

PHYSICS 219

Homework 2

Due in class, Wednesday May 3

Note:

- Makeup lectures on Friday May 12 and 19, usual time. Location will be ISB 231 or 235.
- No lecture: May 8 (I'm away at a meeting) and May 29 (holiday).

1. Toy model of Ising spins

Consider the toy model discussed in class with N spins, μ_i , each of which can take values ± 1 . Let $M = \sum_i \mu_i$ be the total magnetization and $m = M/N$ be the magnetization per spin. We showed in class, that for large N and $m \ll 1$, the log of the number of states of a given magnetization is given by

$$\ln g(N, m) = N \left[\ln 2 - \frac{1}{2} m^2 \right],$$

neglecting terms which are not extensive. This is an agreement with the central limit theorem (*i.e.* g is a Gaussian function of m). Note that $\ln g$ is just the entropy, apart from a multiplicative factor of Boltzmann's constant, k_B .

- (a) Derive an expression for the extensive contribution to $\ln g$, valid for *general* m , *i.e.* not restricted to $m \ll 1$. *Note:* your result will show that the central limit theorem does not apply in the far tails of the distribution where g is extremely small.
- (b) Show that your expression tends to zero for $m \rightarrow \pm 1$ (and explain why it must), and show also that it agrees with the above expression in the limit $m \ll 1$.
- (c) Insert your expression for $g(N, m)$ into the generalized free energy (as discussed in class) when the system is in a magnetic field H . Show that minimization of the generalized free energy leads to the following result for the magnetization:

$$m = \tanh \left(\frac{H}{k_B T} \right).$$

Note: For H small this gives Curie's law, $m = H/k_B T$.

- (d) Also derive this result in a more straightforward way by considering a *single spin* (which is uncorrelated with the others because there are no spin-spin interactions) in a magnetic field.
- 2. An extended version of a very simple problem I set on last year's qualifying exam and which was very badly done. Naturally, I am confident that you, by contrast, will answer this question perfectly!

If the energy stored in the rotational and vibrational modes is not too large, we may approximate the Hamiltonian of the diatomic molecule by

$$\mathcal{H} = \mathcal{H}_{transl} + \mathcal{H}_{rot} + \mathcal{H}_{vib},$$

neglecting any effect of the centrifugal forces on the vibrational modes and the effect of the the vibrational distortions on the moment of inertia, I . In a dilute gas, the density of will be low enough so that the translational motion can be treated classically. The energy of rotation is:

$$\epsilon_j = \frac{\hbar^2 j(j+1)}{2I},$$

where $j = 0, 1, 2, \dots$ is the rotational quantum number. The state with quantum number j has degeneracy $2j+1$ (we have, for simplicity, assumed that the two atoms in the diatomic molecule are different). The vibrational degree of freedom may be taken to be that of a simple harmonic oscillator with frequency ω_{vib} .

- (a) Determine the contribution to the specific heat from the translational motion.
- (b) Obtain an expression for the specific heat from the vibrational part of the motion. Give simpler expressions for the specific heat valid (i) at low T , and (ii) at high T .
- (c) Obtain an expression for the rotational contribution to the energy in the form of an infinite series.
 - i. What is the rotational part of the energy and specific heat at low temperature?
 - ii. Using the Euler-Maclaurin summation formula, see e.g. Numerical Recipes, Sec. 4.2,

$$\sum_{n=n_1}^{n_N} f(n) = \int_{n_1}^{n_N} f(n) dn + \frac{1}{2} [f_N + f_1] + \frac{1}{12} [f'_N - f'_1] - \frac{1}{720} [f'''_N - f'''_1] + \dots,$$

obtain the rotational part of the specific heat at high temperatures.

Note: For Qu. 2(c)iii below you will need the first *three* leading terms in the expansion of the energy in powers of $1/T$. (These can be determined from the terms given in the Euler-Maclaurin summation formula.) This gives the specific heat in the form $A + B/T^2$ where you should calculate A and B .

- iii. Sketch the rotational part of the specific heat as a function of temperature.
- (d) What is the specific heat per molecule in the following limits:

i.

$$T \ll \theta_{rot} \equiv \frac{\hbar^2}{2Ik_B} \ll \theta_{vib} \equiv \frac{\hbar\omega_{vib}}{k_B},$$

ii.

$$\theta_{rot} \ll T \ll \theta_{vib},$$

iii.

$$\theta_{rot} \ll \theta_{vib} \ll T.$$

3. Effect of a potential near the surface due to the walls

The partition function for a classical system of particles is given by

$$Z = \frac{1}{N! (2\pi\hbar)^{3N}} \int \prod_{i=1}^N (d^3 p_i d^3 r_i) \exp(-\mathcal{H}[\vec{p}, \vec{r}]/k_B T) \quad (1)$$

where $\mathcal{H}[\vec{p}, \vec{r}]$ is the Hamiltonian, which depends on the coordinates $\{\vec{r}_i\}$ and momenta $\{\vec{p}_i\}$ of the N particles.

We consider a classical non-interacting gas is repelled by the walls of its container. The force can be represented by a step in the potential energy which is W a short distance ℓ from the wall and zero further away. (Assume that $A\ell \ll V$.)

- (a) Derive Eq. (1) starting from *quantum* statistical mechanics. Explain intuitively the origin of the $N!$ factor and discuss briefly how \hbar arises in an apparently classical formula.
- (b) Find an expression for the additional energy produced by the walls in terms of k_B, T, W, ℓ, N , the volume of the gas V , and the wall area A .
- (c) Show that the corresponding extra specific heat, ΔC , tends to zero when $k_B T$ is very large or very small compared with W , but that

$$\frac{\Delta C}{Nk_B} \sim \frac{\ell A}{V}$$

when $k_B T$ is of order W .

4. Ionization probability

Consider an electron of mass m bound to an atom in a box of volume V . The binding energy is $-E_1$ ($E_1 > 0$) (assume, for now, that there is only one bound state of the electron).

- (a) Find the probability that the atom is ionized (i.e. that the electron is not bound to the atom). (Assume that V is much larger than the volume of the atom).
- (b) What happens to the ionization probability in the limit $V \rightarrow \infty$, even if $k_B T \ll E$? *Note:* The center of mass coordinate of the atom may be ignored.
- (c) Assume now that the atom has other bound states, with energy $-E_2, -E_3$ etc. The interesting case is that $k_B T$ is small compared with both the ionization energy, E_1 , and the atomic excitation energy $|E_2 - E_1|$. Do these other states affect the ionization probability? Discuss your result.

For some interesting comments on this and other problems in physics, see R. E. Peierls, “Surprises in Theoretical Physics”.

5. Debye theory of specific heats

To a good approximation, the lattice vibrations (phonons) of a crystal can be represented by independent simple harmonic oscillators. The problem is that the density of states $\rho(\omega)$ (defined such that the number of modes with frequency between ω and $\omega + \delta\omega$ is $\rho(\omega)\delta\omega$) is complicated. In the Debye theory one notices (i) that the density of states varies as ω^2 for $\omega \rightarrow 0$ because of sound waves whose frequency varies as k as $k \rightarrow 0$ and (ii) the integral of the density of states over all ω is $3N$ where N is the number of atoms. In the Debye theory one just assumes that

$$\begin{aligned}\rho(\omega) &= A\omega^2 & \omega < \omega_D \\ \rho(\omega) &= 0 & \omega > \omega_D\end{aligned}$$

where ω_D is a frequency characteristic of the particular material.

- (a) Determine the constant A .

(b) Writing

$$\hbar\omega_D = k_B\theta_D$$

where θ_D is called the Debye temperature, determine the specific heat, C , as a function of T and θ_D , expressing your answer as a one-dimensional integral.

(c) Show that for $T \gg \theta_D$ one recovers the classical law of Dulong and Petit,

$$\frac{C}{Nk_B} = 3 .$$

Note: The Dulong and Petit law says that the classical specific heat is $k_B/2$ for each quadratic term in the Hamiltonian. Here we have 3 terms in the kinetic energy (one for each cartesian coordinate) and 3 in the potential energy.

(d) Show also that for $T \ll \theta_D$

$$\frac{C}{Nk_B} = B \left(\frac{T}{\theta_D} \right)^3$$

and evaluate the dimensionless number B . What is its numerical value? Note that it is surprisingly large.

Note: Most statistical mechanics books have a section on the Debye theory of specific heats. See also Ashcroft and Mermin “Solid State Physics”, Ch. 23.

6. The Sommerfeld expansion.

In the theory of the fermion systems one frequently needs to expand quantities in powers of the temperature in the limit $k_B T \ll \epsilon_F$, where ϵ_F is the Fermi energy (the $T = 0$ limit of the chemical potential). The problem is a bit complicated because T appears in an exponential in the denominator of the Fermi function but this can be done as follows.

We want to expand the following integral as a power series in T :

$$I = \int_{-\infty}^{\infty} \frac{f(\epsilon)d\epsilon}{e^{\beta(\epsilon-\mu)} + 1} ,$$

where $f(\epsilon)$ is some function which vanishes for ϵ sufficiently large and negative, and varies smoothly in the vicinity of the Fermi energy.

(a) Show that I has the expansion

$$I = \int_{-\infty}^{\mu} f(\epsilon)d\epsilon + \sum_{n=1}^{\infty} a_{2n}(k_B T)^{2n} f^{(2n-1)}(\mu)$$

where

$$a_{2n} = 2 \left(1 - 2^{1-2n} \right) \zeta(2n)$$

where

$$\zeta(n) = 1 + \frac{1}{2^n} + \frac{1}{3^n} + \frac{1}{4^n} + \dots$$

is the Riemann zeta function. Some useful values are $\zeta(2) = \pi^2/6$ and $\zeta(4) = \pi^4/90$. For help see e.g. Appendix C of Ashcroft and Mermin.

- (b) Use this result to find the leading temperature dependence of the chemical potential at low temperature for a free electron gas.
7. *Relativistic Fermi gas.*
- Consider an ideal Fermi gas at zero temperature composed of particles of mass m and spin-1/2 contained in a region of volume V .

- (a) Show that the condition for the gas to be non-relativistic is

$$\frac{N}{V} \ll \left(\frac{mc}{\hbar}\right)^3.$$

Show also that this implies that mean inter-particle spacing is much greater than the Compton wavelength.

- (b) Show that in the non-relativistic region the energy is given by

$$\frac{E}{N} = \frac{3}{10} \left(\frac{3\pi^2 N}{V}\right)^{2/3} \frac{\hbar^2}{m}.$$

- (c) Evaluate the total energy in the extreme relativistic limit.
- (d) By expressing the answer to (b) in terms of the linear dimension R and total mass M , (numerical factors of order unity can be neglected) show that a non-relativistic gas of fixed mass can always find an equilibrium size R_0 such that the sum of the kinetic and gravitational energies is minimized. (Use dimensional arguments to estimate the gravitational energy).
- (e) Show that this is not possible for a relativistic gas and that for M greater than a critical mass M_c , which you should estimate, gravitational collapse occurs. What happens for M smaller than M_c ?