(x_2 - x)\min_x\left(\kappa(x - x_1)^2, \lambda(x - x_2)^2\right),$$

where $x_2 > x_1$ and $\theta(x)$ is the step function and $\kappa, \lambda > 0$. For which energies $E = T + V$ is this system ergodic, non-ergodic? Discuss in both cases the dependence of the time average from the initial conditions.

(ii) Consider a system of N uncoupled harmonic oscillators with total energy $E = \sum_{i=1}^{N} E_i$, where E_i is the energy of the i-th oscillator. Show that the system is not ergodic.

5) Representation of the microcanonical ensemble *(4+3=7 Points)*

In the lecture you derived the probability density of an isolated, ergodic system with conserved energy, at constant particle number N and constant volume V. Energy conservation is expressed in terms of the Hamilton function $H(\vec{\pi}) = H(p, q) = E_0 = \text{const.}$
The probability density is therefore given from the microcanonical ensemble

$$\rho(p, q) = \frac{1}{\Omega(E_0, N, V)}\delta\big(H(\vec{\pi}) - E_0\big).$$

(i) Show that

$$\langle H(\vec{\pi})\rangle = E_0.$$

Hint: Rewrite the phase space integration $d\Gamma$, *splitting the measure into a hypersurface of constant energy* df_{E_0} *and a perpendicular phase space vector to this surface* $d\pi_\perp$, $d\Gamma = df_{E_0} d\pi_\perp$. *Next consider the total differential of the Hamilton function* $H(\vec{\pi})$. *Make use of the direction of the gradient to express* $d\pi_\perp$ *in terms of* dH, *making it possible to integrate the* δ*-distribution.*

An alternative representation of the microcanonical probability density, familiar from the lecture, is given as

$$\rho(p, q) = \begin{cases} \frac{1}{\Delta\Gamma(E_0, V, N)} & E \in [E_0, E_0 + \Delta E] \\ 0 & \text{else.} \end{cases}$$

Instead of a δ-distribution, an energy interval of finite, but small size ΔE is considered.

(ii) Show that in the case $\Delta E \to 0$, we have the same expectation value familiar from (i)

$$\langle H(\vec{\pi})\rangle = E_0.$$

Hint: Proceed as in (i), but keep in mind, that you are now dealing with a finite shell of thickness ΔE.
Make use of the expansion of the phase space volume $\Delta\Gamma(E_0, V, N)$ *at small* ΔE *and identify the density of states* $\Omega(E_0, V, N)$ *in the limit* $\Delta E \to 0$.

6) Properties of the density operator *(7 Points)*

Let $\hat{A}$ be an operator, and the density operator of quantum mechanical system with N particles is defined as

$$\hat{\rho}_N = \sum_i w_i \left|\psi_i\right\rangle \left\langle\psi_i\right| \qquad \text{with} \qquad \sum_i w_i = 1$$

. Prove that

(i) $\mathrm{Tr}(\hat{\rho}_N \hat{A}) = \mathrm{Tr}(\hat{A}\hat{\rho}_N)$.

(ii) $\hat{\rho}_N$ ist hermitian.

(iii) $\hat{\rho}_N$ has only positive eigenvalues.

(iv) $\mathrm{Tr}(\hat{\rho}_N) = 1$, i.e. the probability density is normalized.

(v) $\mathrm{Tr}(\hat{\rho}_N \ln(\hat{\rho}_N)) = \sum_{i=1} w_i \ln w_i$.

(vi) $\mathrm{Tr}(\hat{\rho}_N^2) \leq \mathrm{Tr}(\hat{\rho}_N)$ (when does equality hold?)

(vii) The statistical mean value $\left\langle \hat{A} \right\rangle$ equals the quantum mechanical expectation value of $\hat{A}$, if the system is in a pure state ($w_i = \delta_{ij}$).

Hint: Make use of a complete, discrete set of orthonormal Eigenstates to evaluate the traces.