

HOMEWORK ASSIGNMENT 3

November 25th, 2020

I - On the origin of elasticity in materials

We seek to understand the origin of elasticity, a phenomenon by which materials that are deformed by external systems exert forces to return to their equilibrium shape.

A one-dimensional microscopic model for elasticity

We consider a one-dimensional chain of $N + 1$ atoms linked by N bonds of constant length l . We suppose the number of atoms is very large. The bonds can point either to the right (in which case the next atom is a distance l to the right of the preceding atom) or to the left (the converse). The first atom of the chain is fixed to the origin, and the end of the chain is free. We characterize each configuration of the chain bonds by the algebraic distance L (that is, the difference in coordinates) between the first and the last atom. For example, with $N + 1 = 4$ atoms, the microstate with successive bond directions (right, right, left) will have atoms on coordinates $(0, l, 2l, l)$ from first to last, and thus $L = l$.

1. For a given macrostate L , how many chain configurations $\Omega(L)$ are there?
2. Deduce the entropy of state L .
3. The energy of the chain does not depend on the configuration of the bonds, and the chain can therefore store no energy. In which state L_0 are we most likely to find the chain? How would you geometrically characterize this equilibrium state? We recall the Stirling formula $\ln N! \sim_{N \rightarrow \infty} N \ln N + o(N \ln N)$.

We now consider the chain immersed in a heat bath at temperature T . An external operator uses a micro-manipulation device to exert a force F_{op} on the end of the chain. The other end remains fixed at the origin. This manipulation results in the chain changing in length from its initial state L_0 by a small quantity δL .

4. Write the first law of thermodynamics for the chain in this transformation. With which system(s) did the chain exchange energy?
5. We now consider the heat bath as a system. What is the change in its internal energy δU_{HB} after the transformation? Link this quantity to the corresponding displacement δL . A priori, what are the possible values for δL ?

6. We seek to calculate the state of the heat bath and chain after the operator's action. Write the partition function for the heat bath after the transformation and deduce the average change in energy $\overline{\delta U_{\text{HB}}}$ of the heat bath during the transformation. On average, did the heat bath gain or lose energy? Deduce the average extension $\overline{\delta L}$ of the chain. We denote $R_M = Nl$ the maximum length of the chain.
7. Show that the chain exhibits elastic behavior. What is its stiffness K ? Is the chain more or less stiff at higher temperatures?
8. Discuss in what way the origin of the elastic force can be dubbed as "thermodynamical". In this picture, does this force derive from a fundamental interaction?

The entropic origin of the elastic forces

We seek a more profound explanation to the elastic force.

9. We consider a macrostate in which the chain has small length $\delta L \ll R_M$. What is the expression of the entropy of this macrostate? We advise to introduce $\delta n = \delta L/l \ll N$.
10. Develop $S(\delta L)$ to the lowest order that still depends on $\delta n/N$.
11. Express δS , the difference in entropies between state δL and the equilibrium state, as a function of δL . Express the elastic F_e force as a function of δS and δL .
12. Why can it be said that this elastic force is "entropic"?
13. Do you know of other entropic forces? Think of macroscopic forces exerted by systems of non-interacting particles.