Physics 112 : Lecture 7

Notes for the Fall 2017 Physics 112 Course taught by Professor Holzapfel
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1 Lattices

Suppose we have a lattice of molecules, where it's possible for some of the molecules in the lattice to be 'freed' from the lattice structure. The energy associated with a particular microstate is given by $U = n\epsilon$ where n is the number of molecules that have been displaced out of the lattice structure, and ϵ is the energy associated with displacing one of the lattice molecules out of its intended position. Let N be the number of molecules that are still in their rightful positions, then we have multiplicity given by:

$$g(N, n) = \frac{(N+n)!}{N!n!}$$

since we can choose which n out of the $N + n$ positions are vacant (since the molecules there have been displaced). We can then calculate the entropy and the temperature of the system:

$$\sigma(N, n) = \ln(N, n) = \Bigg[(N+n)\ln(N+n) - N\ln N - n\ln n\Bigg]; \qquad \tau = \frac{\epsilon}{\ln\left(\frac{N+n}{n}\right)}$$

where to find the temperature we have taken the inverse of the partial of σ with respect to the energy (given by $U = n\epsilon$). Note that from this, we have that:

$$\frac{n}{N+n} = e^{-\epsilon/\tau}$$

where $n/(N + n)$ describes physically the 'fractional disorder' of the system, i.e. how many of the lattice particles have been displaced from the lattice structure. At standard conditions, we have that ϵ is on the order of one electronvolt, and that τ is roughly 1/40 electron volts, so:

$$\frac{n}{N+n} \approx e^{-40}$$

i.e. we have very low fractional disorder for ordinary systems in ordinary conditions.

2 Thermal Reservoirs

A reservoir in thermodynamics is defined to be an object so large that no matter how much heat energy you dump into it; or extract form it; it's temperature never changes. Suppose we had a system S consisting of one particle (so it has only one microstate), in contact with a thermal reservoir R. Then we have:

$$g_T = g_S g_R = g_R$$

i.e. the total entropy of the combined system is determined by the reservoir's entropy. Suppose further that the reservoirs multiplicity is a function of it's energy only, it starts at an energy U_0 and transfers ϵ_S amount of energy into the system. So we have:

$$g_T = g_R(U_0 - \epsilon_S)$$

Now we can ask the question 'what is the relative probability that an amount ϵ_1 of energy is transferred to S, rather than an amount ϵ_2 of energy?' The answer is:

$$\frac{P(\epsilon_1)}{P(\epsilon_2)} = \frac{g_R(U_0 - \epsilon_1)}{g_R(U_0 - \epsilon_2)} = \frac{e^{(\sigma_R(U_0-\epsilon_1))}}{e^{(\sigma_R(U_0-\epsilon_2))}} = e^{\Delta\sigma_R}$$

where:

$$\Delta\sigma_R = \sigma_R(U_0 - \epsilon_1) - \sigma_R(U_0 - \epsilon_2)$$

Note that we have the equation:

$$\sigma_R(U_0 - \epsilon) = \sigma_R(U_0) - \epsilon\left(\frac{\partial\sigma_R}{\partial U}\right) = \sigma_R(U_0) - \frac{\epsilon}{\tau}$$

So that we find:

$$\frac{P(\epsilon_1)}{P(\epsilon_2)} = e^{-(\epsilon_1-\epsilon_2)/\tau}$$

This last term is called the Boltzmann Factor.

3 Boltzmann Factor applied to the Harmonic Oscillator

Recall that for a single harmonic oscillator we have energy levels defined by:

$$E_n = (n + 1/2)\hbar\omega$$

So we have Boltmann Factors:

$$\frac{P(E_n)}{P(E_m)} = e^{(m-n)\hbar\omega/(k_B T)}; \qquad \frac{P(E_n)}{P(E_0)} = e^{-n\hbar\omega/(k_B T)}$$

In the regime where $k_BT >> n\hbar\omega$, i.e. when the thermal energy dominates the spacing of the energy levels in the harmonic oscillator, then we have:

$$\frac{P(E_n)}{P(E_0)} \approx 1 - \frac{n\hbar\omega}{k_BT}$$

i.e. the oscillator energy levels for small enough n are roughly equally populated, which makes intuitive sense since the thermal energy is large compared to these small scales. If on the other hand we have that $k_BT << n\hbar\omega$, we have that:

$$\frac{P(E_n)}{P(E_0)} \approx 0$$

for nonzero n, which also makes sense since the thermal energy is much less than the energy needed to excite the harmonic oscillator, so we wouldn't expect much excitation to be happening.

4 Partition Function

We can define the 'partition function' for the above system, which is a function of temperature:

$$Z(\tau) = \sum_s e^{\epsilon_s/\tau}$$

and it can be shown that the probability for the system to have a particular energy ϵ_s is given by:

$$P(\epsilon_s) = \frac{e^{-\epsilon_s/\tau}}{Z}$$

where we can view the partition function as some sort of a normalization constant. If we want to find the average energy, then we can perform the calculation:

$$U = \langle\epsilon\rangle = \sum_s \epsilon_s P(\epsilon_s) = \sum_s \frac{\epsilon_s e^{-\epsilon_s/\tau}}{Z} = \tau^2 \frac{\partial \ln Z}{\partial \tau}$$

But what's the use of all this extra fluff? Suppose we turn to our friend the two state paramagnet, our partition function is given by:

$$Z = e^{mB/\tau} + e^{-mB/\tau} = 2\cosh(\epsilon/\tau)$$

So we can calculate:

$$\langle\epsilon\rangle = -mB\tanh\left(\frac{mB}{k_BT}\right)$$

which is exactly what we found earlier this month; in a much more painful process.