Physics 306: Thermal Physics

Final Exam Stony Brook University

Spring 2024

General Instructions:

You may use one page (front and back) of handwritten notes and a calculator. Graphing calculators are allowed. No other materials may be used.

1 Integrals

Bose and Fermi:

$$\int_0^\infty \mathrm{d}x \, \frac{x}{e^x - 1} = \frac{\pi^2}{6} \tag{1}$$

$$\int_0^\infty dx \, \frac{x^2}{e^x - 1} = 2\zeta(3) \simeq 2.404 \tag{2}$$

$$\int_0^\infty \mathrm{d}x \, \frac{x^3}{e^x - 1} = \frac{\pi^4}{15} \tag{3}$$

$$\int_0^\infty dx \, \frac{x^4}{e^x - 1} = 24 \, \zeta(5) \simeq 24.88 \tag{4}$$

$$\int_0^\infty \mathrm{d}x \, \frac{x^5}{e^x - 1} = \frac{8\pi^6}{63} \tag{5}$$

$$\int_{0}^{\infty} \mathrm{d}x \, \frac{x}{e^x + 1} = \frac{\pi^2}{12} \tag{6}$$

$$\int_0^\infty \mathrm{d}x \, \frac{x^2}{e^x + 1} = \frac{3}{2} \, \zeta(3) \simeq 1.80309 \tag{7}$$

$$\int_0^\infty \mathrm{d}x \, \frac{x^3}{e^x + 1} = \frac{7\pi^4}{120} \tag{8}$$

$$\int_0^\infty dx \, \frac{x^4}{e^x + 1} = \frac{45}{2} \, \zeta(5) \simeq 23.33 \tag{9}$$

$$\int_0^\infty \mathrm{d}x \, \frac{x^5}{e^x + 1} = \frac{31\pi^6}{252} \tag{10}$$

Gamma Function:

$$\Gamma(z) \equiv \int_0^\infty x^{z-1} e^{-x} dx \tag{11}$$

with specific results

$$\Gamma(z+1) = z\Gamma(z)$$
 $\Gamma(n) = (n-1)!$ $\Gamma(\frac{1}{2}) = \sqrt{\pi}$ (12)

Gaussian Integrals:

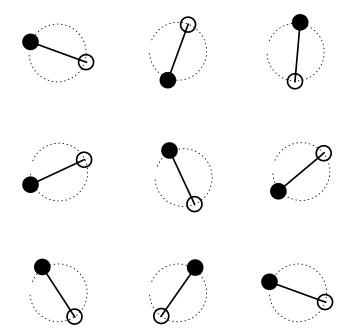
$$I_n = \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\infty} \mathrm{d}x \, e^{-x^2/2\sigma^2} x^n \tag{13}$$

with specific results

$$I_0 = 1$$
 $I_2 = \sigma^2$ $I_4 = 3\sigma^4$ $I_6 = 15\sigma^6$ (14)

Problem 1. 2D Rotors

A molecule in two spatial dimensions of consists of two non-identical atoms, each of mass M. The atoms lie in the xy plane and are separated from each other by a distance r_0 . N such molecules are arranged on a lattice, as shown below. Each molecule is free to rotate in the xy plane around its lattice site, but is otherwise fixed to the site.



The classical energy of a molecule rotating in the xy plane is

$$\epsilon = \frac{1}{2}I\omega^2 = \frac{L_z^2}{2I} \tag{15}$$

where I is the moment of inertia of the molecule and $L_z = I\omega$ is the angular momentum around the z axis. Quantum mechanically, the angular momentum takes on discrete values in units of \hbar labeled by an integer quantum number m:

$$L_z = m\hbar \qquad m = 0, \pm 1, \pm 2, \pm 3, \dots$$
 (16)

The positive and negative values of m describe counter-clockwise and clockwise rotations respectively, while m=0 describes a molecule not rotating at all.

- (a) Approximately evaluate the partition function of the molecule by including just the first two energy levels.
 - (i) Explain why this valid at low temperatures, and define what is meant by low in this context, i.e. low compared to what? Suppose that the atoms in the molecule each have a mass of a Hydrogen atom and assume the a bond length r_0 is a typical atomic distance, estimate the range temperature (in Kelvin where) the low temperature approximation is valid.

¹Note the mass of the atoms M should not be confused with the integer m.

- (b) Determine the mean energy and specific heat of the molecule using the low temperature approximation of (a)
- (c) (i) Briefly explain why at high temperatures the sum over states m can be replaced with an integral. (ii) Evaluate the partition function with this approximation and use the result to find the mean energy the system. Explain the result for the energy using classical reasoning.
- (d) Suppose that the molecules were free to move around in the xy plane as a an ideal gas. What is the specific heat of the gas at constant pressure in the low temperature approximation of part (b) in this case?

(a) The lowest energy level is m=0. The first energy level is $m=\pm 1$ with energy $\Delta=\hbar^2/2I$, with $I=\frac{1}{2}Mr_0^2$ the moment of inertia of the molecule. The partition function is

$$Z = 1 + 2e^{-\beta\Delta} + \dots \tag{17}$$

The two takes into account the two states with the same energy level $m=\pm 1$. The next term in this expression is $2e^{-4\beta\Delta}$ which should be small. The requirement for this to be small is that

$$\beta \Delta \gg 1$$
. (18)

i.e. e^{-x} is small when x is large. So, we must have

$$kT \ll \frac{\hbar^2}{2I} \,. \tag{19}$$

Recognizing that $I = \frac{1}{2}Mr_0^2$, but neglecting constants we have

$$kT \ll \frac{\hbar^2}{Mr_0^2} \,. \tag{20}$$

Using some numbers from the course page (i) $M=m_p\simeq 2000m_e$ (ii) $r_0\simeq 2a_0$

(iii) $\hbar^2/2m_e a_0^2 = 13.6 \,\mathrm{eV}$ (iv) $k_B = \frac{1}{40} \,\mathrm{eV}/300 \,\mathrm{°K}$ we have then

$$T \ll 40^{\circ} \text{K}$$
. (21)

In general this is about right. In diatomic hydrogen, the rotational degrees of freedom freezout at about this temperature.

(b) We have that

$$\langle \epsilon \rangle = -\frac{\partial \ln Z}{\partial \beta} = \frac{2\Delta e^{-\beta \Delta}}{1 + 2e^{-\beta \Delta}}$$
 (22)

And differentiating using the chain rule $\partial X/\partial T = -k\beta^2 \partial X/\partial \beta$:

$$C_V = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T} N \langle \epsilon \rangle = -kN\beta^2 \frac{\partial}{\partial \beta} \langle \epsilon \rangle = kN \frac{2(\beta \Delta)^2 e^{\beta \Delta}}{(e^{\beta \Delta} + 2)^2}$$
 (23)

(c) (i) We have

$$Z = 1 + \sum_{m=1}^{\infty} 2e^{-\beta \Delta m^2} = \sum_{m=-\infty}^{\infty} e^{-\beta \Delta m^2}$$
 (24)

In general if $\beta\Delta$ is very small, $\beta\Delta\ll 1$, then many terms will contribute to the sum. This means $kT\gg\Delta$. The red dots in Fig. 1 show the terms in this sum, when $\beta\Delta=10^{-3}$.

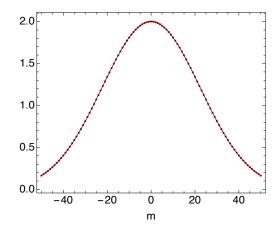


Figure 1: The red dots indicate the terms appear in the partition function sum, Eq. (24). We replace this sum with an integral

(ii) In approximating the sum, we note that the typical m is very large and the sum can repaced by an integral (see figrue)

$$Z \simeq \int_{-\infty}^{\infty} dm \, e^{-\beta \Delta m^2} \tag{25}$$

This integral is Gaussian. Using the Gaussian integrals at the front $\sigma^2 = 1/(2\beta\Delta)$

$$Z \simeq \sqrt{2\pi\sigma^2} = \left(\frac{\pi}{\beta\Delta}\right)^{1/2} \tag{26}$$

Then

$$\langle \epsilon \rangle = -\frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial \beta} \left(\ln \beta^{-1/2} + \text{const} \right) = \frac{1}{2\beta}$$
 (27)

- (iii) This is what we expect at high temperatures. The motion is classical. The Hamiltonian has one quadratic form and thus the mean energy per molecule is $\frac{1}{2}kT$.
- (d) If the molecules the are free to move then the partition function of a single particle factorizes into the a translational piece times a rotational piece, $Z_1 = Z_{1\text{trans}}Z_{1\text{rot}}$, where we computed the rotational part in (a). The energy per particle is a sum of the translational kinetic energy plus the rotational energy we computed in part (b)

$$U = N \langle \epsilon \rangle = \langle \epsilon_{\text{trans}} \rangle + \langle \epsilon_{\text{rot}} \rangle \tag{28}$$

The translational kinetic energy is given by the equipartition theorem, with two degrees of freedom $\epsilon_{\text{trans}} = p_x^2/2m + p_y^2/2m$.

$$\langle \epsilon \rangle = 2N \times \frac{1}{2}kT + N \langle \epsilon \rangle_{(b)}$$
 (29)

So the specific heat per volume is simply

$$C_V = N \frac{\partial \langle \epsilon \rangle}{\partial T} = Nk + C_{\text{part(b)}}$$
 (30)

Finally we use that for an ideal gas $C_p = C_v + Nk$ leading to the final result

$$C_p = 2Nk + C_{\text{part(b)}} \tag{31}$$

Problem 2. Electromagnetic pressure in a transmission line

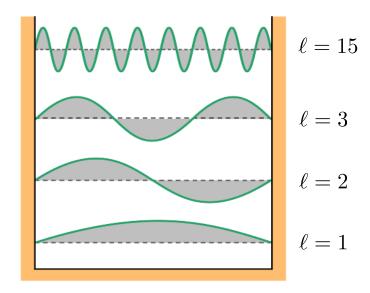
The thermal fluctuations in a electromagnetic transmission line can be described as a gas of photons in a one dimensional box of size L at temperature T. In one dimension, the "volume" (V) of the box is simply the line length, L, and the "pressure" (P) is simply the force the photons exert on the ends of the transmission line, \mathcal{F} .

As photon number is not conserved, you may set the chemical potential to zero throughout this problem.

(a) (i) Starting from the first law of thermodynamics, show that force is related to the derivative of the grand potential², $\Phi_G \equiv U - TS$:

$$\left(\frac{\partial \Phi_G}{\partial L}\right)_T = -\mathcal{F}.$$

- (ii) How could one express the force as a derivative of the energy U?
- (b) Now consider just one Fourier mode in the wire labeled by ℓ , a positive integer. Some of the Fourier modes of the wire are shown below:



The energy of the mode $\varepsilon_{\ell} = cp_{\ell}$ where $p_{\ell} = \pi \hbar \ell / L$ is the magnitude of the momentum of the mode.

Derive grand potential for the ℓ -th mode and show that the force on the ends of the transmission from just this mode is

$$\mathcal{F}_{\ell} = \frac{1}{e^{\beta \varepsilon_{\ell}} - 1} \left(-\frac{d\varepsilon_{\ell}}{dL} \right) . \tag{32}$$

Give a qualitative interpretation of this formula.

²Since the chemical potential is zero the grand potential and free energy are equal.

(c) The total force on the ends of the wire is a sum of the forces from each mode

$$\mathcal{F} = \sum_{\ell} \mathcal{F}_{\ell} \tag{33}$$

By replacing the sum over with an appropriate integral determine the force exerted by the gas.

(a) We have

$$dU = TdS - \mathcal{F}dL \tag{34}$$

Integrating the T dS term by parts, T dS = d(ST) - SdT, we find

$$d\Phi_G = d(U - TS) = -SdT - \mathcal{F}dL \tag{35}$$

Reading from these expressions

$$\mathcal{F} = -\left(\frac{\mathrm{d}U}{\mathrm{d}L}\right)_S \qquad \mathcal{F} = -\left(\frac{\mathrm{d}\Phi_G}{\mathrm{d}L}\right)_T \tag{36}$$

(b) The grand partition function is

$$Z_G = \sum_{n=0}^{\infty} e^{-\beta n\epsilon} = \frac{1}{1 - e^{-\beta \epsilon}}$$
(37)

Taking the logarithm

$$\Phi_G = -kT \ln Z_G = kT \ln(1 - e^{-\beta \epsilon}) \tag{38}$$

Differenentiating with respect to L, and noting that only the energy depends on L we have by the chain rule

$$\mathcal{F}_{\ell} = -\frac{\partial \Phi_G}{\partial \epsilon_{\ell}} \frac{\partial \epsilon_{\ell}}{\partial L} \tag{39}$$

$$= \frac{e^{-\beta \epsilon_{\ell}}}{1 - e^{-\beta \epsilon_{\ell}}} \left(-\frac{\partial \epsilon_{\ell}}{\partial L} \right) \tag{40}$$

$$= \frac{1}{e^{\beta \epsilon_{\ell}} - 1} \left(-\frac{\partial \epsilon_{\ell}}{\partial L} \right) \tag{41}$$

The total force is the number of photons in the mode times the force exerted by each photon $-d\epsilon_{\ell}/dL$.

(c) We note

$$-\frac{d\epsilon_{\ell}}{dL} = \frac{cp_{\ell}}{L} \tag{42}$$

Then

$$\mathcal{F} = \frac{1}{L} \sum_{\text{modes}} n_{BE}(\epsilon) cp = \frac{1}{L} \underbrace{2}_{\text{spin}} \times \int_{-\infty}^{\infty} \frac{Ldp}{2\pi\hbar} \frac{cp}{e^{\beta cp} - 1}$$
 (43)

$$= \frac{(kT)^2}{\pi \hbar c} 2 \int_0^\infty du \, \frac{u}{e^u - 1}$$
 (44)

$$=kT\left(\frac{kT}{\hbar c}\right)\frac{\pi}{3}\tag{45}$$

Problem 3. Absorbing walls

A canister of volume V contains a mono-atomic ideal of mass m. The canister is maintained temperature T and pressure P_0 through a small inlet valve. The walls of the container have N_0 absorbing sites, at fixed locations on the walls. The energy of a site is 0 if no atoms are absorbed and $-\Delta$ if one atom is absorbed from the room.

- (a) Derive the free energy the gas in the volume of the canister and use this result to derive the chemical potential of the gas as a function of the pressure P_0 .
- (b) (i) Determine the mean number of atoms absorbed by the traps. Express your result in terms of the ambient temperature T and pressure P_0 . (ii) At fixed temperature, qualitatively sketch the mean number of atoms absorbed by the gas a function of pressure at fixed temperature. At what pressure are half of the absorbing sites filled?
- (c) If the pressure is increased from P_0 to P_1 how much heat flows from the surrounding gas into the traps. You may leave your result in terms of the chemical potentials μ_0 and μ_1 at the corresponding pressures, P_0 and P_1 .

Hint: What is the relation between heat flow and entropy?

(a) We have

$$Z = \frac{Z_1^N}{N!} \simeq \left(\frac{eZ_1}{N}\right)^N \qquad Z_1 = \int \frac{V d^3 p}{h^3} e^{-\beta p^2/2m} = V n_Q$$
 (46)

where $n_Q = 1/\lambda^3$. Then

$$F = -kT \ln Z = -NkT \ln Z_1 - kT(N \ln N - N)$$
(47)

Differentiating with respect to N

$$\mu = \left(\frac{\partial F}{\partial N}\right)_{T,V} = -kT(\ln V n_Q/N) \tag{48}$$

So we find using p = NkT/V

$$\mu = kT \ln(p/n_O kT) \tag{49}$$

We note that

$$e^{\beta\mu} = \frac{p}{n_Q T} \tag{50}$$

(b) The grand partition function of a single trap is

$$Z_1 = 1 + e^{\beta \Delta} e^{\beta \mu} \tag{51}$$

So the mean number of particles absorbed by a trap is

$$\langle n \rangle = \frac{e^{\beta \Delta} e^{\beta \mu}}{1 + e^{\beta \Delta} e^{\beta \mu}} \tag{52}$$

The total number of particles absorbed is

$$\langle N_{\text{absorbed}} \rangle = N_0 \langle n \rangle = \frac{N_0 e^{\beta \Delta} e^{\beta \mu}}{1 + e^{\beta \Delta} e^{\beta \mu}}$$
 (53)

Using the the results of part (a) we see that this can be

$$\langle N_{\text{absorbed}} \rangle = N_0 \frac{p/p_{\text{ref}}(T)}{1 + p/p_{\text{ref}}(T)}$$
 (54)

where the temperature dependent constant sets the overall pressure scale

$$p_{\rm ref}(T) = T n_Q e^{-\beta \Delta} \tag{55}$$

Setting the aborbed fraction to 1/2 we find:

$$\frac{\langle N_{\text{absorbed}} \rangle}{N_0} = \frac{p/p_{\text{ref}}}{1 + p/p_{\text{ref}}} = \frac{1}{2}$$
 (56)

So the required pressure is simply

$$p = p_{\text{ref}} \tag{57}$$

A sketch of the absorbed fraction is shown in Fig. 2

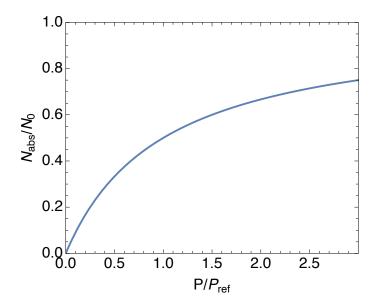


Figure 2: The fraction of sites filled as a function of the pressure. The reference pressure is in Eq. (??)

(c) The heat that flows into of the system at fixed temperature is related to the change in entropy

$$Q = T\Delta S = T N_0(s_1 - s_0) \tag{58}$$

Where s_1 and s_0 is the entropy of a single site at pressure P_1 and P_0 respectively. Differentiating with respect tot temperature, we find

$$s = -\left(\frac{\partial \Phi_G}{\partial T}\right)_{\mu} = -\frac{\partial}{\partial T} \left(-kT \log Z_1\right)$$
 (59)

and thus for P_1 we have

$$\frac{s}{k} = \log Z_1 + kT \partial_T \log Z_1 \tag{60}$$

$$\frac{s}{k} = \log(1 + e^{\beta(\mu_1 + \Delta)}) - \beta(\mu_1 + \Delta) \frac{e^{\beta(\mu_1 + \Delta)}}{1 + e^{\beta(\mu_1 + \Delta)}}$$
(61)

The heat is given by Eq. (58).

Problem 4. Relativistic corrections to a Fermi Gas

The energy of the electron is in general related to its momentum by the relativistic formula

$$\varepsilon(\mathbf{p}) = \sqrt{(mc^2)^2 + (cp)^2} \,. \tag{62}$$

If particles are non-relativistic we have

$$\frac{v}{c} \ll 1$$
, or $\frac{p}{mc} \ll 1$. (63)

(a) Show that for non-relativistic particles we have approximately

$$\varepsilon(\mathbf{p}) \simeq mc^2 + \frac{p^2}{2m} - \frac{p^4}{8m(mc)^2} + \dots$$
 (64)

The leading term is the rest energy of the electron (a constant), the next term is the familiar $\frac{1}{2}mv^2$, and the next term is the first relativistic correction.

Now consider a gas of electrons at zero temperature in a three dimensional volume V and an electron density of n_e . The single particle energy of an electron is in general given by Eq. (62), and is approximated using part (a), Eq. (64).

- (b) Determine the relation between the Fermi momentum and the density of electrons. Explain carefully your steps.
- (c) Determine the energy U of the electron gas in the non-relativistic limit, including the first relativistic correction. Express your result in terms of the Fermi momentum.
- (d) Determine the pressure of the gas including the first relativistic correction. At what density does the correction due to the relativistic term, change the leading result by 10%.

(a) We have the series expansion

$$(1+x)^{\alpha} = 1 + \alpha x + \frac{1}{2!}\alpha(\alpha - 1)x^{2} + \frac{1}{3!}\alpha(\alpha - 1)(\alpha - 2)x^{3}...$$
 (65)

With $\alpha = 1/2$ and $x = (p/mc)^2$ we have

$$\varepsilon(p) = mc^{2} \left(1 + \left(\frac{p}{mc} \right)^{2} \right)^{1/2} = mc^{2} \left[1 + \frac{1}{2} \left(\frac{p}{mc} \right)^{2} - \frac{1}{8} \left(\frac{p}{mc} \right)^{4} + \dots \right]$$
 (66)

(b) So we have

$$N = \sum_{\text{modes}} n_{FD}(p) = \sum_{\text{modes}} \begin{cases} 1 & p < p_F \\ 0 & \text{otherwise} \end{cases}$$
 (67)

Leading to

$$N = 2V \int_{p < p_F} \frac{d^3 p}{(2\pi\hbar)^3} = \frac{2V}{(2\pi\hbar)^3} \frac{4}{3}\pi p_F^3$$
 (68)

So we find after minor algebra

$$p_F = \hbar \left(3\pi^2 n_e\right)^{1/3} \simeq 3.1 \,\hbar n_e^{1/3}$$
 (69)

(c) The energy is

$$U = 2V \int_{p < p_F} \frac{d^3 p}{(2\pi\hbar)^3} \varepsilon(p) \tag{70}$$

$$= \frac{V}{\pi^2 \hbar^3} \int_0^{p_F} p^2 \, \mathrm{d}p \left[mc^2 + \frac{p^2}{2m} - \frac{p^4}{8m(mc)^2} + \dots \right]$$
 (71)

$$= \frac{V}{\pi^2 \hbar^3} \left[\frac{p_F^3}{3} mc^2 - \frac{1}{2 \cdot 5} \frac{p_F^5}{m} - \frac{1}{7 \cdot 8} \frac{1}{m(mc)^2} p_F^7 + \dots \right]$$
 (72)

$$=N\left[mc^2 + \frac{3}{10}\frac{p_F^2}{m} - \frac{3}{56}\frac{1}{m(mc)^2}p_F^4 + \ldots\right]$$
 (73)

(d) The pressure is

$$P = -\left(\frac{\partial U}{\partial V}\right)_{N} = -\left(\frac{\partial U}{\partial p_{F}}\right)_{N} \left(\frac{\partial p_{F}}{\partial V}\right)_{N} \tag{74}$$

Note since $p_F \propto V^{-1/3}$

$$\frac{\partial p_F}{\partial V} = -\frac{1}{3} \frac{p_F}{V} \tag{75}$$

Leading to

$$P = -\left(\frac{\partial U}{\partial V}\right)_{N} = \frac{1}{3} \left(\frac{\partial U}{\partial p_{F}}\right)_{N} \frac{p_{F}}{V} \tag{76}$$

$$= \frac{Np_F^2}{Vm} \left[\frac{1}{5} - \frac{1}{14} \frac{p_F^2}{(mc)^2} + \dots \right]$$
 (77)

We note first of all that the pressure is reduced, which has important physical consequences (see below). Evaluting the result for a 10% correction we find :

$$\frac{1}{14} \frac{1}{m(mc)^2} p_F^4 = 0.1 \frac{1}{5} \frac{p_F^2}{m} \tag{78}$$

Leading to

$$p_F^2 = 0.1 \left(\frac{14}{5}\right) (mc)^2 = 0.28 (mc)^2$$
 (79)

This would have been good enough for the exam. When this is expressed in terms of the density we find

$$n_e^{\text{rel}} \simeq 0.005 \left(\frac{m_e c}{\hbar}\right)^3 \simeq 1.2 \left(\frac{m_e c}{h}\right)^3$$
 (80)