Statistical Mechanics

Midterm Assignment

2023

Thanks to Carlos Baiz, U. Texas at Austin, for allowing the use of the picture "Boltzmann in front of his laptop".

For the midterm assignment you can use the book and other course material including your *own* notes. You are encouraged to solve the exercises using a colab (jupyter) notebook, but this is not a requirement. Mathematica, MATLAB, or another numerical language of choice may also be used. You may use existing libraries as NUMPY and SCIPY. Any code used must be included in the answers and the code handed in should be directly executable (use .ipynb, .m or .n format *not* .pdf). You are welcome to discuss with other students, but each student must hand in an individually written answer (including individual written code). *Answers will be checked for plagiarism and use of ChatGPT.* All provided numbers must include the proper units. All plots must include axis-labels including units. The answers must be given in English and typed. Handwritten answers are not accepted. The final report must be uploaded in the teaching environment as a single .ipynb, .m or .n file including both the answers and the used code. The code must run out of the box, and produce the figures shown in the report.

Norm:
The table below shows the number of points to be given for each of the questions. For the midterm score the total score, M, is converted to the mark using the max score ($M_{\max}$=70) according to the formula $\frac{9M}{M_{\max}} + 1$. The midterm counts for 1/3 of the grade for the full course.

Subquestion	A	B	C	D	E	F	G	H	I	J
Points	5	5	5	10	5	5	10	10	5	10

Phonons in diamond and graphite

Assume a material with 3N phonon-modes with frequency ω_E (the Einstein frequency).

A. Explain why the partition function for the system is given by the equation

$$Q = \prod_{i=1}^{3N} \frac{1}{1 - \exp(-\beta\hbar\omega_E)}.$$

B. Give and explain the analytical expresion for the average occupation number for each phonon mode

C. Derive the total internal energy of the system.

D. Show that the heat capacity of the system is given by:

$$C_V = 3Nk\hbar^2\omega_E^2\beta^2 \left(\frac{\exp(-\beta\hbar\omega_E)}{(\exp(-\beta\hbar\omega_E) - 1)^2} \right) \tag{1}$$

E. In the associated datafile 'diamond.dat' the experimentally measured specific heat of diamond is provided as a function of temperature. Assuming the Einstein specific heat model of Eq. 1 find the Einstein temperature ($T_E = \hbar\omega_E/k_B$) for diamond by fitting. Pay attention to the units of the provided data.

F. Use the Debye model for the specific heat capacity to determine the Debye temperature T_D. Hint: The expression in the book is not very suited for numerical approaches as $\exp(T_D/T)$ diverges for small values of T. The fit will be more stable if you reformulate the expression in terms of $\exp(-T_D/T)$.

G. Plot the experimental data in one plot with the Einstein and Debye models and discuss which model gives the best approximation and why.

H. In the associated file 'graphite.dat' the experimentally specific heat of graphite is provided as a function of temperature. Fit these data to the Einstein and Debye models, find the best Einstein and Debye temperature, and plot the fitted data together with the experimental data. Pay attention to the units of the provided data.

I. The resulting fits for graphite are significantly worse than for diamond. Give an explanation based on the crystal structure of diamond and graphite.

J. Use the determined Debye functions to determine the entropy at room temperature for diamond and graphite.