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SoSe 05

Set 7
5/30/05

T IV: Thermodynamik und Statistik
(Prof. E. Frey)

Problem set 7

Problem 7.1 *Quantum harmonic oscillator*

The Hamiltonian of a harmonic oscillator is represented in terms of creation/anihilation operators

$$\mathcal{H} = \frac{\hbar\omega}{2}\left(\hat{a}\hat{a}^+ + \hat{a}^+\hat{a}\right), \qquad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^+), \quad \hat{p} = -i\sqrt{2\hbar m\omega}(\hat{a} - \hat{a}^+)$$

Derive expressions for the quantum thermal averages $\langle \hat{x}^2 \rangle = Z^{-1}\mathsf{Tr}(e^{-\mathcal{H}/k_BT}\hat{x}^2)$ and $\langle \hat{x}^4 \rangle$. Discuss the crossover from pure quantum fluctuations, $k_BT \ll \hbar\omega$, to classical thermal fluctuations, $k_BT \gg \hbar\omega$. Can you guess what the full probability distribution for the coordinate, $P(x) = \langle \delta(x - \hat{x}) \rangle$, should be?

Problem 7.2 *Two-dimensional rotor*

The Lagrangian of a classical rotator characterized by an angle, $-\pi < \varphi \le \pi$ in an external field, E, is given by

$$\mathcal{L} = \frac{I}{2}\dot{\varphi}^2 + \mu E \cos\varphi$$

where I denotes the moment of inertia and μ is the coupling parameter to the field.

1. Derive the Hamilton function $\mathcal{H}$ corresponding to the Lagrangian.
2. Write down the canonical partition function and evaluate the integral over the canonical momentum.
3. The configurational integral can be performed in terms of special functions only. Expand the configurational integral for high temperatures $k_BT \gg \mu E$ in powers of inverse temperature $\beta = 1/k_BT$. For low temperatures $k_BT \ll \mu E$ the fluctuations of φ are strongly localized and are reasonably well approximated by a Gaussian. Derive the leading terms of the low-temperature expansion for the configurational integral.
4. Give corresponding expansions for the free energy.
5. Discuss the heat capacity and the mean alignment $\langle \cos\varphi \rangle$ for high and low temperatures, respectively.

Problem 7.3 *Diesel engine*

Before you consider this problem study carefully the Carnot process which you can look up in the textbooks.

The Diesel cycle can approximately be regarded as a sequence of four steps: 1. adiabatic compression, 2. isobaric expansion (ignition), 3. adiabatic expansion, 4. isochoric cooling. Sketch the cycle in a S–V and a P–V diagram. Calculate the heat and the corresponding work for each of the steps for an ideal gas. Determine the efficiency of the Diesel engine.

[For an ideal gas the equation of state reads $PV = Nk_BT$. The specific heats C_P and C_V are independent of pressure and temperature. Adiabats fulfill $PV^\gamma = const.$ with $\gamma = C_P/C_V, C_P - C_V = Nk_B$.]

Problem 7.4

For a particular system it is found that if the volume is kept constant at the value V_0 and the pressure is changed from P_0 to an arbitrary pressure P', the heat transfer to the system is

$$Q' = A(P' - P_0)\,, \qquad A > 0\,.$$

In addition it is known that the adiabates of the system are of the form

$$PV^\gamma = const.\,, \qquad \gamma > 0\,.$$

Find the energy $E(P, V)$ for an arbitrary point in the P–V plane, expressing $E(P, V)$ in terms of $P_0, V_0, A, E_0 \equiv E(P_0, V_0)$ and γ (as well as P and V).
Answer:

$$E - E_0 = A(Pr^\gamma - P_0) + PV(1 - r^{\gamma-1})/(\gamma - 1)\,, \qquad r = V/V_0$$

Problem 7.5

Show that if a single-component system is such that PV^k is constant in the adiabatic process (k is a positive constant) the energy is

$$E = \frac{1}{k-1}PV + Nf(PV^k/N^k)$$

where f is an undetermined function.
Hint: Write the adiabat in terms of intensive variables. The constant depends only on the entropy density.

Problem 7.6 *Kelvin and Clausius*

Argue that Kelvin's statement of the second law of thermodynamics follows from Clausius and vice versa. Assume that Kelvin is wrong to infer that Clausius has to be wrong too. Assume that Clausius is wrong and argue that Kelvin's statement would be invalid. Use reversible Carnot cycles to construct your argument.