PHYSICS 140A : STATISTICAL PHYSICS FINAL EXAMINATION SOLUTIONS 100 POINTS TOTAL

(1) Consider a system of N independent, distinguishable S = 1 objects, each described by the Hamiltonian

$$\label{eq:hamiltonian} \hat{h} = \Delta\,S^2 - \mu_0 \mathsf{H}\,S \ ,$$

where $S \in \{-1, 0, 1\}$.

- (a) Find F(T, H, N). [10 points]
- (b) Find the magnetization M(T, H, N). . [5 points]
- (c) Find the zero field susceptibility, $\chi(T) = \frac{1}{N} \frac{\partial M}{\partial H}\Big|_{H=0}$. [5 points]
- (d) Find the zero field entropy S(T, H = 0, N). (*Hint* : Take $H \rightarrow 0$ first.) [5 points]

Solution: The partition function is $Z = \zeta^N$, where ζ is the single particle partition function,

$$\zeta = \operatorname{Tr} e^{-\beta \hat{h}} = 1 + 2 e^{-\Delta/k_{\rm B}T} \cosh\left(\frac{\mu_0 \mathsf{H}}{k_{\rm B}T}\right) \,. \tag{1}$$

Thus,

(a)
$$F = -Nk_{\rm B}T\ln\zeta = -Nk_{\rm B}T\ln\left[1 + 2e^{-\Delta/k_{\rm B}T}\cosh\left(\frac{\mu_0\mathsf{H}}{k_{\rm B}T}\right)\right]$$
(2)

The magnetization is

(b)
$$M = -\frac{\partial F}{\partial \mathsf{H}} = \frac{k_{\mathrm{B}}T}{Z} \cdot \frac{\partial Z}{\partial \mathsf{H}} = \frac{2\mu_0 \sinh\left(\frac{\mu_0 \mathsf{H}}{k_{\mathrm{B}}T}\right)}{e^{\Delta/k_{\mathrm{B}}T} + 2\cosh\left(\frac{\mu_0 \mathsf{H}}{k_{\mathrm{B}}T}\right)}$$
(3)

To find the zero field susceptibility, we expand M to linear order in H, which entails expanding the numerator of M to first order in H and setting H = 0 in the denominator. We then find

(c)
$$\chi(T) = \frac{2\mu_0^2}{k_{\rm B}T} \cdot \frac{1}{e^{\Delta/k_{\rm B}T} + 2}$$
 (4)

To find the entropy in zero field, it is convenient to set $H \to 0$ first. The free energy is then given by $F(T, H = 0, N) = -Nk_{\rm B}T \ln \left(1 + 2e^{-\Delta/k_{\rm B}T}\right)$, and therefore

(d)
$$S = -\frac{\partial F}{\partial T} = Nk_{\rm B} \ln\left(1 + 2e^{-\Delta/k_{\rm B}T}\right) + \frac{N\Delta}{T} \cdot \frac{1}{2 + e^{\Delta/k_{\rm B}T}}$$
(5)

(2) A classical gas consists of particles of two species: A and B. The dispersions for these species are

$$arepsilon_{_{
m A}}(oldsymbol{p}) = rac{oldsymbol{p}^2}{2m} ~~,~~arepsilon_{_{
m B}}(oldsymbol{p}) = rac{oldsymbol{p}^2}{4m} - \Delta ~.$$

In other words, $m_{\rm A} = m$ and $m_{\rm B} = 2m$, and there is an additional energy offset $-\Delta$ associated with the B species.

- (a) Find the grand potential $\Omega(T, V, \mu_{\rm A}, \mu_{\rm B})$. [10 points]
- (b) Find the number densities $n_A(T, \mu_A, \mu_B)$ and $n_B(T, \mu_A, \mu_B)$. [5 points]
- (c) If $2A \rightleftharpoons B$ is an allowed reaction, what is the relation between n_A and n_B ? (*Hint* : What is the relation between μ_A and μ_B ?) [5 points]
- (d) Suppose initially that n_A = n and n_B = 0. Find n_A in equilibrium, as a function of T and n and constants.
 [5 points]

Solution : The grand partition function Ξ is a product of contributions from the A and B species, and the grand potential is a sum:

(a)
$$\Omega = -Vk_{\rm B}T \,\lambda_T^{-3} e^{\mu_{\rm A}/k_{\rm B}T} - 2^{3/2} \,Vk_{\rm B}T \,\lambda_T^{-3} e^{(\mu_{\rm B}+\Delta)/k_{\rm B}T}$$
(6)

Here, we have defined the thermal wavelength for the A species as $\lambda_T \equiv \lambda_{T,A} = \sqrt{2\pi\hbar^2/mk_{\rm B}T}$. For the B species, since the mass is twice as great, we have $\lambda_{T,B} = 2^{-1/2} \lambda_{T,A}$.

The number densities are

$$n_{\rm A} = -\frac{1}{V} \cdot \frac{\partial \Omega}{\partial \mu_{\rm A}} = V \lambda_T^{-3} e^{\mu_{\rm A}/k_{\rm B}T} \tag{7}$$

$$n_{\rm B} = -\frac{1}{V} \cdot \frac{\partial \Omega}{\partial \mu_{\rm B}} = 2^{3/2} \, V \lambda_T^{-3} \, e^{(\mu_{\rm B} + \Delta)/k_{\rm B}T} \ . \tag{8}$$

If the reaction $2A \rightleftharpoons B$ is allowed, then the chemical potentials of the A and B species are related by $\mu_{\rm B} = 2\mu_{\rm A} \equiv 2\mu$. We then have

(b)
$$n_{\rm A}\lambda_T^3 = e^{\mu/k_{\rm B}T}$$
 (9)

and

(b)
$$n_{\rm B} \lambda_T^3 = 2^{3/2} e^{(2\mu + \Delta)/k_{\rm B}T}$$
 (10)

The relation we seek is therefore

(c)
$$n_{\rm B} = 2^{3/2} \left(n_{\rm A} \lambda_T^3 \right)^2 e^{\Delta/k_{\rm B}T}$$
 (11)

If we initially have $n_{\scriptscriptstyle\rm A}=n$ and $n_{\scriptscriptstyle\rm B}=0,$ then in general we must have

$$n_{\rm A} + 2n_{\rm B} = n \qquad \Longrightarrow \qquad n_{\rm B} = \frac{1}{2} \left(n - n_{\rm A} \right) \,.$$
 (12)

Thus, eliminating $n_{\rm B}$, we have a quadratic equation,

$$2^{3/2} \lambda_T^3 e^{\Delta/k_{\rm B}T} n_{\rm A}^2 = \frac{1}{2} (n - n_{\rm A}) , \qquad (13)$$

the solution of which is

(d)
$$n_{\rm A} = \frac{-1 + \sqrt{1 + 16\sqrt{2} n \lambda_T^3 e^{\Delta/k_{\rm B}T}}}{8\sqrt{2} \lambda_T^3 e^{\Delta/k_{\rm B}T}}$$
 (14)

(3) A branch of excitations for a three-dimensional system has a dispersion $\varepsilon(\mathbf{k}) = A |\mathbf{k}|^{2/3}$. The excitations are bosonic and are not conserved; they therefore obey photon statistics.

- (a) Find the single excitation density of states per unit volume, g(ε). You may assume that there is no internal degeneracy for this excitation branch.
 [10 points]
- (b) Find the heat capacity $C_V(T,V)$. [5 points]
- (c) Find the ratio E/pV. [5 points]
- (d) If the particles are bosons with number conservation, find the critical temperature T_c for Bose-Einstein condensation.
 [5 points]

Solution : We have, for three-dimensional systems,

$$g(\varepsilon) = \frac{1}{2\pi^2} \frac{k^2}{d\varepsilon/dk} = \frac{3}{4\pi^2 A} k^{7/3} .$$
 (15)

Inverting the dispersion to give $k(\varepsilon) = (\varepsilon/A)^{3/2}$, we obtain

(a)
$$g(\varepsilon) = \frac{3}{4\pi^2} \frac{\varepsilon^{7/2}}{A^{9/2}}$$
 (16)

The energy is then

$$E = V \int_{0}^{\infty} d\varepsilon \ g(\varepsilon) \ \frac{\varepsilon}{e^{\varepsilon/k_{\rm B}T} - 1}$$
$$= \frac{3V}{4\pi^2} \Gamma\left(\frac{11}{2}\right) \zeta\left(\frac{11}{2}\right) \frac{(k_{\rm B}T)^{11/2}}{A^{9/2}} . \tag{17}$$

Thus,

(b)
$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = \frac{3V}{4\pi^2} \Gamma\left(\frac{13}{2}\right) \zeta\left(\frac{11}{2}\right) k_{\rm B} \left(\frac{k_{\rm B}T}{A}\right)^{9/2}$$
(18)

The pressure is

$$p = -\frac{\Omega}{V} = -k_{\rm B}T \int_{0}^{\infty} d\varepsilon \ g(\varepsilon) \ \ln\left(1 - e^{-\varepsilon/k_{\rm B}T}\right)$$
(19)
$$= -k_{\rm B}T \int_{0}^{\infty} d\varepsilon \ \frac{3}{4\pi^{2}} \ \frac{\varepsilon^{7/2}}{A^{9/2}} \ \ln\left(1 - e^{-\varepsilon/k_{\rm B}T}\right)$$
$$= -\frac{3}{4\pi^{2}} \ \frac{(k_{\rm B}T)^{11/2}}{A^{9/2}} \int_{0}^{\infty} ds \ s^{7/2} \ \ln\left(1 - e^{-s}\right)$$
$$= \frac{3V}{4\pi^{2}} \Gamma\left(\frac{9}{2}\right) \zeta\left(\frac{11}{2}\right) \ \frac{(k_{\rm B}T)^{11/2}}{A^{9/2}} \ .$$
(20)

Thus,

(c)
$$\frac{E}{pV} = \frac{\Gamma(\frac{11}{2})}{\Gamma(\frac{9}{2})} = \frac{9}{2}$$
 (21)

To find $T_{\rm c}$ for BEC, we set $z=1~(i.e.~\mu=0)$ and $n_0=0,$ and obtain

$$n = \int_{0}^{\infty} d\varepsilon \ g(\varepsilon) \ \frac{\varepsilon}{e^{\varepsilon/k_{\rm B}T_{\rm c}} - 1}$$
(22)

Substituting in our form for $g(\varepsilon)$, we obtain

$$n = \frac{3}{4\pi^2} \Gamma\left(\frac{9}{2}\right) \zeta\left(\frac{9}{2}\right) \left(\frac{k_{\rm B}T}{A}\right)^{9/2} , \qquad (23)$$

and therefore

(d)
$$T_{\rm c} = \frac{A}{k_{\rm B}} \left(\frac{4\pi^2 n}{3\Gamma(\frac{9}{2})\,\zeta(\frac{9}{2})} \right)^{2/9}$$
 (24)

(4) Short answers:

(a) What are the conditions for a dynamical system to exhibit Poincaré recurrence?[3 points]

The time evolution of the dynamics must be invertible and volume-preserving on a phase space of finite total volume. For $\dot{\varphi} = X(\varphi)$ this requires that the phase space divergence vanish: $\nabla \cdot X = 0$.

(b) Describe what the term *ergodic* means in the context of a dynamical system.[3 points]

Ergodicity means that time averages may be replaced by phase space averages, *i.e.* $\langle f(\varphi) \rangle_T = \langle f(\varphi) \rangle_S$, where

$$\langle f(\boldsymbol{\varphi}) \rangle_T = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \, f(\boldsymbol{\varphi}(t))$$
 (25)

$$\langle f(\boldsymbol{\varphi}) \rangle_S = \int d\mu \, \varrho(\boldsymbol{\varphi}) \, f(\boldsymbol{\varphi}) \,,$$
 (26)

where $\rho(\boldsymbol{\varphi})$ is a phase space distribution. For the microcanonical ensemble,

$$\varrho(\varphi) = \frac{\delta(E - H(\varphi))}{\int d\mu \,\delta(E - H(\varphi))} , \qquad (27)$$

- (c) What is the microcanonical ensemble? [3 points] The microcanonical ensemble is defined by the phase space probability distribution $\rho(\varphi) = \delta(E - H(\varphi))$, which says that all states that lie on the same constant energy hypersurface in phase space are equally likely.
- (d) A system with L = 6 single particle levels contains N = 3 bosons. How many distinct many-body states are there? [3 points] The general result for bosons is $\Omega_{\text{BE}}(L, N) = \binom{N+L-1}{N}$, so we have $\Omega = \binom{8}{3} = 56$.
- (e) A system with L = 6 single particle levels contains N = 3 fermions. How many distinct many-body states are there? [3 points] The general result for bosons is $\Omega_{\rm FD}(L, N) = {L \choose N}$, so we have $\Omega = {6 \choose 3} = 20$.
- (f) Explain how the Maxwell-Boltzmann limit results, starting from the expression for $\Omega_{\text{BE/FD}}(T, V, \mu)$. [3 points] We have

$$\Omega_{\rm BE/FD} = \pm k_{\rm B} T \sum_{\alpha} \ln\left(1 \mp z \, e^{-\varepsilon_{\alpha}/k_{\rm B}T}\right) \,. \tag{28}$$

The MB limit occurs when the product $z e^{-\varepsilon_{\alpha}/k_{\rm B}T} \ll 1$, in which case

$$\Omega_{\rm BE/FD} \longrightarrow \Omega_{\rm MB} = -k_{\rm B}T \sum_{\alpha} e^{(\mu - \varepsilon_{\alpha})/k_{\rm B}T} , \qquad (29)$$

where the sum is over all energy eigenstates of the single particle Hamiltonian.

(g) For the Dieterici equation of state, $p(1-bn) = nk_{\rm B}T \exp(-an/k_{\rm B}T)$, find the second virial coefficient $B_2(T)$. [3 points] We must expand in powers of the density n:

$$p = nk_{\rm B}T \frac{e^{-an/k_{\rm B}T}}{1 - bn} = nk_{\rm B}T \left(1 - \frac{an}{k_{\rm B}T} + \dots\right) \left(1 + bn + \dots\right)$$
$$= nk_{\rm B}T + \left(b k_{\rm B}T - a\right) n^2 + \mathcal{O}(n^3) .$$
(30)

The virial expansion of the equation of state is

$$p = nk_{\rm B}T(1 + B_2(T) + B_3(T)n^2 + \dots) , \qquad (31)$$

and so we identify

$$B_2(T) = b - \frac{a}{k_{\rm B}T} . (32)$$

(h) Explain the difference between the Einstein and Debye models for the specific heat of a solid. [4 points]

The Einstein model assumes a phonon density of states $g(\varepsilon) = C_{\rm E} \,\delta(\varepsilon - \varepsilon_0)$, while for the Debye model one has $g(\varepsilon) = C_{\rm D} \,\varepsilon^2 \,\Theta(\varepsilon_{\rm D} - \varepsilon)$, where $C_{\rm E,D}$ are constants, and $\varepsilon_{\rm D}$ is a cutoff known as the Debye energy. At high temperatures, both models yield a Dulong-Petit heat capacity of $3Nk_{\rm B}$, where N is the number of atoms in the solid. At low temperatures, however, the Einstein model yields an exponentially suppressed specific heat, while the specific heat of the Debye model obeys a T^3 power law.

(i) Who composed the song yerushalayim shel zahav? [50 quatloos extra credit] The song was composed by Naomi Shemer in 1967. In 2005, it was revealed that it was based in part on a Basque folk song.