

Thermodynamics and Statistical Physics

FMF150 VT2013

Projects

- **1. Rotational and vibrational states in molecules [RB]** Start by answering the questions in exercise problem 29. Then search the literature for realistic values of rotational and vibrational energies in two-atomic molecules. Then, choose a suitable two-atomic gas and calculate the heat capacity (or specific heat) as a function of temperature. Investigate in particular what happens when rotational and vibrational states start to get excited. At what temperatures does it happen? Compare your results to figure 1.13 in the textbook and to tabulated values for the specific heat at room temperature. (30, 234-236, 370-372)
- **2. van der Waals equation of states [RB]** Study its relation to the ideal gas law and to phase transitions. Why can van der Waals equation be used in cases where the ideal gas law does not work? Determine the temperature, pressure and volume at the critical point and use the "Maxwell construction" to calculate the pressure at which the phase transition takes place. (180-185)
- **3. The Ising model [RB]** Read the relevant pages in the textbook. Then, treat some of the computer problems presented in the textbook (problems 8.26 – 8.32). Discuss the choice of problems with me before you start your calculations. (340-356)
- **4. Distribution functions [RB]** Compare the Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein distributions at different temperatures for different number of particles. When does the Maxwell-Boltzmann distribution give the same result as the quantum distributions? Calculate also how the Fermi energy depends on the temperature and the number of particles. (266-271)
- **5. Planets in the habitable zone around the star Gliese 581 [RB]** Start by studying the exercise problems 43–45. Then, search the literature to find relevant data for Gliese 581 (size and surface temperature) and its planets (size and distance to the star). Then, calculate the average temperature of the planets. Does any of the planets lie in the habitable zone (where liquid water can exist on the surface of the planet)? (288-307)
- **6. The cosmic microwave background radiation [RB]** Search the literature for relevant experimental data. The measured average temperature is low and the fluctuations are very small. Calculate spectral curves like the one in figure 7.20 in the textbook for the highest and lowest temperatures and estimate what accuracy is needed in the experimental data to distinguish the two temperatures. Discuss also the technical difficulties associated with the experiments (COBE and WMAP). (288-307)
- **7. Density of states [RB]** Investigate the infinite square well and the harmonic oscillator potentials in one, two and three dimensions. Focus your attention to differences and similarities. How do you explain the results? (279-282)

- **8. Weakly interacting gases [MH]** van der Waals gas is an example of weakly interacting gas. Investigate the microscopic theory and the method of cluster expansion of partition function, diagrammatic rules and exponential summations. Discuss the virial expansion (related to problem 1.17). Compare the second virial coefficient for Lennard-Jones potential and the "hard spheres" (problem 8.11). Try to search in the literature what the virial means (hint: virial theorem). (328-339)
- **9. Equivalence of statistical ensembles [MH]** Study microcanonical, canonical and grandcanonical ensembles. Use saddle point approximation and derive the first thermodynamical law. Investigate also fluctuations of energy in the canonical ensemble and fluctuations of density in the grandcanonical ensemble and show their relation to the "susceptibilities". Show that such fluctuations are negligible in thermodynamical limit and all ensembles are equivalent. (Huang textbook 144-154)
- **10. The Darwin-Fowler method [MH]** The canonical ensemble can be derived from combinatorial arguments. This derivation is based on Stirling's formula (Reif 229-231). The derivation of canonical ensemble can be done more rigorously by The Darwin-Fowler method. Study and discuss the derivation, this involves more mathematics. (Huang textbook 193-199)
- **11. The Szilard engine.** In 1929, Leo Szilard suggested (as a thought experiment) an information-driven heat engine that seems to violate the second law of thermodynamics. This engine has today become a paradigm for describing information-to-work conversion in thermodynamic systems. Discuss/describe the engine cycle for a single classical particle (assuming the ideal gas law is applicable) in a hard-walled one-dimensional container of length L that can be divided by a movable wall, and is coupled to a single heat bath of temperature T . In addition, discuss some (or all) of the following matters in more detail: The currently accepted theory of why the second law is not violated for such an engine. The efficiency η of the engine. The theoretical description of a Szilard engine operating in the quantum regime (i.e. for a quantum particle in a one-dimensional box). The average information-to-work conversion, as a function of T , for an engine with two (or three) particles (ideal gas and/or quantum). (Observe that, at least in the quantum case, W needs to be computed numerically.) The difference in W between different quantum particles, e.g. spin-polarized fermions and spin-0 bosons. [Hint, see the work of: Landauer and Bennett, as well as Kim, Sagawa, De Liberato and Ueda]