(1) A noninteracting system consists of $N$ dimers. Each dimer consists of two spins, $S$ and $\sigma$, 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 $\chi_S(T) = \frac{\partial \langle S \rangle}{\partial H} \bigg|_{H=0}$.

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

(d) Examine the $J \rightarrow 0$ 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.

<table>
<thead>
<tr>
<th>$S$</th>
<th>$\sigma$</th>
<th>$\hat{h}(S, \sigma)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>+1</td>
<td>+1</td>
<td>$-J - \mu_0 H$</td>
</tr>
<tr>
<td>0</td>
<td>+1</td>
<td>0</td>
</tr>
<tr>
<td>-1</td>
<td>+1</td>
<td>$+J + \mu_0 H$</td>
</tr>
</tbody>
</table>

Table 1: Energy table for problem 1.

Thus, the single dimer partition function is

$$\zeta = \text{Tr} e^{-\beta \hat{h}} = e^{\beta J \mu_0 H} + 1 + e^{-\beta J} e^{-\beta \mu_0 H} + e^{-\beta J} e^{\beta \mu_0 H} + 1 + e^{\beta J} e^{-\beta \mu_0 H} + e^{\beta J} e^{\beta \mu_0 H} = 2 + 4 \cosh(\beta \mu_0 J) \cosh(\beta H).$$

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

$$F(T, N) = -Nk_B T \ln \left( 2 + 4 \cosh \left( \frac{J}{k_B T} \right) \cosh \left( \frac{\mu_0 H}{k_B T} \right) \right).$$

(b) We have

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

1
so

\[ \langle S \rangle = \frac{\cosh(J/k_B T) \sinh(\mu_0 H/k_B T)}{\cosh(J/k_B T) \cosh(\mu_0 H/k_B T) + \frac{1}{2}} \]

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

\[ \chi_S(T) = \frac{\partial \langle S \rangle}{\partial H} \bigg|_{H=0} = \frac{\cosh(J/k_B T)}{\cosh(J/k_B T) + \frac{1}{2}} \cdot \frac{\mu_0}{k_B T} \]

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 \( \mu_0 \).

(c) We have

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

so

\[ \langle \sigma \rangle = \frac{\sinh(J/k_B T) \sinh(\mu_0 H/k_B T)}{\cosh(J/k_B T) \cosh(\mu_0 H/k_B T) + \frac{1}{2}} \]

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

\[ \chi_\sigma(T) = \frac{\partial \langle \sigma \rangle}{\partial H} \bigg|_{H=0} = \frac{\sinh(J/k_B T)}{\cosh(J/k_B T) + \frac{1}{2}} \cdot \frac{\mu_0}{k_B T} \]

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

\[ \chi_S(T, J = 0) = \frac{2\mu_0}{3k_B T} \quad , \quad \chi_\sigma(T, J = 0) = 0 \]

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 \( \chi_S \) is due to the fact that \( S = 0 \) in \( \frac{1}{3} \) of the states. The \( \sigma \) 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

\[ \left( p + \frac{a}{v^2} \right) (v - b) = RT \]

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

\[ \varepsilon(T, v) = \frac{1}{2} f RT - \frac{a}{v} \]

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, \( W_{\text{cyc}} \). Hint: you only need to know \( Q_{AB} \) and the cycle efficiency \( \eta \).

Solution:

(a) We have

\[
0 = T\, ds = d\varepsilon + p\, dv \\
= \frac{1}{2} fR\, dT + \left( p + \frac{a}{v^2} \right)\, dv \\
= \frac{1}{2} fR\, dT + \frac{RT\, dv}{v-b} = \frac{1}{2} fRT\, d\ln \left[ (v-b)T^{f/2} \right],
\]

where \( s = N_A S/N \) is the molar entropy. Thus, the adiabatic equation of state for the van der Waals gas is

\[
ds = 0 \Rightarrow (v-b)T^{f/2} = \text{const.}
\]

Setting \( b = 0 \), we recover the ideal gas result.

(b) Since BC is an adiabat, we have

\[
(v_B - b)T_2^{f/2} = (v_C - b)T_1^{f/2} \Rightarrow v_C = b + (v_B - b) \left( \frac{T_2}{T_1} \right)^{f/2}
\]

(c) We have, from the First Law,

\[
Q_{AB} = E_B - E_A + W_{AB} \\
= \nu \left( \frac{a}{v_A} - \frac{a}{v_B} \right) + \nu \int_{v_A}^{v_B} dv \, p \\
= \nu \left( \frac{a}{v_A} - \frac{a}{v_B} \right) + \nu \int_{v_A}^{v_B} dv \left[ \frac{RT_2}{v-b} - \frac{a}{v^2} \right],
\]
hence

\[ Q_{AB} = \nu R T_2 \ln \left( \frac{v_B - b}{v_A - b} \right) \]

with \( \nu = 1 \).

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

\[ \eta = \frac{W_{\text{cyc}}}{Q_{AB}} \Rightarrow W_{\text{cyc}} = \nu R (T_2 - T_1) \ln \left( \frac{v_B - b}{v_A - b} \right) \]

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

\[ \Xi(T, V, \mu) = \prod_{\alpha} \left( \frac{1 - e^{(q+1)(\mu - \epsilon_{\alpha})/k_B T}}{1 - e^{(\mu - \epsilon_{\alpha})/k_B T}} \right), \]

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 \( n(\epsilon, T) \) of \( q \)-state paraphotons of energy \( \epsilon \)?

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

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

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

(d) Show that \( p = C_q n k_B T \), 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

\[ n = -\frac{\partial Q}{\partial \mu} = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln \Xi \]

\[ = \frac{1}{e^{\beta(\epsilon - \mu) - 1} - 1} - \frac{q + 1}{e^{(q+1)\beta(\epsilon - \mu) - 1} - 1} . \]

Setting \( \mu = 0 \), we find

\[ n(\epsilon, T) = \frac{1}{e^{\epsilon/k_B T} - 1} - \frac{q + 1}{e^{(q+1)\epsilon/k_B T} - 1} \]
(b) With $g = 1$, we have

$$
g(\varepsilon) \, d\varepsilon = \frac{d^3k}{(2\pi)^3} = \frac{k^2 \, dk}{2\pi^2} \quad \Rightarrow \quad g(\varepsilon) = \frac{k^2}{2\pi^2} \frac{dk}{d\varepsilon} = \frac{\varepsilon^2}{2\pi^2 (hc)^3}
$$

(c) The pressure is

$$
p = -\frac{\Omega}{V} = k_B T \int_0^\infty d\varepsilon \, g(\varepsilon) \left\{ \ln \left(1 - e^{-(q+1)\varepsilon/k_B T}\right) - \ln \left(1 - e^{-\varepsilon/k_B T}\right) \right\}
$$

$$
= \frac{k_B T}{2\pi^2 (hc)^3} \int_0^\infty d\varepsilon \, \varepsilon^2 \left\{ \ln \left(1 - e^{-(q+1)\varepsilon/k_B T}\right) - \ln \left(1 - e^{-\varepsilon/k_B T}\right) \right\}
$$

$$
= \frac{\zeta(4) (k_B T)^4}{\pi^2 (hc)^3} \cdot \left(1 - \frac{1}{(q + 1)^3}\right).
$$

Thus,

$$
p(T) = \left(1 - (q + 1)^{-3}\right) \cdot \frac{\zeta(4) (k_B T)^4}{\pi^2 (hc)^3}
$$

(d) We need to evaluate

$$
n = \int_0^\infty d\varepsilon \, g(\varepsilon) \left\{ \frac{1}{e^{\varepsilon/k_B T} - 1} - \frac{q + 1}{e^{(q+1)\varepsilon/k_B T} - 1} \right\}
$$

$$
= \frac{1}{2\pi^2 (hc)^3} \int_0^\infty d\varepsilon \, \varepsilon^2 \left\{ \frac{1}{e^{\varepsilon/k_B T} - 1} - \frac{q + 1}{e^{(q+1)\varepsilon/k_B T} - 1} \right\}
$$

$$
= \left(1 - (q + 1)^{-2}\right) \cdot \frac{\zeta(3) (k_B T)^3}{\pi^2 (hc)^3}
$$

From this we derive

$$
C_q = \frac{p}{nk_B T} = \frac{\zeta(4)}{\zeta(3)} \cdot \frac{q^2 + 3q + 3}{q^2 + 3q + 2}
$$

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

(a) A particle in $d = 3$ dimensions has the dispersion $\varepsilon(k) = \varepsilon_0 \exp(ka)$. 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 $T = 300 \text{ K}$ 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 $\Delta C_V$ 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 $\Delta C_V$.

**Solution:**

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

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

Thus,

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

The result is plotted in Fig. 2.

(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

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

Now

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

Thus, the information entropy is

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

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 $E = \frac{1}{2} f N k_b T$ is independent of volume for the ideal gas, there is no change in temperature, i.e.

$$T_{\text{final}} = T_{\text{initial}} = 100 \text{ K}.$$
(d) The characteristic temperatures for the vibrational mode (vibron) and Schottky defect are given by \( \Theta = \frac{\hbar \omega_0}{k_B} \) and \( \Theta = \frac{\Delta}{k_B} \), respectively. A detailed derivation of the heat capacity for these systems is provided in §§4.10.5-6 of the Lecture Notes. One finds

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

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, \( \Delta C_V \) 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 quahtloos extra credit]

Solution:

Using conventional notation, my best shot would be

\[
9^{9^{9^{9^9}}}
\]

This is a very big number indeed: \( 9^9 \approx 3.7 \times 10^8 \), so \( 9^{9^9} \approx 10^{3.5 \times 10^8} \), and \( 9^{9^{9^9}} \approx 10^{10^{10^{2.7 \times 10^8}}} \). 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 \( 9^{9^{9^9}} \), 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.