PHYSICS 140A : STATISTICAL PHYSICS
FINAL EXAMINATION SOLUTIONS

Instructions: *Do problem 4 (34 points) and any two of problems 1, 2, and 3 (33 points each)*

(1) A noninteracting system consists of N dimers. Each dimer consists of two spins, S and σ, where $S \in \{-1, 0, +1\}$ and $\sigma \in \{-1, +1\}$. The Hamiltonian is

$$\hat{H} = -J \sum_{i=1}^{N} S_i \, \sigma_i - \mu_0 H \sum_{i=1}^{N} S_i \, .$$

Thus, the individual dimer Hamiltonian is $\hat{h} = -JS\sigma - \mu_0 HS$.

(a) Find the N-dimer free energy $F(T, N)$.

(b) Find the average $\langle S \rangle$ and the zero field susceptibility $\chi_S(T) = \frac{\partial \langle S \rangle}{\partial H}\Big|_{H=0}$.

(c) Find the average $\langle \sigma \rangle$ and the zero field susceptibility $\chi_\sigma(T) = \frac{\partial \langle \sigma \rangle}{\partial H}\Big|_{H=0}$.

(d) Examine the $J \to 0$ limits of $\chi_S(T)$ and $\chi_\sigma(T)$ and interpret your results physically.

Solution :

(a) There are six energy states for each dimer, listed in Tab. 1

S	σ	$\hat{h}(S,\sigma)$	S	σ	$\hat{h}(S,\sigma)$
$+1$	$+1$	$-J - \mu_0 H$	$+1$	-1	$J - \mu_0 H$
0	$+1$	0	0	-1	0
-1	$+1$	$+J + \mu_0 H$	-1	-1	$-J + \mu_0 H$

Table 1: Energy table for problem 1.

Thus, the single dimer partition function is

$$\begin{aligned}\zeta = \mathsf{Tr}\, e^{-\beta \hat{h}} &= e^{\beta J} e^{\beta \mu_0 H} + 1 + e^{-\beta J} e^{-\beta \mu_0 H} + e^{-\beta J} e^{\beta \mu_0 H} + 1 + e^{\beta J} e^{-\beta \mu_0 H} \\ &= 2 + 4 \cosh(\beta \mu_0 J) \cosh(\beta \mu_0 H) \, .\end{aligned}$$

For N noninteracting dimers, $Z = \zeta^N$ (the dimers are regarded as distinguishable). Thus,

$$\boxed{F(T,N) = -N k_B T \ln\Big(2 + 4 \cosh\big(J/k_B T\big) \cosh\big(\mu_0 H/k_B T\big)\Big)}$$

(b) We have

$$\langle S \rangle = \frac{\mathsf{Tr}\ S\, e^{-\beta \hat{h}(S,\sigma)}}{\mathsf{Tr}\ e^{-\beta \hat{h}(S,\sigma)}} = \frac{e^{\beta J} e^{\beta \mu_0 H} - e^{-\beta J} e^{-\beta \mu_0 H} + e^{-\beta J} e^{\beta \mu_0 H} - e^{\beta J} e^{-\beta \mu_0 H}}{2 + 4 \cosh(\beta J) \cosh(\beta H)} \, ,$$

so

$$\boxed{\langle S\rangle = \frac{\cosh(J/k_{\rm B}T)\sinh(\mu_0 H/k_{\rm B}T)}{\cosh(J/k_{\rm B}T)\cosh(\mu_0 H/k_{\rm B}T)+\frac{1}{2}}}$$

Expanding to linear order in H and taking the coefficient, we have

$$\boxed{\chi_S(T) = \frac{\partial\langle S\rangle}{\partial H}\bigg|_{H=0} = \frac{\cosh\big(J/k_{\rm B}T\big)}{\cosh\big(J/k_{\rm B}T\big)+\frac{1}{2}}\cdot\frac{\mu_0}{k_{\rm B}T}}$$

Note that usually we define $\chi = \frac{\partial M}{\partial T}$ with $M = \mu_0\,\langle S\rangle$, so our result above differs by a factor of μ_0.

(c) We have

$$\langle\sigma\rangle = \frac{\mathsf{Tr}\ \sigma\, e^{-\beta\hat{h}(S,\sigma)}}{\mathsf{Tr}\ e^{-\beta\hat{h}(S,\sigma)}} = \frac{e^{\beta J}e^{\beta\mu_0 H} + e^{-\beta J}e^{-\beta\mu_0 H} - e^{-\beta J}e^{\beta\mu_0 H} - e^{\beta J}e^{-\beta\mu_0 H}}{2+4\cosh(\beta J)\cosh(\beta H)}\ ,$$

so

$$\boxed{\langle \sigma\rangle = \frac{\sinh(J/k_{\rm B}T)\sinh(\mu_0 H/k_{\rm B}T)}{\cosh(J/k_{\rm B}T)\cosh(\mu_0 H/k_{\rm B}T)+\frac{1}{2}}}$$

Expanding to linear order in H and taking the coefficient, we have

$$\boxed{\chi_\sigma(T) = \frac{\partial\langle \sigma\rangle}{\partial H}\bigg|_{H=0} = \frac{\sinh\big(J/k_{\rm B}T\big)}{\cosh\big(J/k_{\rm B}T\big)+\frac{1}{2}}\cdot\frac{\mu_0}{k_{\rm B}T}}$$

(d) As $J\to 0$ we have

$$\boxed{\chi_S(T,J=0) = \frac{2\mu_0}{3k_{\rm B}T}\quad,\quad \chi_\sigma(T,J=0)=0}$$

The physical interpretation of these results is as follows. When $J=0$, the individual dimer Hamiltonian is $\hat{h} = -\mu_0 HS$. The factor of $\frac{2}{3}$ in χ_S is due to the fact that $S=0$ in $\frac{1}{3}$ of the states. The σ spins don't couple to the field at all in this limit, so $\chi_\sigma = 0$.

(2) Recall that a van der Waals gas obeys the equation of state

$$\Big(p + \frac{a}{v^2}\Big)\big(v-b\big) = RT\ ,$$

where v is the molar volume. We showed that the energy per mole of such a gas is given by

$$\varepsilon(T,v) = \tfrac{1}{2}fRT - \frac{a}{v}\ ,$$

where T is temperature and f is the number of degrees of freedom per particle.

(a) For an ideal gas, the adiabatic equation of state is $v\,T^{f/2} = \text{const}$. Find the adiabatic equation of state (at fixed particle number) for the van der Waals gas.

(b) One mole of a van der Waals gas is used as the working substance in a Carnot engine (see Fig. 1). Find the molar volume at v_{C} in terms of v_{B}, T_1, T_2, and constants.

(c) Find the heat Q_{AB} absorbed by the gas from the upper reservoir.

(d) Find the work done per cycle, W_{cyc}. *Hint: you only need to know Q_{AB} and the cycle efficiency η.*

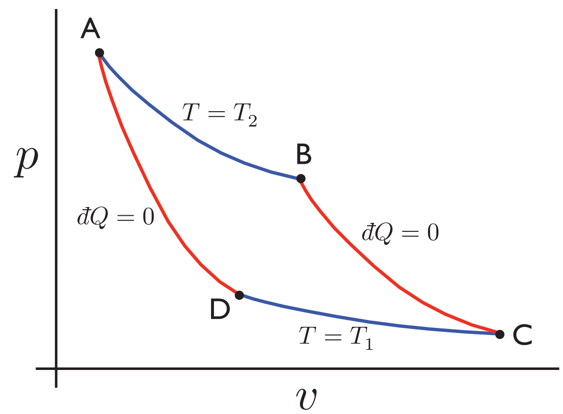

Figure 1: The Carnot cycle.

Solution :

(a) We have

$$
\begin{aligned}
0 = T\,ds &= d\varepsilon + p\,dv \\
&= \tfrac{1}{2} f R\,dT + \left(p + \frac{a}{v^2}\right) dv \\
&= \tfrac{1}{2} f R\,dT + \frac{RT\,dv}{v-b} = \tfrac{1}{2} f RT\,d\ln\!\left[(v-b)\,T^{f/2}\right] ,
\end{aligned}
$$

where $s = N_{\mathsf{A}} S/N$ is the molar entropy. Thus, the adiabatic equation of state for the van der Waals gas is

$$
\boxed{ds = 0 \quad \Rightarrow \quad (v-b)\,T^{f/2} = \text{const.}}
$$

Setting $b = 0$, we recover the ideal gas result.

(b) Since BC is an adiabat, we have

$$
(v_{\mathsf{B}} - b)\,T_2^{f/2} = (v_{\mathsf{C}} - b)\,T_1^{f/2} \quad \Rightarrow \quad \boxed{v_{\mathsf{C}} = b + (v_{\mathsf{B}} - b)\left(\frac{T_2}{T_1}\right)^{f/2}}
$$

(c) We have, from the First Law,

$$
\begin{aligned}
Q_{\mathsf{AB}} &= E_{\mathsf{B}} - E_{\mathsf{A}} + W_{\mathsf{AB}} \\
&= \nu\left(\frac{a}{v_{\mathsf{A}}} - \frac{a}{v_{\mathsf{B}}}\right) + \nu \int\limits_{v_{\mathsf{A}}}^{v_{\mathsf{B}}} dv\, p \\
&= \nu\left(\frac{a}{v_{\mathsf{A}}} - \frac{a}{v_{\mathsf{B}}}\right) + \nu \int\limits_{v_{\mathsf{A}}}^{v_{\mathsf{B}}} dv \left[\frac{RT_2}{v-b} - \frac{a}{v^2}\right] ,
\end{aligned}
$$

hence

$$\boxed{Q_{\mathsf{AB}} = \nu R T_2 \ln\left(\frac{v_{\mathsf{B}} - b}{v_{\mathsf{A}} - b}\right)}$$

with $\nu = 1$.

(d) Since the cycle is reversible, we must have

$$\eta = \frac{W_{\mathsf{cyc}}}{Q_{\mathsf{AB}}} \quad \Rightarrow \quad \boxed{W_{\mathsf{cyc}} = \nu R (T_2 - T_1) \ln\left(\frac{v_{\mathsf{B}} - b}{v_{\mathsf{A}} - b}\right)}$$

(3) In homework assignment #9, you showed that the grand partition function for a gas of q-state parafermions is

$$\Xi(T, V, \mu) = \prod_\alpha \left(\frac{1 - e^{(q+1)(\mu - \varepsilon_\alpha)/k_{\mathrm{B}} T}}{1 - e^{(\mu - \varepsilon_\alpha)/k_{\mathrm{B}} T}}\right) ,$$

where the product is over all single particle states. Consider now the case where the number of parafermions is not conserved, hence $\mu = 0$. We call such particles *paraphotons*.

(a) What is the occupancy $n(\varepsilon, T)$ of q-state paraphotons of energy ε?

(b) Suppose the dispersion is the usual $\varepsilon(\boldsymbol{k}) = \hbar c k$. Assuming g $= 1$, find the single particle density of states $g(\varepsilon)$ in three space dimensions.

(c) Find the pressure $p(T)$. You may find the following useful:

$$\int_0^\infty \! dt \, \frac{t^{r-1}}{e^t - 1} = \Gamma(r)\,\zeta(r) \qquad , \qquad \int_0^\infty \! dt \, t^{r-1} \, \ln\left(\frac{1}{1 - e^{-t}}\right) = \Gamma(r)\,\zeta(r+1) \, .$$

(d) Show that $p = C_q \, n k_{\mathrm{B}} T$, where n is the number density, and C_q is a dimensionless constant which depends only on q.

Solution :

(a) For $\mu \neq 0$, for a single parafermion state, we have

$$\begin{aligned} n &= -\frac{\partial \Omega}{\partial \mu} = \frac{1}{\beta} \frac{\partial \ln \Xi}{\partial \mu} \\ &= \frac{1}{e^{\beta(\varepsilon - \mu)} - 1} - \frac{q+1}{e^{(q+1)\beta(\varepsilon - \mu)} - 1} \, . \end{aligned}$$

Setting $\mu = 0$, we find

$$\boxed{n(\varepsilon, T) = \frac{1}{e^{\varepsilon / k_{\mathrm{B}} T} - 1} - \frac{q+1}{e^{(q+1)\,\varepsilon / k_{\mathrm{B}} T} - 1}}$$

(b) With g = 1, we have

$$g(\varepsilon)\, d\varepsilon = \frac{d^3\!k}{(2\pi)^3} = \frac{k^2\, dk}{2\pi^2} \quad \Rightarrow \quad \boxed{\; g(\varepsilon) = \frac{k^2}{2\pi^2}\,\frac{dk}{d\varepsilon} = \frac{\varepsilon^2}{2\pi^2(\hbar c)^3} \;}$$

(c) The pressure is

$$\begin{aligned}
p = -\frac{\Omega}{V} &= k_{\rm B}T \int\limits_0^\infty \! d\varepsilon\; g(\varepsilon) \left\{ \ln\!\big(1 - e^{-(q+1)\varepsilon/k_{\rm B}T}\big) - \ln\!\big(1 - e^{-\varepsilon/k_{\rm B}T}\big) \right\} \\
&= \frac{k_{\rm B}T}{2\pi^2(\hbar c)^3} \int\limits_0^\infty \! d\varepsilon\; \varepsilon^2 \left\{ \ln\!\big(1 - e^{-(q+1)\varepsilon/k_{\rm B}T}\big) - \ln\!\big(1 - e^{-\varepsilon/k_{\rm B}T}\big) \right\} \\
&= \frac{\zeta(4)\,(k_{\rm B}T)^4}{\pi^2(\hbar c)^3} \cdot \left(1 - \frac{1}{(q+1)^3} \right) .
\end{aligned}$$

Thus,

$$\boxed{\; p(T) = \Big(1 - (q+1)^{-3} \Big) \cdot \frac{\zeta(4)\,(k_{\rm B}T)^4}{\pi^2(\hbar c)^3} \;}$$

(d) We need to evaluate

$$\begin{aligned}
n &= \int\limits_0^\infty \! d\varepsilon\; g(\varepsilon) \left\{ \frac{1}{e^{\varepsilon/k_{\rm B}T} - 1} - \frac{q+1}{e^{(q+1)\,\varepsilon/k_{\rm B}T} - 1} \right\} \\
&= \frac{1}{2\pi^2(\hbar c)^3} \int\limits_0^\infty \! d\varepsilon\; \varepsilon^2 \left\{ \frac{1}{e^{\varepsilon/k_{\rm B}T} - 1} - \frac{q+1}{e^{(q+1)\,\varepsilon/k_{\rm B}T} - 1} \right\} \\
&= \Big(1 - (q+1)^{-2} \Big) \cdot \frac{\zeta(3)\,(k_{\rm B}T)^3}{\pi^2(\hbar c)^3}
\end{aligned}$$

From this we derive

$$\boxed{\; C_q = \frac{p}{n k_{\rm B}T} = \frac{\zeta(4)}{\zeta(3)} \cdot \frac{q^2 + 3q + 3}{q^2 + 3q + 2} \;}$$

(4) Provide brief but substantial answers to the following:

(a) A particle in $d = 3$ dimensions has the dispersion $\varepsilon(\boldsymbol{k}) = \varepsilon_0 \exp(ka)$. Find the density of states per unit volume $g(\varepsilon)$. Sketch your result.

(b) Find the information entropy in the distribution $p_n = C\, e^{-\lambda n}$, where $n \in \{0, 1, 2, \ldots\}$. Choose C so as to normalize the distribution.

(c) An ideal gas at temperature $T = 300\,\mathrm{K}$ undergoes an adiabatic free expansion which results in a doubling of its volume. What is the final temperature?

(d) For an N-particle noninteracting system, sketch the contributions ΔC_V to the heat capacity *versus* temperature for (i) a vibrational mode at energy $\hbar\omega_0$, and (ii) a two-level (Schottky) defect with energy splitting $\Delta = \varepsilon_1 - \varepsilon_0$. Take care to identify any relevant characteristic temperatures, as well as the limiting values of ΔC_V.

Solution :

(a) Inverting the dispersion relation, we obtain the expression $k(\varepsilon) = a^{-1} \ln\big(\varepsilon/\varepsilon_0\big)\,\Theta(\varepsilon - \varepsilon_0)$. We then have

$$g(\varepsilon) = \frac{k^2}{2\pi}\,\frac{dk}{d\varepsilon} = \frac{k^2}{2\pi}\cdot\frac{1}{a\varepsilon_0 e^{ak}}\ .$$

Thus,

$$\boxed{g(\varepsilon) = \frac{1}{2\pi^2 a^3}\,\frac{1}{\varepsilon}\,\ln^2\!\left(\frac{\varepsilon}{\varepsilon_0}\right)\Theta(\varepsilon - \varepsilon_0)}$$

The result is plotted in Fig. 2.

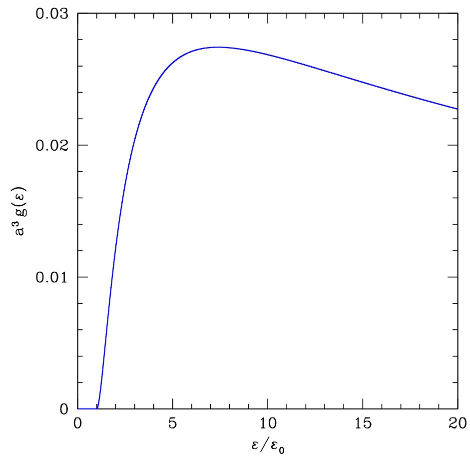

Figure 2: DOS for problem 4.a.

(b) Normalizing the distribution,

$$1 = \sum_{n=0}^{\infty} p_n = C\sum_{n=0}^{\infty} e^{-n\lambda} = \frac{C}{1 - e^{-\lambda}}\ ,$$

hence $C = 1 - e^{-\lambda}$. The information entropy is

$$S = -\sum_{n=0}^{\infty} p_n \ln p_n = -\ln\big(1 - e^{-\lambda}\big) + C\lambda\sum_{n=0}^{\infty} n\,e^{-\lambda n}\ .$$

Now

$$f(\lambda) = \sum_{n=0}^{\infty} e^{-n\lambda} = \frac{1}{1 - e^{-\lambda}} \qquad\Rightarrow\qquad \sum_{n=0}^{\infty} n\,e^{-n\lambda} = -\frac{df}{d\lambda} = \frac{1}{(e^{\lambda} - 1)(1 - e^{-\lambda})}\ .$$

Thus, the information entropy is

$$S(\lambda) = \frac{\lambda}{e^{\lambda} - 1} - \ln\big(1 - e^{-\lambda}\big)\ .$$

Note that $S(\lambda \to 0) \sim 1 - \ln\lambda$ which diverges logarithmically with $1/\lambda$. This is approaching the uniform distribution. For $\lambda \to \infty$, we have $p_n = \delta_{n,0}$, and $S(\lambda \to \infty) = 0$.

(c) Under an adiabatic free expansion, $\Delta E = Q = W = 0$ with N conserved. Since $E = \frac{1}{2} f N k_{\mathrm{B}} T$ is independent of volume for the ideal gas, there is no change in temperature, *i.e.*

$$\boxed{T_{\mathrm{final}} = T_{\mathrm{initial}} = 100\,\mathrm{K}}$$

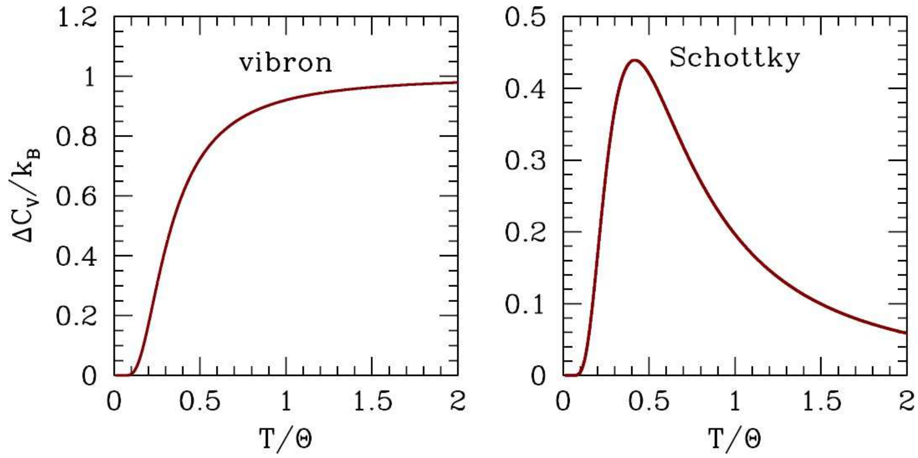

Figure 3: Heat capacities for a N identical vibrational modes (left) and Schottky defects (right).

(d) The characteristic temperatures for the vibrational mode (vibron) and Schottky defect are given by $\Theta = \hbar\omega_0/k_B$ and $\Theta = \Delta/k_B$, respectively. A detailed derivation of the heat capacity for these systems is provided in §§ 4.10.5-6 of the Lecture Notes. One finds

$$\Delta C_V = N k_B \left(\frac{\Theta}{T}\right)^2 \frac{e^{\Theta/T}}{(e^{\Theta/T} \mp 1)^2} ,$$

where the top sign is for the vibron and the bottom sign for the Schottky defect. All you were asked to do, however, was to provide a sketch (see Fig. 3). The $T \to \infty$ limit of the vibron result is given by the Dulong-Petit value of k_B per oscillator mode. For the Schottky defect, ΔC_V vanishes in both the $T \to 0$ and $T \to \infty$ limits.

(5) Write a well-defined expression for the greatest possible number expressible using only five symbols. *Examples:* $1+2+3$, 10^{100}, $\Gamma(99)$. [50 quatloos extra credit]

Solution :

Using conventional notation, my best shot would be

$$\boxed{9^{9^{9^{9^9}}}}$$

This is a very big number indeed: $9^9 \approx 3.7 \times 10^8$, so $9^{9^9} \sim 10^{3.5\times 10^8}$, and $9^{9^{9^{9^9}}} \sim 10^{10^{10^{3.7\times 10^8}}}$. But in the world of big numbers, this is still tiny. For a fun diversion, use teh google to learn about the Ackermann sequence and Knuth's up-arrow notation. Using Knuth's notation (see `http://en.wikipedia.org/wiki/Knuth's_up-arrow_notation`), one could write $9 \uparrow^{99} 9$, which is vastly larger. But even *these* numbers are modest compared with something called the "Busy Beaver sequence", which is a concept from computer science and Turing machines. For a very engaging essay on large numbers, see `http://www.scottaaronson.com/writings/bignumbers.html`.