33-341 — Thermal Physics I

Department of Physics, Carnegie Mellon University, Fall Term 2018, Deserno

Problem sheet #15

45. Electric dipole in a homogeneous electric field *(5 points, due on Monday)*

A three-dimensional electric dipole, characterized by a *unit vector* $\boldsymbol{d}$, has the energy $H(\boldsymbol{d}) = -\boldsymbol{d}\cdot\boldsymbol{E}$ when placed in a homogeneous electric field $\boldsymbol{E}$. It will also have some translational and rotational kinetic energy, but we will ignore this for now.

1. Choosing the direction of the electric field as the $\hat{z}$-axis, express the dipole's energy in spherical polar coordinates.
2. Write down the canonical partition function Z for this system; ignore the momentum integrals and factors of h.
   Hint: don't forget that this choice of coordinates implies a Jacobian *(functional determinant) in your integral.*
3. Define the polarization $d_{||} = \boldsymbol{d}\cdot(\boldsymbol{E}/E)$, which is the *projection* of the dipole moment along the direction of the external field. *Without explicitly evaluating* Z, prove that $\langle d_{||}\rangle = -\partial F/\partial E$, where $F = -k_{\rm B}T\,\ln(Z)$ is the free energy.
   Hint: Explicitly write down the canonical average and use parameter differentiation to rewrite your expression. (You know anyways what you want to find—work backwards if you need to.)
4. Now evaluate the partition function and derive an *explicit* formula for $\langle d_{||}\rangle$. Express your answer using the function $\mathscr{L}(x) = \coth(x) - x^{-1}$, which is often called the "*Langevin function*". Plot the result using suitably normalized axes!

46. Electric dipole in a homogeneous electric field—continued *(5 points, due on Tuesday)*

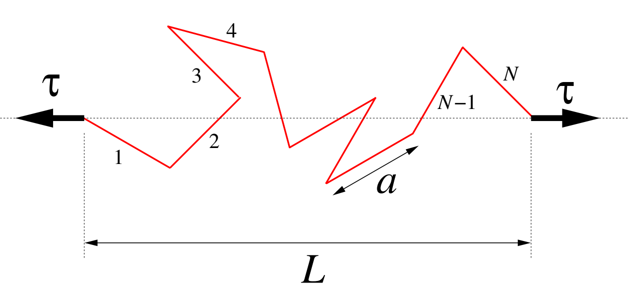
1. Expand the average polarization $\langle d_{||}\rangle$ from the previous problem to lowest nontrivial order for small values of βdE.
2. The (isothermal) *susceptibility* of the polarization can be defined as $\chi_T = \left(\frac{\partial\langle d_{||}\rangle}{\partial E}\right)_T = -\left(\frac{\partial^2 F}{\partial E^2}\right)$. Show that in the limit $E\to 0$ or $T\to\infty$ this converges towards a constant that does not depend on the applied field.
3. The susceptibility is a response function. Derive the associated fluctuation-response-theorem $k_{\rm B}T\,\chi_T = \langle d_{||}^2\rangle - \langle d_{||}\rangle^2$.

47. Heat capacity of stick-like molecules *(5 points, due on Wednesday)*

At not too low and not too high temperature, linear molecules (such as O_2, N_2, or CO_2) can be viewed as linear sticks. Their motion can be decomposed into some overall *translation* and some *rotation*. For the latter, the kinetic energy can be written as $E_{\rm rot} = \frac{1}{2I}(L_1^2 + L_2^2)$, where L_1 and L_2 are the angular momentum of rotation about the two axes perpendicular to the molecule's axis (rotation around its axis makes no sense, says quantum mechanics). Given that the kinetic degrees of freedom of each individual molecule are hence $(p_x, p_y, p_z, L_1, L_2)$, what is the average kinetic energy of such a molecule in the canonical state? And what is therefore the isochoric specific heat of diatomic gases such as O_2? *Hint: Remember problem 44!*

48. A microscopic model of rubber elasticity *(5 points, due on Friday)*

A simple model of a *polymer* is a chain of N links, each of length a, which are connected via perfectly flexible "hinges". Let's say we pull on this chain with some tension τ. Each link i can be characterized by two angles ϑ_i and φ_i that describe its orientation relative to the pulling direction.



1. If a link is not perfectly aligned with the pulling direction, it has to do work against the external pulling force, and this suggests an obvious potential energy for each link and, consequently, for the entire chain. Write it down!
2. Calculate the canonical partition function Z and the free energy F of this system; ignore the momentum part.
3. What is the expected length $\langle L\rangle$ of the chain, *i. e.*, the distance between the two end points of the chain (which must be aligned with the pulling direction)? Explicitly calculate $\langle L\rangle$ as a function of τ, T, a, and N.
4. Calculate $\left(\frac{\partial\langle L\rangle}{\partial T}\right)_\tau$ in the limit of small forces. Marvel at the sign. You've begun to unravel the mystery of problem 38!