

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #1

(1) To measure the heat capacity of an object, all you usually have to do is put it in thermal contact with another object whose heat capacity is known. Suppose that a 100 g chunk of metal is immersed in boiling water (100° C). After a time, the metal is removed and quickly transferred to a Styrofoam cup containing 250 g of water at 20° C. After a little while, the temperature of the contents of the cup is found to be 24° C. You may assume that the heat transferred from contents of the cup to its surroundings, and the heat capacity of the cup itself are both negligible.

- (a) How much heat is gained by the water in the Styrofoam cup?
- (b) How much heat is lost by the metal?
- (c) What is the heat capacity of the metal?
- (d) What is the specific heat (in J/g K) of the metal?

(2) The heat capacity of Albertson's *Rotini Tricolore* is approximately 1.8 J/g °C. Suppose you toss 340 g of pasta at 15° C into 1.5 liters of boiling water. What effect does this have on the temperature of the water, before the stove has time to provide any more heat?

Hint: You will need to look up some constants in order to solve this problem. Part of the problem is in understanding what constants you need. Once you know, try Google.

(3) Consider the van der Waals equation of state,

$$\left(p + \frac{a\nu^2}{V^2}\right)(V - \nu b) = \nu RT$$

where $\nu = N/N_A$ is the number of moles. Find expressions for each of the following quantities in terms of the specific volume $v = V/\nu$, the temperature T , and constants. Don't confuse the symbols ν and v !

(a) $-V\left(\frac{\partial p}{\partial V}\right)_T$ (b) $\left(\frac{\partial p}{\partial T}\right)_V$ (c) $\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p$

(4) A peculiar molecule discovered in Santa Barbara, consisting of uranium, carbon, and antimony (UCSb) is found in its gas phase to obey the modified van der Waals equation,

$$p(V - \nu b) = \nu RT .$$

From calorimetry, the energy is determined to be

$$E(T, V, \nu) = \nu \varepsilon_0 e^{T/T_0} ,$$

which is volume-independent, with $\varepsilon_0 = 1000 \text{ J/mol}$ and $T_0 = 300 \text{ K}$.

- (a) Find an expression for the molar specific heat c_p .
- (b) How much heat energy Q is required to raise $\nu = 5$ moles of the UCSb gas from $T_A = 300 \text{ K}$ to $T_B = 600 \text{ K}$ and at constant pressure?
- (c) (Challenging!) Find an expression for the adiabatic speed of sound $c_S(v, T)$ in terms of the molar volume $v = V/\nu$, the temperature T , and other constants (including the molecular mass M). For a discussion of sound in fluids (and gases), see §14.5.5 of my lecture notes from Physics 110B (still available online).

(5) Which of the following quantities is a 'state function' for driving? Explain your answers.

- (a) travel time
- (b) elevation
- (c) aggravation

(6) For each of the following differentials, identify whether it is exact or inexact. If you can, find the integrating factor L for which $dU = e^{-L} dW$ is exact.

- (a) $dW = 2x^2y dx + x^3 dy$
- (b) $dW = \frac{y^2z}{(x+y)^2} dx + \frac{x^2z}{(x+y)^2} dy + \frac{xy}{x+y} dz$
- (c) $dW = e^{xy} dx + \left(2x + \frac{x}{y} e^{xy}\right) dy$

PHYSICS 140A : ASSIGNMENT #1 SOLUTIONS

Problem 1.

Solution:

(a) $Q_w = m_w C_w \Delta T_w = 4.2 \times 10^3 J$, where the specific heat of water is :

$$C_w = 4.2 \times 10^3 J / kg \cdot ^\circ C$$

(b) When we neglect the heat loss, the heat received by water should be the exact the same as the heat lost by the metal. Therefore:

$$Q_m = Q_w = 4.2 \times 10^3 J$$

(c) Capacity of the metal is:

$$C_m = \frac{Q_m}{T_0 - T_1} = 55.3 J / K$$

(d) Specific heat is:

$$c_m = \frac{C_m}{m} = 0.55 J / g \cdot K$$

Problem 2.

Solution:

When you toss pasta into boiling water, there will be heat transferring from boiling water to pasta. In this process, the total thermal energy should be conserved.

$$m_p C_p \Delta T_p + m_w C_w \Delta T_w = 0, \text{ where } p=\text{pasta, } w=\text{water}$$

Necessary constants are:

$$m_w = \rho V = 1.0 kg / L * 1.5 L = 1.5 kg$$

$$C_w = 4.2 \times 10^3 J / kg \cdot ^\circ C$$

$$\Rightarrow T_{Final} = 92.5^\circ C$$

So if the stove provides no heat to the system before thermal equilibrium, the final temperature would be $92.5^\circ C$.

Problem 3.

Solution:

$$(a) \left(p + \frac{av^2}{V^2} \right) (V - vb) = \nu RT \Rightarrow \left[\left(\frac{\partial p}{\partial V} \right)_T - \frac{2av^2}{V^3} \right] (V - vb) + \left(p + \frac{av^2}{V^2} \right) = 0$$

$$\Rightarrow \left(\frac{\partial p}{\partial V} \right)_T = -\frac{vRT}{(V - vb)^2} + \frac{2av^2}{V^3}$$

$$\Rightarrow -V \left(\frac{\partial p}{\partial V} \right)_T = \frac{uRT}{(u - b)^2} - \frac{2a}{u^2}$$

$$(b) \left(p + \frac{av^2}{V^2} \right) (V - vb) = vRT \Rightarrow \left(\frac{\partial p}{\partial T} \right)_V (V - vb) = vR$$

$$\Rightarrow \left(\frac{\partial p}{\partial T} \right)_V = \frac{R}{(u - b)}$$

$$(c) \left(p + \frac{av^2}{V^2} \right) (V - vb) = vRT \Rightarrow -\frac{2av^2}{V^3} \left(\frac{\partial V}{\partial T} \right)_p (V - vb) + \left(p + \frac{av^2}{V^2} \right) \left(\frac{\partial V}{\partial T} \right)_p = vR$$

$$\Rightarrow -\frac{2av^2}{V^3} \left(\frac{\partial V}{\partial T} \right)_p (V - vb) + \frac{vRT}{V - vb} \left(\frac{\partial V}{\partial T} \right)_p = vR$$

$$\Rightarrow \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_p = \frac{R}{\frac{2ab}{u^2} - \frac{2a}{u} + \frac{RTu}{u - b}}$$

where $u = \frac{V}{v}$ is the molar volume.

Problem 4.

Solution:

$$(a) C_p = \left(\frac{\partial E}{\partial T} \right)_p + p \left(\frac{\partial V}{\partial T} \right)_p = \frac{v\varepsilon_0}{T_0} e^{T/T_0} + vR$$

$$\Rightarrow c_p = \frac{\varepsilon_0}{T_0} e^{T/T_0} + R$$

The term $p \left(\frac{\partial V}{\partial T} \right)_p$ can be obtained by the similar method employed in Problem 3.

$$(b) Q = \int_{T_A}^{T_B} v c_p dT = \int_{T_A}^{T_B} \left(\frac{v\varepsilon_0}{T_0} e^{T/T_0} + vR \right) dT = E(T_B, V, v) - E(T_A, V, v) + vR(T_B - T_A)$$

$$= 3.58 \times 10^4 J$$

$$(c) c_s^2 = \left(\frac{\partial p}{\partial \rho} \right)_{dQ=0}, \quad \rho \text{ is density defined by } M/V = M_0/u, \quad M_0 \text{ is molar mass.}$$

$$c_s^2 = \frac{\partial p}{\partial u} \frac{\partial u}{\partial \rho} = -\frac{u^2}{M_0} \left(\frac{\partial p}{\partial u} \right)_{\#Q=0} \quad (1)$$

Therefore, in order to compute c_s , we must know the relationship between p and v .

$dE = dQ - pdV = -pdV$, also we know:

$$E = v\varepsilon_0 e^{T/T_0}$$

$$\Rightarrow dT = -\frac{pT_0}{\varepsilon_0} e^{-T/T_0} du \quad (2)$$

From equation of state,

$(u-b)dp + pdu = RdT$, then substituting (2) into this expression, we get:

$$dp = -\frac{RT}{(u-b)^2} \left(1 + \frac{RT_0}{\varepsilon_0} e^{-T/T_0} \right) du \quad (3)$$

Then from (1) we can get the complete solution:

$$c_s^2 = \frac{RT}{M_0} \left(\frac{u}{u-b} \right)^2 \left(1 + \frac{RT_0}{\varepsilon_0} e^{-T/T_0} \right)$$

Problem 5.

Solution:

(a) Travel time is not a state function because it depends on the path taken and not on the endpoints alone.

(b) Elevation is a state function. No matter what path you take between A and B, the net elevation change will be the same.

© Aggravation most certainly is not a state function. You can become more aggravated if your path takes you along a highly congested stretch of road.

Problem 6.

Solution:

For a differential as: $dW = \sum_i A_i dx_i$

A simple rule to identify it "exact" or "inexact" is:

$$\frac{\partial A_i}{\partial x_j} = \frac{\partial A_j}{\partial x_i}$$

(1) $dW = 2x^2 y dx + x^3 dy$

$$\therefore \frac{\partial A_x}{\partial y} = 2x^2 \neq 3x^2 = \frac{\partial A_y}{\partial x}$$

\therefore Inexact differential.

It is easy to find if we employ a factor " $\frac{1}{x}$ ", the new differential becomes:

$$dU = 2xydx + x^2 dy = d(x^2 y)$$

Now it is an exact differential. $L = \ln x$

$$(2) \quad dW = \frac{y^2 z}{(x+y)^2} dx + \frac{x^2 z}{(x+y)^2} dy + \frac{xy}{x+y} dz$$

According to the rule above, it is an exact differential.

$$\text{In fact, it can be written as } dW = d\left(\frac{xyz}{x+y}\right)$$

$$(3) \quad dW = e^{xy} dx + \left(2x + \frac{x}{y} e^{xy}\right) dy$$

Obviously, it is an inexact differential.

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #2

(1) One mole of a diatomic ($\gamma = \frac{7}{5}$) ideal gas is driven along a cycle depicted in fig. 1. Stage AB is an isotherm at temperature $T_A = 500$ K. Stage BC is an isobar, and stage CA is an isochore. The volumes at A and B are $V_A = 1.00$ L and $V_B = 4.00$ L.

- (a) What is the pressure p_B at point B?
- (b) What is the total work done per cycle?
- (c) What is the entropy change $S_C - S_B$?

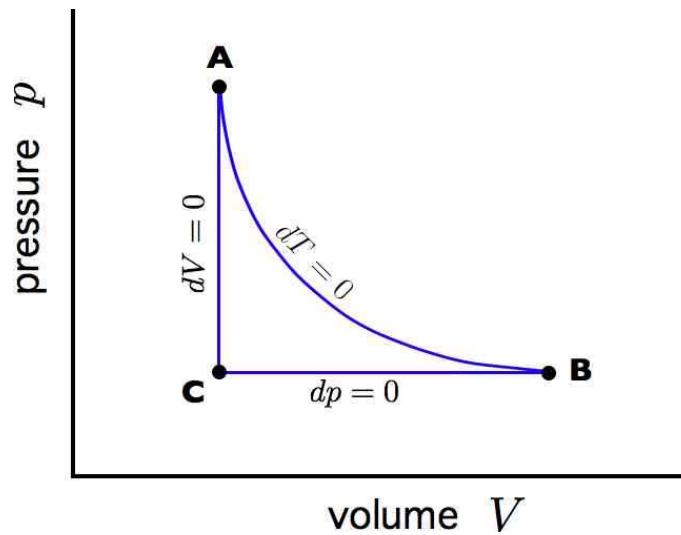


Figure 1: A three-stage cycle consisting of an isotherm (AB), an isobar (BC), and an isochore (CA).

(2) Consider the Diesel cycle of fig. 2. Define the *compression ratio* $r = V_B/V_D$ and the *cutoff ratio* $s = V_A/V_D$. Derive a formula for the efficiency $\eta = W/Q_{DA}$ for an ideal gas Diesel cycle in terms of r , s , and the ideal gas parameter $\gamma = 1 + \frac{2}{f}$. Compare your result with the efficiency of an Otto cycle with the same compression ratio, and show that the Otto cycle has a greater efficiency. However, an optimized Otto cycle with real fuel has a compression ratio of about $r = 8$. Compare its efficiency with that of a Diesel cycle with $r = 18$ and $s = 2$.

(3) Scientists discover a novel extraterrestrial molecule, illudium phosdex, in the Murchison meteorite. They are overjoyed. The thermodynamics of this new material follow from the relation

$$E(S, V, N) = \frac{a S^5}{V^2 N^2}.$$

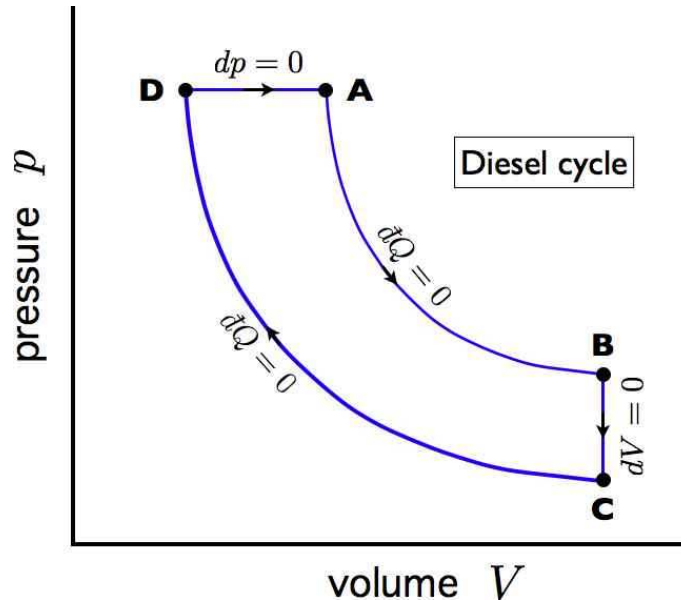


Figure 2: A Diesel cycle consists of two adiabats, an isobar, and an isochore.

- (a) Let $a = 10^{48}$ in MKS units. What are the MKS units of the constant a ?
- (b) Derive the analog of the ideal gas law for this system – an equation of state relating p , T , N , and V .
- (c) How much work is required to isothermally expand 3.00 moles of illudium phosdex from $V_i = 2.00 \text{ m}^3$ to $V_f = 3.00 \text{ m}^3$ at a temperature of $T = 300 \text{ K}$? Recall $N_A = 6.02 \times 10^{23}$.
- (d) At a pressure of $p = 1.00 \times 10^5 \text{ Pa}$, a quantity of illudium phosdex is placed in a sealed chamber. The chamber is thermally insulated so that no heat is exchanged between sample and environment. Additional pressure is applied and the change in volume is recorded. What is the measured compressibility $\kappa = -V^{-1}\partial V/\partial p$?

(4) Consider the relation

$$E(S, V, N) = \varepsilon_0 \frac{N^{1+\alpha}}{V^\alpha} \exp\left(\frac{\alpha S}{N k_B}\right),$$

where ε_0 and α are constants.

- (a) Show that this system obeys the ideal gas law.
- (b) Find the adiabatic equation of state in terms of p and V .
- (c) Find the molar heat capacities c_V and c_p .

(5) *Challenging!* Consider the modified ideal gas Carnot cycle in fig. 3. The upper isotherm AB is broken into two separate stages. AA' is an adiabatic free expansion, and all other stages are quasistatic. Define the parameter

$$x = \frac{V_{A'} - V_A}{V_B - V_A}.$$

When $x = 0$, the entire cycle is reversible, and when $x = 1$, the entire upper isotherm is taken up by the adiabatic free expansion. Also define the expansion ratio

$$r = \frac{V_B}{V_A}.$$

- Show that $V_A V_C = V_B V_D$.
- What is the work W done per cycle? Express your answer in terms of the temperatures T_1 and T_2 , the ratios x and r , and the number of moles of gas ν .
- Suppose $V_A = 1.00$ L and $V_B = 10.0$ L. Suppose further that $T_1 = 50^\circ$ C and $T_2 = 400^\circ$ C. At what value of $V_{A'}$ would the work done per cycle vanish?
- The efficiency of this cycle is defined as $\eta = W/Q_{A'B}$. Derive an expression for $\eta(x, r, T_1/T_2)$.

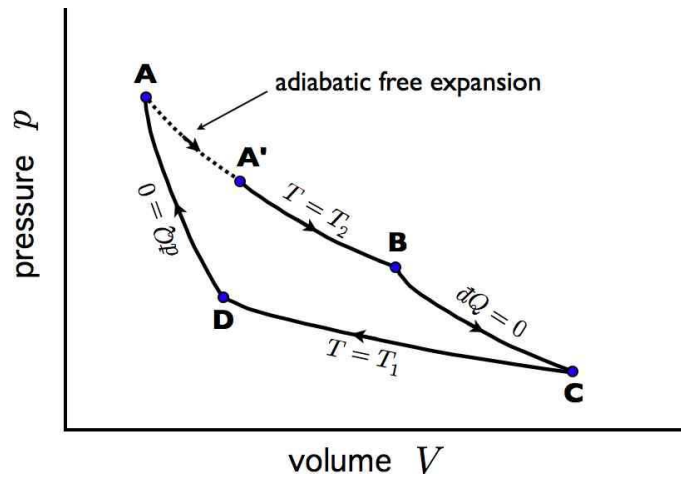
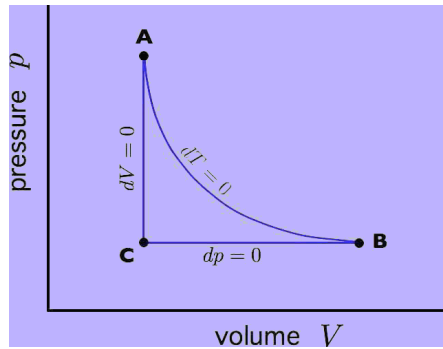


Figure 3: In this modified Carnot cycle, the upper isotherm is itself broken into two stages. AA' is an adiabatic free expansion, and A'B is a quasistatic isotherm. Stages BC, CD, and DA are all quasistatic.

PHYSICS 140A : ASSIGNMENT #2 SOLUTIONS

Problem 1. Solution:



(a) As we know V_B and T_B , we can directly use:

$$P_B = \frac{\nu RT_B}{V_B} = 1.04 \times 10^6 \text{ Pa}$$

(b) We can compute the area under the curve to get the work in this process.

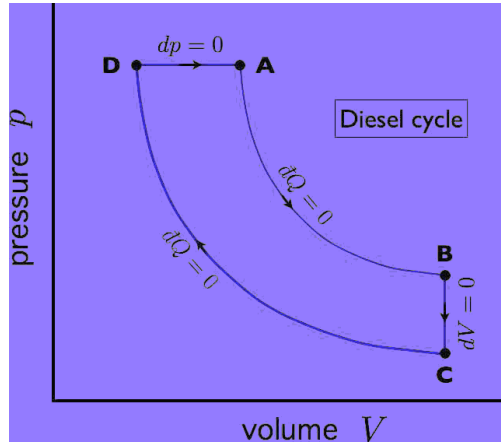
$$\begin{aligned} W &= \int_A^B P dV = \int_A^B P dV - P_B (V_B - V_C) \\ &= \int_{V_A}^{V_B} \frac{\nu RT_A}{V} dV - \nu RT_B \left(1 - \frac{V_C}{V_B}\right) \\ &= \nu RT_B \left\{ \ln\left(\frac{V_B}{V_A}\right) - 1 + \frac{V_C}{V_B} \right\} = 2.64 \times 10^3 \text{ J} \end{aligned}$$

$$(c) \Delta S = \int_B^C dS = \int_B^C \frac{dQ}{T} = \int_B^C \frac{dE + PdV}{T} \quad (1)$$

where $E = \frac{PV}{\gamma - 1}$, take it into (1), we get:

$$\begin{aligned} \Delta S &= \int_B^C \frac{PdV + VdP}{(\gamma - 1)T} + \frac{P}{T} dV = \int_B^C \frac{\gamma}{\gamma - 1} \nu R \frac{dV}{V} + \frac{\nu R}{\gamma - 1} \frac{dP}{P} \\ &= \frac{\gamma}{\gamma - 1} \nu R \ln\left(\frac{V_C}{V_B}\right) = -40.3 \text{ J / K} \end{aligned}$$

Problem 2. Solution:



First of all, let's consider the work during this period, i.e. S_{ABCD}

$$\begin{aligned}
 W &= S_{ABCD} = \int_A^B PdV + \int_B^C PdV + \int_C^D PdV + \int_D^A PdV \\
 &= \int_A^B \frac{P_A V_A^\gamma}{V^\gamma} dV + \int_C^D \frac{P_A V_D^\gamma}{V^\gamma} dV + P_A (V_A - V_D) \\
 &= \frac{\gamma}{\gamma-1} P_A (V_A - V_D) - \frac{1}{\gamma-1} P_A V_B^{1-\gamma} (V_A^\gamma - V_D^\gamma)
 \end{aligned}$$

Secondly, in this period, the ideal gas absorb heat during D->A, therefore:

$$Q = \int_D^A dQ = \int_D^A dE + PdV = \int_D^A d\left(\frac{PV}{\gamma-1}\right) + P_A (V_A - V_D) = \frac{\gamma}{\gamma-1} P_A (V_A - V_D)$$

Finally, we get:

$$\eta = \frac{W}{Q} = 1 - \frac{1}{\gamma} \frac{r^{1-\gamma} (s^\gamma - 1)}{s-1}, \text{ where } s \text{ and } r \text{ have been defined in the problem.}$$

$$\text{Otto cycle has the efficiency of } \eta = 1 - \left(\frac{V_{\min}}{V_{\max}}\right)^{\gamma-1}$$

If $r=18, s=2, \eta_{\text{Diesel}} = 81\% < \eta_{\text{Otto}} = 85\%$, however an optimized Otto Cycle has the parameter of $r=8, \eta_{\text{max of Otto}} = 75\%$, which is less than the efficiency in Diesel cycle.

Problem 3. Solution:

(a) The unit of S is J/K, V is m^3 and E is J, therefore, a should has the unit of:

$$m^6 K^5 / J^4.$$

$$(b) \quad E = \frac{aS^5}{V^2N^2} \Rightarrow dE = \frac{5aS^4}{V^2N^2}dS - \frac{2aS^5}{V^3N^2}dV \quad (1)$$

On the other hand, we know:

$$dE = TdS - PdV \quad (2)$$

Compare (1) and (2), we can easily get the relation:

$$T = \frac{5aS^4}{V^2N^2}, \quad P = \frac{2aS^5}{V^3N^2}$$

Then we can get the equation of state:

$$P\left(\frac{V}{N}\right)^{1/2} 5^{5/4} a^{1/4} = 2T^{5/4}$$

(c) As a isotherm process, the equation of state should be:

$$PV^{1/2} = C = \text{const.}$$

Therefore, the work in this isotherm process is:

$$W = \int PdV = \int \frac{C}{V^{1/2}} dV = 2C(V_f^{1/2} - V_i^{1/2})$$

(d) Always be aware of the difference between isotherm process and adiabatic process!

First, let's rewrite the equation of state as:

$$P^4V^2a = \frac{16}{3125}N^2T^5$$

We can then get the differential relation:

$$4P^3V^2adP + 2P^4VadV = \frac{16}{625}N^2T^4dT \quad (1)$$

$$\text{As adiabatic process, } dE = -PdV \quad (2)$$

Where $E = \frac{aS^5}{V^2N^2} = \frac{(VN)^{1/2}}{5^{5/4}a^{1/4}}T^{5/4}$, and P is determined by the equation of state

as above.

The (2) can give us the relation of dV and dT, $dT = -\frac{2T}{V}dV$

Invoking this relation to (1), we can get:

$$-\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{dQ=0} = \frac{1}{3P}$$

Problem 4. Solution:

(a) Similar as the problem 3, $dE = TdS - PdV$

$$T = \left(\frac{\partial E}{\partial S}\right)_V = \frac{\alpha\epsilon_0}{k_B}\left(\frac{N}{V}\right)^\alpha \exp\left(\frac{\alpha S}{Nk_B}\right)$$

$$P = -\left(\frac{\partial E}{\partial V}\right)_S = \alpha \varepsilon_0 \left(\frac{N}{V}\right)^{1+\alpha} \exp\left(\frac{\alpha S}{Nk_B}\right)$$

Therefore, $PV = NkT = \nu RT$. \Rightarrow This system obeys the ideal gas law.

(b) As for adiabatic process, $dE = dQ - PdV = -PdV = -\frac{Nk_B T}{V} dV$ (1)

In addition, we can rewrite $E = \frac{Nk_B T}{\alpha}$ by using the relation in (a).

Therefore, $dE = \frac{Nk_B}{\alpha} dT$, invoking this expression into (1):

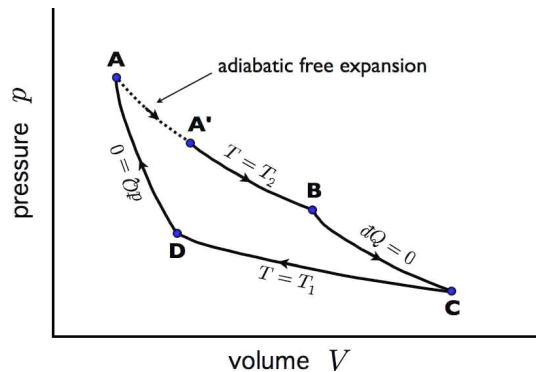
$$\frac{Nk_B}{\alpha} dT = -\frac{Nk_B T}{V} dV \Rightarrow TV^\alpha = \text{const.}$$

(c) From the derivation above, we can get $c_V = \frac{1}{\nu} \left(\frac{\partial E}{\partial T}\right)_V = \frac{R}{\alpha}$

$$c_P = c_V + p \left(\frac{\partial V}{\partial T}\right)_p = \frac{1+\alpha}{\alpha} R$$

Problem 5. Solution:

(a)



The volume relation should be the same as the normal Carot Cycle. i.e.

$\oint \frac{dQ}{T} = 0$, where only A \rightarrow B and C \rightarrow D contribute dQ. Thus,

$$\oint \frac{dQ}{T} = \frac{\int_A^B \frac{nRT_2}{V} dV}{T_2} + \frac{\int_C^D \frac{nRT_1}{V} dV}{T_1} = nR \ln \left(\frac{V_B V_D}{V_A V_C} \right) \Rightarrow V_A V_C = V_B V_D$$

(b) Let's analysis the work in details.

$$AA': Q_{AA'} = W_{AA'} = 0$$

$$A'B: Q_{A'B} = W_{A'B} = nRT_2 \ln\left(\frac{V_B}{V_{A'}}\right)$$

$$BC: Q_{BC} = 0; W_{BC} = \frac{nR(T_2 - T_1)}{\gamma - 1}$$

$$CD: Q_{CD} = W_{CD} = -nRT_1 \ln\left(\frac{V_C}{V_D}\right) = -nRT_1 \ln\left(\frac{V_B}{V_A}\right)$$

$$DA: Q_{DA} = 0; W_{DA} = -\frac{nR(T_2 - T_1)}{\gamma - 1}$$

The total work in this cycle is:

$$W = W_{AA'} + W_{A'B} + W_{BC} + W_{CD} + W_{DA} = nRT_2 \ln\left(\frac{V_B}{V_{A'}}\right) - nRT_1 \ln\left(\frac{V_B}{V_A}\right)$$

By using the defined parameter x and r , we can get:

$$W = nR(T_2 - T_1) \ln r - nRT_2 \ln(1 + (r - 1)x)$$

(c) Let $W = nR(T_2 - T_1) \ln r - nRT_2 \ln(1 + (r - 1)x) = 0$, we can solve this problem, and the

$$\text{answer is } x = \frac{r^{1-T_1/T_2} - 1}{r - 1} \approx 0.26$$

(d) $Q_{A'B} = nRT_2 \ln\left(\frac{V_B}{V_A + x(V_B - V_A)}\right) = nRT_2 \ln\left(\frac{r}{1 + x(r - 1)}\right)$, therefore

$$\eta = \frac{W}{Q_{A'B}} = 1 - \frac{T_1}{T_2} \frac{\ln r}{\ln r - \ln(1 + (r - 1)x)} < 1 - \frac{T_1}{T_2}$$

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #3

(1) For an ideal gas, show explicitly that

$$\frac{\partial(T, S, N)}{\partial(p, V, N)} = \left(\frac{\partial T}{\partial p}\right)_{V, N} \left(\frac{\partial S}{\partial V}\right)_{p, N} - \left(\frac{\partial T}{\partial V}\right)_{p, N} \left(\frac{\partial S}{\partial p}\right)_{V, N} = 1.$$

(2) A thermodynamic process takes place at constant φ , where φ is a particular function of some state variables. In each of the following cases, find the heat capacity at constant φ , *i.e.* C_φ . You may assume N is constant in all cases, and furthermore that the gas is ideal.

(a) $\varphi(T, V) = VT^{-2}$.

(b) $\varphi(p, T) = T e^{p/p_0}$.

(c) $\varphi(p, V) = p^3 V$.

(3) The entropy of a thermodynamic system $S(E, V, N)$ is given by

$$S(E, V, N) = a E^\alpha V^\beta N^\gamma,$$

where a is a dimensionful constant.

(a) Extensivity of S imposes a condition on (α, β, γ) . Find this constraint.

(b) Even with the extensivity condition satisfied, the system may violate one or more stability criteria. Find the general conditions on (α, β, γ) which are thermodynamically permissible.

(4) Express $V\left(\frac{\partial T}{\partial V}\right)_H$ in terms of c_p , α_p , and κ_T . See §1.10.1 of the notes if you have forgotten the definitions of the latter two quantities.

(5) An ideal gas expands isothermally from volume V_i to volume V_f .

(a) Assuming N is constant, what is the change in the Helmholtz free energy F ?

(b) Assuming μ is constant, what is the change in the Landau free energy Ω ?

PHYSICS 140A : ASSIGNMENT #3 SOLUTIONS

Problem 1. Solution:

First, let's derive the expression of S.

$dE = TdS - PdV$, for ideal gas, it can be written as:

$$dS = nC_V \frac{dT}{T} + p \frac{dV}{T} \Rightarrow dS = nC_V \frac{dT}{T} + nR \frac{dV}{V} \Rightarrow$$

$$S = nC_V \ln T + nR \ln V + C' = nC_V \ln P + n(C_V + R) \ln V + C$$

$$\text{Therefore, we can get: } \left(\frac{\partial S}{\partial V} \right)_{p,N} = \frac{n(C_V + R)}{V}, \left(\frac{\partial S}{\partial p} \right)_{V,N} = \frac{nC_V}{p}$$

$$\text{In addition, from the equation of state: } \left(\frac{\partial T}{\partial V} \right)_{p,N} = \frac{p}{nR}, \left(\frac{\partial T}{\partial p} \right)_{V,N} = \frac{V}{nR}$$

$$\text{Finally we get: } \frac{\partial(T, S, N)}{\partial(p, V, N)} = 1$$

Problem 2. Solution:

$$C_\varphi = \left(\frac{dQ}{dT} \right)_\varphi = \left(\frac{dE + pdV}{dT} \right)_\varphi = C_V + p \left(\frac{\partial V}{\partial T} \right)_\varphi$$

Consider ideal gas for the following derivation.

$$(a) \quad \varphi(T, V) = VT^{-2} = C$$

$$\Rightarrow \left(\frac{\partial V}{\partial T} \right)_\varphi = 2CT$$

$$\Rightarrow C_\varphi = C_V + p \left(\frac{\partial V}{\partial T} \right)_\varphi = C_V + 2pCT = C_V + 2R$$

$$(b) \quad \varphi(T, p) = Te^{p/p_0} = \text{Const}$$

$$\Rightarrow \ln T + \frac{p}{p_0} = \ln T + \frac{RT}{p_0 V} = \ln \text{Const.} \Rightarrow \frac{1}{T} + \frac{R}{p_0 V} - \frac{RT}{p_0 V^2} \left(\frac{\partial V}{\partial T} \right)_\varphi = 0$$

$$\Rightarrow C_\varphi = C_V + p \left(\frac{\partial V}{\partial T} \right)_\varphi = C_V + R + \frac{p_0 V}{T}$$

$$(c) \quad \varphi(T, p) = p^3 V = \text{const.} \Leftrightarrow VT^{-3/2} = C$$

$$\text{The same procedure as (a) we can get: } C_\varphi = C_V + \frac{3}{2}R$$

Problem 3. Solution:

(a) The extensivity of S imposes a relation of:

$$S(\lambda E, \lambda V, \lambda N) = \lambda S(E, V, N)$$

So we can easily get the constraint:

$$\alpha + \beta + \gamma = 1$$

(b) Usually the stability of a system depends on the second order differential of a given function, e.g. potential energy, entropy.

As a standard procedure, we should evaluate $\frac{\partial^2 S}{\partial x_i \partial x_j}$, in which x_i are dimensionless

variables, e.g: $E = E_0 x_1$. Since S tends to reach maximum, the matrix of $\left(\frac{\partial^2 S}{\partial x_i \partial x_j} \right)$ should

be non-positive matrix. In other words, the eigenvalues of the following matrix should be non-positive.

$$\begin{pmatrix} \alpha(\alpha - 1) & \alpha\beta & \alpha\gamma \\ \alpha\beta & \beta(\beta - 1) & \beta\gamma \\ \alpha\gamma & \beta\gamma & \gamma(\gamma - 1) \end{pmatrix}$$

The final answer is $\alpha, \beta, \gamma \in [0, 1]$

Problem 4. Solution:

$$dH = TdS + Vdp, \text{ if } H = \text{const, then } 0 = TdS + Vdp \quad (*)$$

So we should express dS and dp in terms of dT and dV.

$$dS = \left(\frac{\partial S}{\partial T} \right)_V dT + \left(\frac{\partial S}{\partial V} \right)_T dV = \frac{C_V}{T} dT + \frac{\alpha_p}{\kappa_T} dV$$

$$dV = \left(\frac{\partial V}{\partial T} \right)_p dT + \left(\frac{\partial V}{\partial p} \right)_T dp = V\alpha_p dT - V\kappa_T dp \Rightarrow dp = \frac{\alpha_p}{\kappa_T} dT - \frac{1}{V\kappa_T} dV$$

Invoking them into (*), we can get:

$$V \left(\frac{\partial T}{\partial V} \right)_H = \frac{1 - \alpha_p T}{\alpha_p + \frac{C_p \kappa_T}{V} - T\alpha_p^2}$$

Problem 5. Solution:

(a) For isothermal process of ideal gas with fixed N, $\Delta F = -T\Delta S = -nRT \ln \left(\frac{V_f}{V_i} \right)$, where

ΔS have obtained in the Problem 1. Or we can directly get the result from the expression:

$$dF = -SdT - pdV + \mu dN = -pdV \Rightarrow \Delta F = -nRT \ln\left(\frac{V_f}{V_i}\right)$$

(b) $d\Omega = -SdT - pdV - Nd\mu = -pdV = dF$

$$\Rightarrow \Delta\Omega = -nRT \ln\left(\frac{V_f}{V_i}\right)$$

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #4

(1) The latent heat of vaporization of hexane (C_6H_{14}) is $\ell = 30.8 \text{ kJ/mol}$. The boiling point at $p = 1.00 \text{ atm}$ is $T^* = 68.9^\circ\text{C}$. Assuming that ℓ is roughly constant over this part of the vaporization curve, what will be boiling point be at a pressure $p = 0.50 \text{ atm}$?

(2) A chemical reaction among σ species may be written symbolically as an equation of the form

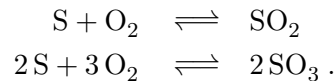
$$\zeta_1 A_1 + \zeta_2 A_2 + \cdots + \zeta_\sigma A_\sigma = 0,$$

where A_a is a chemical formula, and ζ_a is a stoichiometric coefficient. Chemical reactions are discussed in section §1.13 of the notes.

(a) Show that the dimension of the coexistence space for a system with σ species, φ coexisting phases, in which there are ρ chemical reactions is

$$d_{\text{coex}}(\sigma, \varphi, \rho) = 2 + \sigma - \varphi - \rho.$$

(b) Consider a chemically reactive system containing solid sulfur S and three gases O_2 , SO_2 , and SO_3 . Two possible reactions take place:



What is the maximum number of phases of this system that can coexist at any point in thermodynamic state space?

(3) A small college dormitory contains five different rooms. Each room houses two persons. Ten students live in the dorm: four physics majors and six chemistry majors.

(a) Suppose the dormitory rules forbid physics and chemistry majors from sharing a room. How many possible distinct room assignments are there? Note that the rooms are themselves distinct.

(b) If the rules are relaxed and physics and chemistry majors are allowed to room together, how many possible distinct room assignments are there?

(c) Generalize to the case of $M + N$ rooms, $2M$ physics majors, and $2N$ chemistry majors. What is the numbers of possible room assignments $W_1(M, N)$ assuming the rule from part (a) is enforced? What is the number of possible room assignments $W_2(M, N)$ assuming the rule is relaxed? Writing $M = x \cdot (M + N)$, what is the change in dimensionless entropy $\ln W_2 - \ln W_1$ upon relaxing the rule in the limit where $M + N$ is large and x is finite?

PHYSICS 140A : ASSIGNMENT #4 SOLUTIONS

Problem 1. Solution:

$$\left(\frac{dp}{dT}\right) = \frac{l}{T\Delta S} \approx \frac{pl}{RT^2} \Rightarrow \frac{dp}{p} = \frac{l}{R} \frac{dT}{T^2}$$

Suppose $l = \text{const.}$, we can get:

$$\ln \frac{p}{p_0} = -\frac{l}{R} \left(\frac{1}{T} - \frac{1}{T_0}\right) \Rightarrow T = 321.4K = 48.4^\circ C$$

Problem 2. Solution:

(a) From the lecture note we know $\zeta_1 A_1 + \zeta_2 A_2 + \dots + \zeta_\sigma A_\sigma = 0$ is equivalent to

$$\sum_{a=1}^{\sigma} \zeta_a \mu_a = 0$$

, i.e. one chemical reaction results in one equation which will lead to degree of freedom decrease by one. Therefore if we have ρ reaction, the degree will decrease by ρ . As a result, we can just simply revise the existed relation:

$$d_{\text{coex}} = 2 + \sigma - \varphi \text{ to } d_{\text{coex}} = 2 + \sigma - \varphi - \rho$$

(b) $d = 2 + \sigma - \varphi - \rho$, if $\sigma = 4$ and $\rho = 2$, $\Rightarrow \varphi_{\text{max}} = 4$

Problem 3. Solution:

(a) Select two rooms for chemistry C_5^2 , chemistry students assigned in this two rooms C_4^2 , the remained six physics students are assigned in three rooms: $C_6^2 C_4^2$. There are totally

$$C_5^2 C_4^2 C_6^2 C_4^2 = 5400$$

(b) If we don't distinguish majors, the problem is equivalent to: How should we assign 10 people to 5 rooms? Therefore, we can easily write down the answer as: $C_{10}^2 C_8^2 C_6^2 C_4^2 = 113400$.

(c) According to the analysis above, if there are M+N rooms corresponding (a) assignment rule:

$$W_1 = C_{M+N}^M C_{2M}^2 C_{2M-2}^2 \dots C_2^2 \times C_{2N}^2 C_{2N-2}^2 \dots C_2^2 = \frac{(M+N)! (2M)! (2N)!}{M! N! 2^M 2^N}$$

If (b) assignment rule:

$$W_2 = C_{2(M+N)}^2 C_{2(M+N)-2}^2 \dots C_2^2 = \frac{(2M+2N)!}{2^{M+N}}$$

Using the formula $\ln(N!) \approx N(\ln N - 1)$ where N is large enough, we can get:

$$\ln W_2 - \ln W_1 = M \ln \frac{M+N}{M} + N \ln \frac{M+N}{N}$$

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #5 SOLUTIONS

(1) Consider a modified version of the Kac ring model where each spin now exists in one of three states: A, B, or C. The flippers rotate the internal states cyclically: $A \rightarrow B \rightarrow C \rightarrow A$.

- (a) What is the Poincaré recurrence time for this system? *Hint*: the answer depends on whether or not the total number of flippers is a multiple of 3.

SOLUTION: If the number of flippers N_f is a multiple of 3, then each spin will have made an integer number of complete cyclic changes $A \rightarrow B \rightarrow C \rightarrow A$ after one complete passage around the ring. The recurrence time is then N , where N is the number of sites. If the number of flippers N_f is not a multiple of 3, then the recurrence time is simply $3N$.

- (b) Simulate the system numerically. Choose a ring size on the order of $N = 10,000$ and investigate a few flipper densities: $x = 0.001$, $x = 0.01$, $x = 0.1$, $x = 0.99$. Remember that the flippers are located randomly at the start, but do not move as the spins evolve. Starting from a configuration where all the spins are in the A state, plot the probabilities $p_A(t)$, $p_B(t)$, and $p_C(t)$ versus the discrete time coordinate t , with t ranging from 0 to the recurrence time. If you can, for each value of x , plot the three probabilities in different colors or line characteristics (e.g. solid, dotted, dashed) on the same graph.

SOLUTION: See figs. 1, 2, 3.

- (c) Let's call $a_t = p_A(t)$, etc. Explain in words why the *Stosszahlansatz* results in the equations

$$\begin{aligned} a_{t+1} &= (1-x)a_t + x c_t \\ b_{t+1} &= (1-x)b_t + x a_t \\ c_{t+1} &= (1-x)c_t + x b_t . \end{aligned}$$

This describes what is known as a *Markov process*, which is governed by coupled equations of the form $P_i(t+1) = \sum_j Q_{ij} P_j(t)$, where Q is the *transition matrix*. Find the 3×3 transition matrix for this Markov process.

SOLUTION: According to the *Stosszahlansatz*, the probability a_{t+1} that a given spin will be in state A at time $(t+1)$ is the probability a_t it was in A at time t times the probability $(1-x)$ that it did not encounter a flipper, plus the probability c_t it was in state C at time t times the probability x that it did encounter a flipper. This explains the first equation. The others follow by cyclic permutation.

The transition matrix is

$$Q = \begin{pmatrix} 1-x & 0 & x \\ x & 1-x & 0 \\ 0 & x & 1-x \end{pmatrix} .$$

- (d) Show that the total probability is conserved by a Markov process if $\sum_i Q_{ij} = 1$ and verify this is the case for the equations in (c).

SOLUTION: The total probability is $\sum_i P_i$. Assuming $\sum_i Q_{ij} = 1$, we have

$$\sum_i P_i(t+1) = \sum_i \sum_j Q_{ij} P_j(t) = \sum_j \left(\sum_i Q_{ij} \right) P_j(t) = \sum_j P_j(t)$$

and the total probability is conserved. That's a Good Thing.

- (e) One can then eliminate $c_t = 1 - a_t - b_t$ and write these as two coupled equations. Show that if we define

$$\tilde{a}_t \equiv a_t - \frac{1}{3} \quad , \quad \tilde{b}_t \equiv b_t - \frac{1}{3} \quad , \quad \tilde{c}_t \equiv c_t - \frac{1}{3}$$

that we can write

$$\begin{pmatrix} \tilde{a}_{t+1} \\ \tilde{b}_{t+1} \end{pmatrix} = R \begin{pmatrix} \tilde{a}_t \\ \tilde{b}_t \end{pmatrix} ,$$

and find the 2×2 matrix R . Note that this is *not* a Markov process in A and B, since total probability for the A and B states is not itself conserved. Show that the eigenvalues of R form a complex conjugate pair. Find the amplitude and phase of these eigenvalues. Show that the amplitude never exceeds unity.

SOLUTION: Substituting $a_t = \tilde{a}_t + \frac{1}{3}$, *etc.* into the Markov process and eliminating $\tilde{c}_t = -(\tilde{a}_t + \tilde{b}_t)$, we obtain

$$R = \begin{pmatrix} 1 - 2x & -x \\ x & 1 - x \end{pmatrix} .$$

The characteristic polynomial for R is

$$\begin{aligned} P(\lambda) &= \det(\lambda \cdot 1 - R) = (\lambda - 1 + 2x)(\lambda - 1 + x) + x^2 \\ &= \lambda^2 - (2 - 3x)\lambda + (1 - 3x + 3x^2) . \end{aligned}$$

The eigenvalues are the two roots of $P(\lambda)$:

$$\lambda_{\pm} = 1 - \frac{3}{2}x \pm i\frac{\sqrt{3}}{2}x .$$

Note that we can write

$$\lambda_{\pm}(x) = e^{-1/\tau(x)} e^{\pm i\phi(x)}$$

where

$$\tau(x) = -\frac{2}{\ln(1 - 3x + 3x^2)} \quad , \quad \phi(x) = \tan^{-1} \left(\frac{\sqrt{3}x}{2 - 3x} \right) .$$

Since $x(1-x)$ achieves its maximum volume on the unit interval $x \in [0, 1]$ at $x = \frac{1}{2}$, where $x(1-x) = \frac{1}{4}$, we see that $\frac{1}{2} \leq |\lambda(x)| \leq 1$, hence $0 \leq \tau(x) \leq \ln 2$. We plot $\tau(x)$ and $\phi(x)$ in fig. 3.

If you managed to get this far, then you've done all that was asked. However, one can go farther and analytically solve the equations for the Markov chain. In so doing, we will discuss the linear algebraic aspects of the problem.

The matrix R is real but not symmetric. For such a matrix, the characteristic polynomial satisfies $[P(\lambda)]^* = P(\lambda^*)$, hence if λ is a root of $P(\lambda = 0)$, which is to say λ is an eigenvalue, then so is λ^* . Accordingly, the eigenvalues of a real asymmetric matrix are either real or come in complex conjugate pairs. We can decompose such a matrix R as a sum over its eigenvectors,

$$R_{ij} = \sum_{\alpha} \lambda_{\alpha} \psi_i^{\alpha} \phi_j^{\alpha},$$

where

$$\begin{aligned} \sum_j R_{ij} \psi_j^{\alpha} &= \lambda_{\alpha} \psi_i^{\alpha} \\ \sum_i \phi_i^{\alpha} R_{ij} &= \lambda_{\alpha} \phi_j^{\alpha}. \end{aligned}$$

Thus, ψ_j^{α} is the j^{th} component of the α^{th} right eigenvector of R , while ϕ_i^{α} is the i^{th} component of the α^{th} left eigenvector of R . Note that ϕ^{α} is a right eigenvector for the transposed matrix R^t . We can further impose the normalization condition,

$$\langle \phi^{\alpha} | \psi^{\beta} \rangle = \sum_i \psi_i^{\alpha} \phi_i^{\beta} = \delta^{\alpha\beta}.$$

One can check that the following assignment of eigenvectors is valid for our $R(x)$ matrix:

$$\begin{aligned} \vec{\psi}_+ &= \begin{pmatrix} 1 \\ -e^{i\pi/3} \end{pmatrix} & \vec{\psi}_- &= \begin{pmatrix} 1 \\ -e^{-i\pi/3} \end{pmatrix} \\ \vec{\phi}_+ &= \frac{1}{\sqrt{3}} e^{i\pi/6} (1 \quad e^{i\pi/3}) & \vec{\phi}_- &= \frac{1}{\sqrt{3}} e^{-i\pi/6} (1 \quad e^{-i\pi/3}). \end{aligned}$$

Let us write the vector

$$\vec{\eta}_t = \begin{pmatrix} \tilde{a}_t \\ \tilde{b}_t \end{pmatrix}.$$

We then may expand $\vec{\eta}_t$ in the right eigenvectors of R , writing

$$\vec{\eta}_t = \sum_{\alpha} C_{\alpha} \lambda_{\alpha}^t \vec{\psi}^{\alpha}.$$

Suppose we begin in a state where $a_{t=0} = 1$ and $b_{t=0} = c_{t=0} = 0$. Then we have $\tilde{a}_{t=0} = \frac{2}{3}$ and $\tilde{b}_{t=0} = -\frac{1}{3}$, hence

$$C_{\alpha} = \langle \vec{\phi}^{\alpha} | \begin{pmatrix} +2/3 \\ -1/3 \end{pmatrix} \rangle.$$

We thereby find $C_+ = C_- = \frac{1}{3}$, and

$$\begin{aligned}\tilde{a}_t &= \frac{2}{3} e^{-t/\tau} \cos(t\phi) \\ \tilde{b}_t &= \frac{2}{3} e^{-t/\tau} \sin\left(t\phi - \frac{\pi}{6}\right),\end{aligned}$$

with $\tilde{c}_t = -(\tilde{a}_t + \tilde{b}_t)$.

- (f) The fact that the eigenvalues of R are complex means that the probabilities should *oscillate* as they decay to their equilibrium values $p_A = p_B = p_C = \frac{1}{3}$. Can you see this in your simulations?

SOLUTION: Yes! The oscillation is particularly clear in the lower panel of fig. 1.

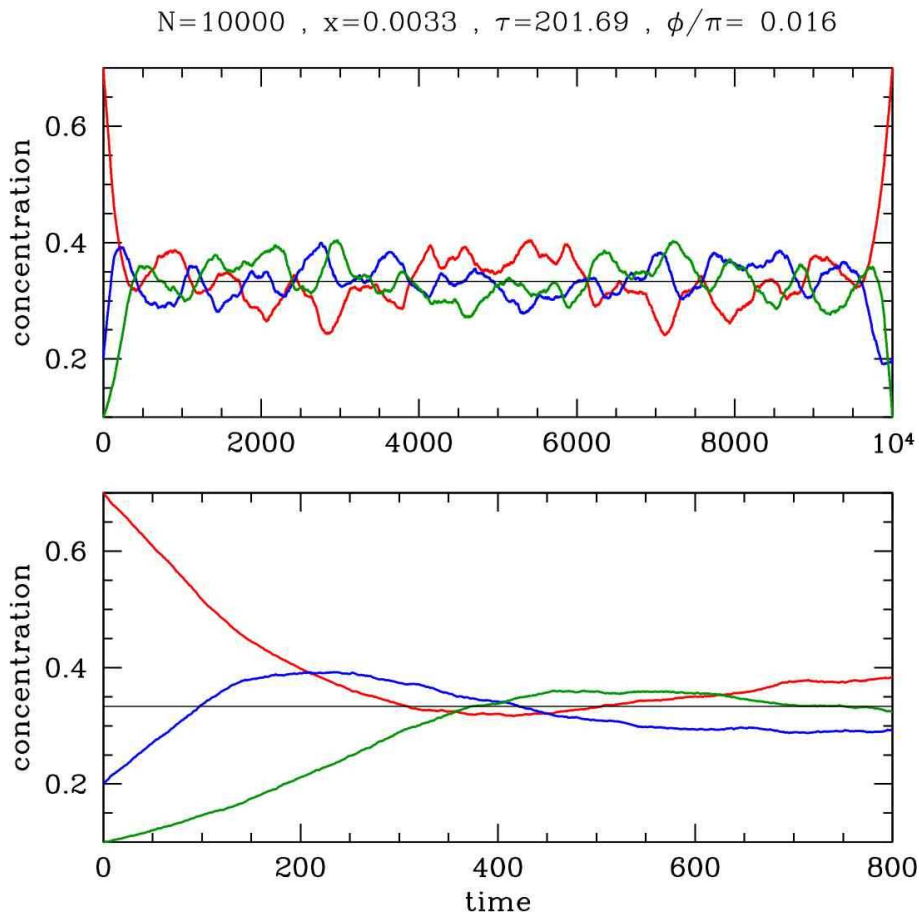


Figure 1: Simulation of three state Kac ring model with initial conditions $a_{t=0} = 0.7, b_{t=0} = 0.2, c_{t=0} = 0.1$. Note the oscillations as equilibrium is approached.

- (2) Create your own pixelated image to iterate under the cat map. Don't do anything extravagant – something with less than 25 black pixels should be fine. Choose a denominator k which is minimally acceptable to convey your image. Then iterate the pixel coordinates

$N=10000$, $x=0.0330$, $\tau=19.87$, $\phi/\pi= 0.052$

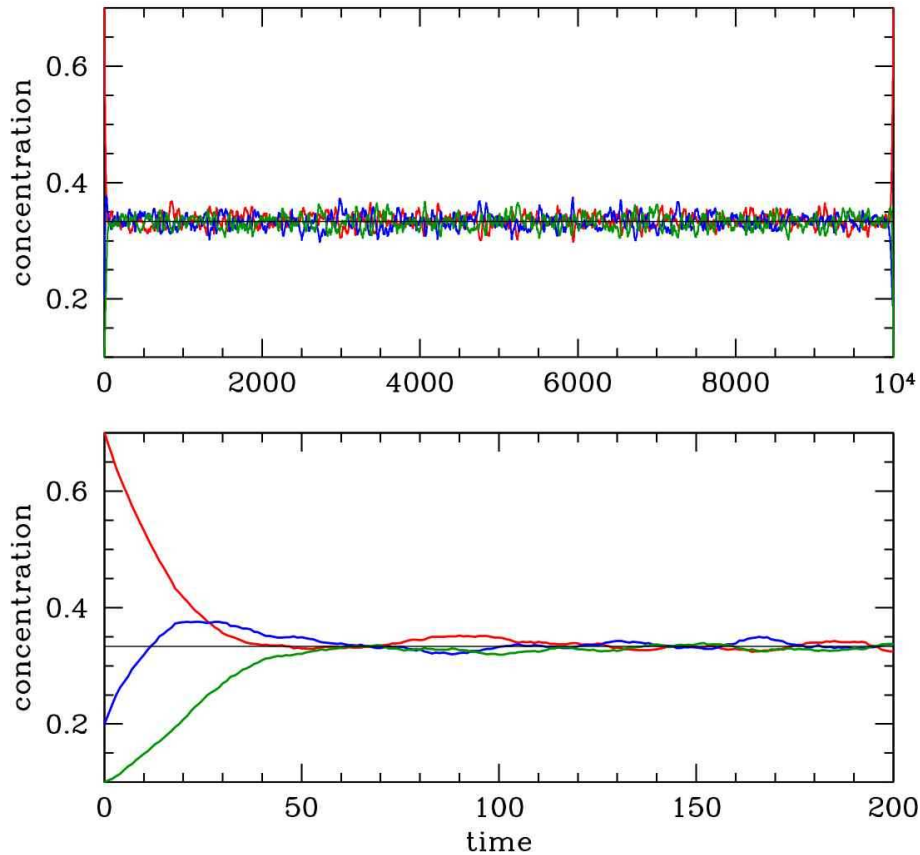


Figure 2: Simulation of three state Kac ring model with initial conditions $a_{t=0} = 0.7$, $b_{t=0} = 0.2$, $c_{t=0} = 0.1$.

under the cat map. Show how your image gets messed up after a few iterations of the map, but is nevertheless recurrent. You'll need to write a computer code to do this problem.

SOLUTION: Thomas Tran has kindly agreed to make his solution public. His iterated cat map, acting on an image of a blobfish, can be viewed at

<https://physics-forums.ucsd.edu/showthread.php?t=73>

I've uploaded Thomas' image files to the Physics 140 web page and included a link from the homework page:

<http://physics.ucsd.edu/students/courses/fall2008/physics140/CATMAP/catmap.html>

(3) Find $\mu(T, p)$ for the nonrelativistic ideal gas in d dimensions, and for the ultrarelativistic ideal gas in d dimensions.

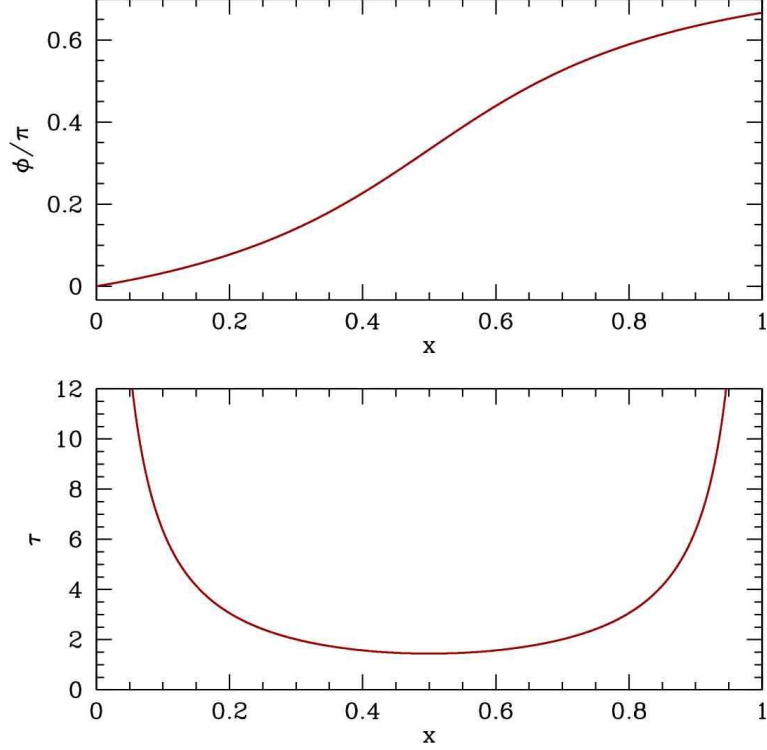


Figure 3: Phase angle and relaxation time for the Markov process derived via the *Stosszahlansatz* from the three state Kac ring model.

SOLUTION: We have

$$S_{\text{NR}}(E, V, N) = \frac{1}{2} d N k_B \ln \left[\frac{m}{d \pi \hbar^2} \cdot \frac{E}{N} \cdot \left(\frac{V}{N} \right)^{2/d} \right]$$

$$S_{\text{UR}}(E, V, N) = d N k_B \ln \left[\frac{[\Omega_d \Gamma(d)]^{1/d}}{d \hbar c} \cdot \frac{E}{N} \cdot \left(\frac{V}{N} \right)^{1/d} \right].$$

Recall the differential relation

$$dS = \frac{1}{T} dE + \frac{p}{T} dV - \frac{\mu}{T} dN.$$

This says

$$\frac{\mu}{T} = - \left(\frac{\partial S}{\partial N} \right)_{E,V} = \begin{cases} -\frac{1}{2} d k_B \ln \left(\frac{m}{d \pi \hbar^2} \cdot \frac{E}{N} \cdot \left(\frac{V}{N} \right)^{2/d} \right) + \left(1 + \frac{d}{2} \right) k_B & \text{(NR)} \\ -d k_B \ln \left(\frac{[\Omega_d \Gamma(d)]^{1/d}}{d \hbar c} \cdot \frac{E}{N} \cdot \left(\frac{V}{N} \right)^{1/d} \right) + (1 + d) k_B & \text{(UR)}. \end{cases}$$



Figure 4: Iterated cat map acting on a pixelated image of a blobfish. (Credit: Thomas Tran)

We need to eliminate E/N and V/N . To this end, we write

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_{V,N} = \begin{cases} \frac{1}{2} dk_B \cdot \frac{N}{E} & \text{(NR)} \\ dk_B \cdot \frac{N}{E} & \text{(UR)} \end{cases}$$

and

$$\frac{p}{T} = \left(\frac{\partial S}{\partial V} \right)_{E,N} = \begin{cases} k_B \cdot \frac{N}{V} & \text{(NR)} \\ k_B \cdot \frac{N}{V} & \text{(UR)} \end{cases}$$

Thus,

$$\frac{\mu}{T} = \begin{cases} -\frac{1}{2} dk_B \ln \left(\frac{m}{2\pi\hbar^2} \cdot p^{-2/d} \cdot (k_B T)^{1+\frac{2}{d}} \right) + \left(1 + \frac{d}{2}\right) k_B & \text{(NR)} \\ -dk_B \ln \left(\frac{[\Omega_d \Gamma(d)]^{1/d}}{\hbar c} \cdot p^{-1/d} \cdot (k_B T)^{1+\frac{1}{d}} \right) + (1+d)k_B & \text{(UR)}. \end{cases}$$

Thus, we have

$$\mu(T, p) = \begin{cases} k_B T \left(\ln p - \left(1 + \frac{1}{2}d\right) \ln T + \mathcal{C} \right) & \text{(NR)} \\ k_B T \left(\ln p - (1+d) \ln T + \mathcal{C}' \right) & \text{(UR)}, \end{cases}$$

where \mathcal{C} and \mathcal{C}' are constants.

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #6 SOLUTIONS

(1) Consider a monatomic ideal gas, represented within the grand canonical ensemble. Show that the probability of finding the system to have N atoms is given by the Poisson distribution,

$$P_N = \frac{1}{N!} e^{-\langle N \rangle} \langle N \rangle^N .$$

Solution : The grand partition function is $\Xi = \sum_N z^N Z_N$, where $z = \exp(\beta\mu)$ is the fugacity. The ordinary canonical partition function is $Z_N = (V/\lambda_T^3)^N/N!$, where $\lambda_T = \sqrt{2\pi\hbar^2/mk_B T}$ is the thermal wavelength. Thus, $\Xi = \exp(zV/\lambda_T^3)$, and the average number of particles is

$$\langle N \rangle = z \frac{\partial}{\partial z} \ln \Xi = \frac{zV}{\lambda_T^3} .$$

The probability that there are N particles in the system is clearly

$$P_N = \frac{z^N Z_N}{\Xi} = \frac{1}{N!} e^{-\langle N \rangle} \langle N \rangle^N .$$

(2) Derive the grand canonical distribution when there are several types of particles present.

Solution : Let $Z(N_1, N_2, \dots, N_K)$ be the OCE partition function for K species of particles when there are N_j particles of species j . Then introduce K chemical potentials μ_j (or K fugacities $z_j = \exp(\beta\mu_j)$) and write

$$\Xi(T, V, \mu_1, \dots, \mu_K) = \sum_{N_1} \dots \sum_{N_K} e^{N_1\beta\mu_1} \dots e^{N_K\beta\mu_K} Z(N_1, \dots, N_K) .$$

(3) An ideal paramagnet is described by the model in §3.11 of the notes, *i.e.*

$$\hat{H} = -\mu_0 H \sum_{j=1}^{\mathcal{N}} \sigma_j ,$$

where each $\sigma_j = \pm 1$. Suppose the system starts off at a temperature $T = 10$ mK and a field $H = 20$ T. The field is then lowered *adiabatically* to $H = 1$ T. What is the final temperature of the system?

Solution : This problem may be solved by dimensional analysis. Clearly the entropy S is a function of T and H , and the only dimensionally correct possibility is $S(T, H, \mathcal{N}) = \mathcal{N}k_B f(\mu_0 H/k_B T)$. We conclude that during an adiabatic process that the ration H/T is constant. Thus,

$$T_f = T_i \cdot \frac{H_f}{H_i} = \frac{T_i}{20} = 500 \text{ nK} .$$

Explicitly, we have

$$Z = \left(\sum_{\sigma=\pm 1} e^{\mu_o H \sigma / k_B T} \right)^{\mathcal{N}} = 2^{\mathcal{N}} \cosh^{\mathcal{N}} \left(\frac{\mu_o H}{k_B T} \right). \quad (1)$$

The free energy is then

$$F = -k_B T \ln Z = -\mathcal{N} k_B T \ln 2 - \mathcal{N} k_B T \ln \cosh \left(\frac{\mu_o H}{k_B T} \right).$$

The entropy is

$$S = - \left(\frac{\partial F}{\partial T} \right)_{H, \mathcal{N}} = \mathcal{N} k_B \left\{ \ln 2 + \ln \cosh \left(\frac{\mu_o H}{k_B T} \right) + \left(\frac{\mu_o H}{k_B T} \right) \sinh \left(\frac{\mu_o H}{k_B T} \right) \right\}.$$

This is of the required form, $S(T, H, \mathcal{N}) = \mathcal{N} k_B f(\mu_o H / k_B T)$, with $f(x) = \ln(2 \cosh x) + x \sinh x$.

(4) Consider a nonrelativistic ideal gas. From dimensional analysis, we conclude that

$$\langle |\mathbf{p}|^k \rangle = C_k (m k_B T)^{k/2}.$$

Find the constants C_k . Use the OCE.

Solution : Canceling factors common to both numerator and denominator, we have

$$\langle |\mathbf{p}|^k \rangle = \frac{\int_0^{\infty} dp p^{2+k} e^{-p^2/2m k_B T}}{\int_0^{\infty} dp p^2 e^{-p^2/2m k_B T}}.$$

Thus, after writing $p = x \sqrt{m k_B T}$, we have

$$C_k = \frac{\int_0^{\infty} dx x^{2+k} e^{-x^2/2}}{\int_0^{\infty} dx x^2 e^{-x^2/2}}.$$

We now change variables, writing $x = \sqrt{2y}$. Then $dx = dy/\sqrt{2y}$ and

$$C_k = \frac{2^{k/2} \int_0^{\infty} dy y^{\frac{k}{2} + \frac{1}{2}} e^{-y}}{\int_0^{\infty} dx y^{\frac{1}{2}} e^{-y}} = 2^{k/2} \frac{\Gamma\left(\frac{3+k}{2}\right)}{\Gamma\left(\frac{3}{2}\right)}.$$

Note $C_0 = 1$, as required by normalization, $C_1 = \sqrt{\frac{8}{\pi}}$, and $C_2 = 3$, which yields the familiar result $\langle \mathbf{p}^2 / 2m \rangle = \frac{3}{2} k_B T$.

(5) Show that

$$C_V = -k_B \beta^2 \frac{\partial^2}{\partial \beta^2} (\beta F) .$$

Solution : We have

$$C_V = -T \frac{\partial^2 F}{\partial T^2} .$$

We now write $\beta = 1/k_B T$, hence

$$\frac{\partial}{\partial T} = -k_B \beta^2 \frac{\partial}{\partial \beta} . \quad (2)$$

Then

$$\begin{aligned} C_V &= -\frac{1}{k_B \beta} \left(-k_B \beta^2 \frac{\partial}{\partial \beta} \right)^2 F \\ &= k_B \beta \frac{\partial}{\partial \beta} \left(\beta^2 \frac{\partial F}{\partial \beta} \right) = -k_B \left(\beta^3 \frac{\partial^2 F}{\partial \beta^2} + 2\beta^2 \frac{\partial F}{\partial \beta} \right) \\ &= -k_B \beta^2 \frac{\partial^2}{\partial \beta^2} (\beta F) = k_B \beta^2 \frac{\partial^2 \ln Z}{\partial \beta^2} . \end{aligned}$$

(6) Consider a three state system with energy levels at $\varepsilon = 0$, $\varepsilon = \Delta$, and $\varepsilon = W$, with $0 \leq \Delta \leq W$. Compute the free energy for such a system, $f(T)$. Derive an expression for the heat capacity $c(T)$. You may find the results from problem (5) useful. Plot the specific heat $c(T)$ versus $k_B T/\Delta$ for $W = \Delta$, $W = 2\Delta$, and $W = 6\Delta$.

Solution : The partition function is

$$\zeta = \text{Tr} e^{-\beta \hat{H}} = 1 + e^{-\beta \Delta} + e^{-\beta W} .$$

Thus,

$$f(T) = -k_B T \ln \zeta = -k_B T \ln \left(1 + e^{-\Delta/k_B T} + e^{-W/k_B T} \right) . \quad (3)$$

The heat capacity is

$$\begin{aligned} c(T) &= k_B \beta^2 \frac{\partial^2}{\partial \beta^2} \ln \zeta \\ &= k_B \beta^2 \frac{\Delta^2 e^{-\beta \Delta} + W^2 e^{-\beta W} + (W - \Delta)^2 e^{-\beta(\Delta+W)}}{(1 + e^{-\beta \Delta} + e^{-\beta W})^2} . \end{aligned}$$

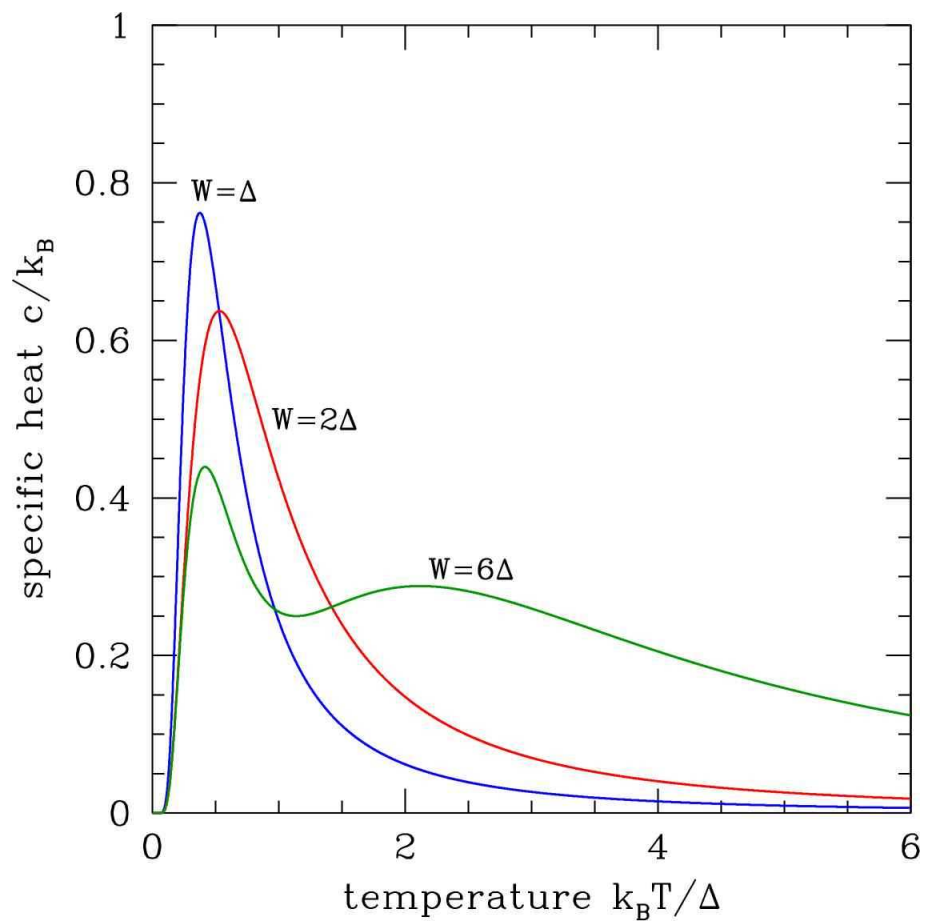


Figure 1: Specific heat $c(T)$ for $W = \Delta$, $W = 2\Delta$, and $W = 6\Delta$.

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #7 SOLUTIONS

(1) Calculate, under equilibrium conditions, the number of photons in a cavity of volume 1 m^3 at a temperature of $T = 293 \text{ K}$. Compare this number with the number of ideal gas molecules under the same conditions.

From the notes, eqn. 4.82, we have $n(T) = 20.405 \times (T[\text{K}])^3 \text{ cm}^{-3}$. With a volume $V = 10^6 \text{ cm}^3$, we have $N = 5.13 \times 10^{14}$. For a classical gas at $T = 293 \text{ K}$ and $p = 1 \text{ atm}$, we have

$$N = \frac{pV}{k_B T} = \frac{(1.013 \times 10^5 \text{ Pa})(1.0 \text{ m}^3)}{(1.38 \times 10^{-23} \text{ J/K})(293 \text{ K})} = 2.51 \times 10^{25}. \quad (1)$$

(2) Thanksgiving turkey typically cooks at a temperature of 350° F . Calculate the total electromagnetic energy inside an oven of volume $V = 1.0 \text{ m}^3$ at this temperature. Compare it to the thermal energy of the air in the oven at the same temperature.

The total electromagnetic energy is

$$E = 3pV = \frac{\pi^2}{15} \frac{V (k_B T)^4}{(\hbar c)^3} = 3.78 \times 10^{-5} \text{ J}. \quad (2)$$

For air, which is a diatomic ideal gas, we have $E = \frac{5}{2}pV$. What do we take for p ? If we assume that oven door is closed at an initial temperature of 63° F which is 300 K , then with a final temperature of $350^\circ \text{ F} = 450 \text{ K}$, we have an increase in the absolute temperature by 50%, hence a corresponding pressure increase of 50%. So we set $p = \frac{3}{2} \text{ atm}$ and we have

$$E = \frac{5}{2} \cdot \frac{3}{2} (1.013 \times 10^5 \text{ Pa})(1.0 \text{ m}^3) = 3.80 \times 10^5 \text{ J}, \quad (3)$$

which is about ten orders of magnitude larger.

(3) Let L denote the number of single particle energy levels and N the total number of particles for a given system. Find the number of possible N -particle states $\Omega(L, N)$ for each of the following situations:

(a) Distinguishable particles with $L = 3$ and $N = 3$.

$$\Omega_D(3, 3) = 3^3 = 27.$$

(b) Bosons with $L = 3$ and $N = 3$.

$$\Omega_{BE}(3, 3) = \binom{5}{3} = 10.$$

(c) Fermions with $L = 10$ and $N = 3$.

$$\Omega_{FD}(10, 3) = \binom{10}{3} = 120.$$

(d) Find a general formula for $\Omega_D(L, N)$, $\Omega_{BE}(L, N)$, and $\Omega_{FD}(L, N)$.

The general results are

$$\Omega_D(L, N) = L^N, \quad \Omega_{BE}(L, N) = \binom{N+L-1}{N}, \quad \Omega_{FD}(L, N) = \binom{L}{N}. \quad (4)$$

(4) A species of noninteracting quantum particles in $d = 2$ dimensions has dispersion $\varepsilon(\mathbf{k}) = \varepsilon_0 |\mathbf{k}\ell|^{3/2}$, where ε_0 is an energy scale and ℓ a length.

(a) Assuming the particles are $S = 0$ bosons obeying photon statistics, compute the heat capacity C_V .

The density of states is

$$g(\varepsilon) = \frac{1}{2\pi} \frac{k}{d\varepsilon/dk} = \frac{k^{1/2}}{3\pi\varepsilon_0 \ell^{3/2}} = \frac{\varepsilon^{1/3}}{3\pi\ell^2\varepsilon_0^{4/3}}. \quad (5)$$

The total energy is

$$E = A \int_0^\infty d\varepsilon g(\varepsilon) \frac{\varepsilon}{e^{\varepsilon/k_B T} - 1} \quad (6)$$

$$= \frac{A}{3\pi\ell^2} \Gamma\left(\frac{7}{3}\right) \zeta\left(\frac{7}{3}\right) \frac{(k_B T)^{7/3}}{\varepsilon_0^{4/3}}, \quad (7)$$

where A is the system area. Thus,

$$C_A(T) = \left(\frac{\partial E}{\partial T}\right)_A = \frac{A k_B}{3\pi\ell^2} \Gamma\left(\frac{10}{3}\right) \zeta\left(\frac{7}{3}\right) \left(\frac{k_B T}{\varepsilon_0}\right)^{4/3}. \quad (8)$$

(b) Assuming the particles are $S = 0$ bosons, is there an Bose condensation transition? If yes, compute the condensation temperature $T_c(n)$ as a function of the particle density. If no, compute the low-temperature behavior of the chemical potential $\mu(n, T)$.

The following integral may be useful:

$$\int_0^\infty \frac{u^{s-1} du}{e^u - 1} = \Gamma(s) \sum_{n=1}^\infty n^{-s} \equiv \Gamma(s) \zeta(s),$$

where $\Gamma(s)$ is the gamma function and $\zeta(s)$ is the Riemann zeta-function.

The condition for Bose-Einstein condensation is

$$n = \int_0^\infty d\varepsilon g(\varepsilon) \frac{1}{e^{\varepsilon/k_B T_c} - 1} = \frac{1}{3\pi\ell^2} \Gamma\left(\frac{4}{3}\right) \zeta\left(\frac{4}{3}\right) \left(\frac{k_B T_c}{\varepsilon_0}\right)^{1/3}. \quad (9)$$

Thus,

$$T_c = \frac{\varepsilon_0}{k_B} \left(\frac{3\pi\ell^2 n}{\Gamma\left(\frac{4}{3}\right) \zeta\left(\frac{4}{3}\right)} \right)^3. \quad (10)$$

(5) Recall how we derived the GCE probability distribution based on the maximization of the entropy S under the constraint of fixed average energy E and particle number N .

(a) Show that one obtains the Bose-Einstein distribution $n_\alpha = [e^{\beta(\varepsilon_\alpha - \mu)} - 1]^{-1}$ if one extremizes the entropy function

$$S = -k_B \sum_\alpha [n_\alpha \ln n_\alpha - (1 + n_\alpha) \ln(1 + n_\alpha)]$$

subject to fixed average E and N .

The variation of the entropy is

$$\delta S = -k_B \sum_\alpha \ln\left(\frac{n_\alpha}{1 + n_\alpha}\right) \delta n_\alpha \quad (11)$$

We also have

$$\delta N = \sum_\alpha \delta n_\alpha \quad (12)$$

$$\delta E = \sum_\alpha \varepsilon_\alpha \delta n_\alpha. \quad (13)$$

We then write

$$S^* = S - \lambda_N \left(\sum_\alpha n_\alpha - N \right) - \lambda_E \left(\sum_\alpha \varepsilon_\alpha n_\alpha - E \right) \quad (14)$$

and compute

$$\delta S^* = - \sum_\alpha \left[k_B \ln\left(\frac{n_\alpha}{1 + n_\alpha}\right) + \lambda_N + \lambda_E \varepsilon_\alpha \right] \delta n_\alpha = 0. \quad (15)$$

Setting

$$\lambda_E = \frac{1}{T}, \quad \lambda_N = -\frac{\mu}{T}, \quad (16)$$

we recover the Bose-Einstein distribution,

$$n_\alpha = \frac{1}{e^{(\varepsilon_\alpha - \mu)/k_B T} - 1}. \quad (17)$$

(b) Show that one obtains the Fermi-Dirac distribution $n_\alpha = [e^{\beta(\varepsilon_\alpha - \mu)} + 1]^{-1}$ if one extremizes the entropy function

$$S = -k_B \sum_\alpha [n_\alpha \ln n_\alpha + (1 - n_\alpha) \ln(1 - n_\alpha)]$$

subject to fixed average E and N .

The variation of the entropy is

$$\delta S = -k_B \sum_\alpha \ln\left(\frac{n_\alpha}{1 - n_\alpha}\right) \delta n_\alpha \quad (18)$$

As in the Bose-Einstein case, we have

$$\delta N = \sum_{\alpha} \delta n_{\alpha} \quad (19)$$

$$\delta E = \sum_{\alpha} \varepsilon_{\alpha} \delta n_{\alpha} . \quad (20)$$

We then write

$$S^* = S - \lambda_N \left(\sum_{\alpha} n_{\alpha} - N \right) - \lambda_E \left(\sum_{\alpha} \varepsilon_{\alpha} n_{\alpha} - E \right) \quad (21)$$

and compute

$$\delta S^* = - \sum_{\alpha} \left[k_B \ln \left(\frac{n_{\alpha}}{1 - n_{\alpha}} \right) + \lambda_N + \lambda_E \varepsilon_{\alpha} \right] \delta n_{\alpha} = 0 . \quad (22)$$

Setting

$$\lambda_E = \frac{1}{T} \quad , \quad \lambda_N = -\frac{\mu}{T} , \quad (23)$$

we recover the Bose-Einstein distribution,

$$n_{\alpha} = \frac{1}{e^{(\varepsilon_{\alpha} - \mu)/k_B T} + 1} . \quad (24)$$

(6) Hydrogen (H_2) freezes at 14 K and boils at 20 K under atmospheric pressure. The density of liquid hydrogen is 70 kg/m^3 . Hydrogen molecules are bosons. No evidence has been found for Bose-Einstein condensation of hydrogen. Why not?

If we treat the H_2 molecules as bosons, and we ignore the rotational freedom, which is appropriate at temperatures below $\Theta_{\text{rot}} = 85.4 \text{ K}$, we have

$$T_c = \frac{2\pi\hbar^2}{mk_B} \left(\frac{n}{\zeta(\frac{3}{2})} \right)^{2/3} = 6.1 \text{ K} . \quad (25)$$

Thus, the critical temperature for ideal gas Bose-Einstein condensation is significantly below the freezing temperature for H_2 . The freezing transition into a regular solid preempts any BEC phenomena.

**PHYSICS 140A : STATISTICAL PHYSICS
MIDTERM EXAM : DO ANY TWO PROBLEMS**

(1) For each of the following situations, explain clearly and fully why it is or is not thermodynamically possible.

- (a) Energy function $E(S, V, N) = a S V N$ with a constant. [6 points]
No! $E(\lambda S, \lambda V, \lambda N) = \lambda^3 E(S, V, N)$ is homogeneous of degree 3 – not extensive.
- (b) Equation of state $V = a N p T$ with a constant. [6 points]
No! The isothermal compressibility $\kappa_T = -\frac{1}{V} \left(\frac{\partial V}{\partial p} \right)_T = -1/p$ is negative, which violates $\kappa_T > \kappa_S > 0$.
- (c) A system where $\left(\frac{\partial V}{\partial T} \right)_{p, N} < 0$ over some range of T and p . [6 points]
Yes! Many systems, such as water, contract upon a temperature increase over some range of temperature.
- (d) The phase diagram for a single component system depicted in fig. 1 (left panel). (You only need know that a superfluid is a distinct thermodynamic phase.) [6 points]
No! This one is tricky. From the Clapeyron equation, we have $\left(\frac{dp}{dT} \right)_{\text{coex}} = \frac{\Delta s}{\Delta v}$. Nernst's law says that the entropy of both the solid and superfluid phases must vanish at $T = 0$. Therefore all coexistence curves which intersect the pressure axis at $T = 0$ must do so with zero slope.
- (e) The phase diagram for a single component system in fig. 1 (right panel). (You only need know that BCC, HCP, and FCC solids are distinct phases.) [6 points]
No! The Gibbs phase rule $d = 2 + \sigma - \varphi$ gives the dimension of thermodynamic space over which φ distinct phases among σ species can coexist. For $\sigma = 1$ we have $\varphi \leq 3$, since $d \geq 0$. So four phase coexistence with a single component is impossible.
- (f) $E(S, V, N) = a N^2 V^{-1} \exp(S/Nb)$ with a and b constant. [6 points]
Yes! E is properly extensive and convex. One can derive $E = pV = NbT$, which is the ideal gas law with k_B replaced by b .
- (g) 15 Joules of heat energy are required to raise the temperature of a system by $\Delta T = 1^\circ\text{C}$ at constant volume. 10 Joules of heat energy are required to raise the temperature of the same system by $\Delta T = 1^\circ\text{F}$ at constant pressure. [6 points]
Yes! The heat capacity at constant volume is $C_V = \left(\frac{dQ}{dT} \right)_V = 15 \text{ J/K}$. The heat capacity at constant pressure is $C_p = \left(\frac{dQ}{dT} \right)_p = 10 \text{ J} / \frac{5}{9} \text{ K} = 18 \text{ J/K}$. Stability requires $C_p > C_V$, which is satisfied.
- (h) A heat engine operating between reservoirs at temperatures $T_1 = 400 \text{ K}$ and $T_2 = 600 \text{ K}$. During each cycle, the engine does work $W = 300 \text{ J}$ and the entropy of the upper reservoir decreases by 2.00 J/K . [8 points]
Yes! The only possible obstacle here is whether the engine's efficiency is greater than

that of the corresponding Carnot cycle, for which $\eta_C = 1 - \frac{T_1}{T_2} = \frac{1}{3}$. We have $\eta = \frac{W}{Q_2}$ and $\Delta S_2 = -\frac{Q_2}{T_2}$. Thus, $\eta = W/[T_2(-\Delta S_2)] = 300 \text{ J}/[(600 \text{ K})(2.00 \text{ J/K})] = \frac{1}{4} < \eta_C$.

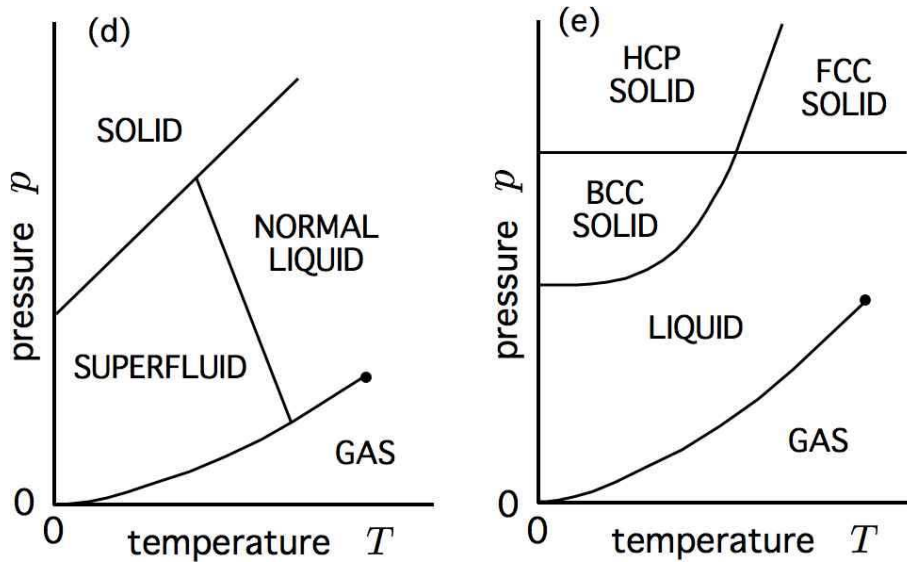


Figure 1: Phase diagrams for parts (d) and (e) of problem 1.

(2) A thermodynamic system obeys

$$E(S, V, N) = \frac{aS^4}{NV^2}.$$

(a) Find $T(S, V, N)$. [10 points]

We have

$$T = \left(\frac{\partial E}{\partial S} \right)_{V, N} = \frac{4aS^3}{NV^2}.$$

(b) Find $p(T, V, N)$. [10 points]

To obtain the equation of state $p = p(T, V, N)$, we first have to find

$$p = - \left(\frac{\partial E}{\partial V} \right)_{S, N} = \frac{2aS^4}{NV^3}$$

then eliminate S . Clearly

$$\frac{T^4}{p^3} = \frac{256 a^4 S^{12}}{N^4 V^8} \cdot \frac{N^3 V^9}{8 a^3 S^{12}} = 32 a \frac{V}{N}.$$

(c) Find $\mu(T, p)$. [10 points]

$$\mu = \left(\frac{\partial E}{\partial N} \right)_{S, V} = -\frac{aS^4}{N^2V^2}.$$

Eliminating the S^4 term by dividing this by the expression for p , we have

$$\frac{\mu}{p} = -\frac{aS^4}{N^2V^2} \cdot \frac{NV^3}{2aS^4} = \frac{V}{2N} = \frac{T^4}{64ap^3}.$$

Note that we used the equation of state to eliminate the ratio V/N in terms of the other intensive variables T and p . Thus,

$$\mu(T, p) = \frac{T^4}{64ap^2}.$$

(d) Suppose the volume is isothermally expanded by a factor of eight ($V \rightarrow 8V$ at constant T). Then the temperature is isobarically increased by a factor of two ($T \rightarrow 2T$ at constant p). By what factor does the entropy change? Be sure to indicate whether S increases or decreases. [10 points]

From part (a) we have $S(T, V, N) = (NV^2T/4a)^{1/3}$, hence isothermal expansion by a factor of eight leads to a quadrupling ($8^{2/3}$) of the entropy. We next need $S(T, p, N)$, which we obtain by eliminating V using part (b):

$$\frac{T^3}{p^2} = \frac{64a^3S^9}{N^3V^6} \cdot \frac{N^2V^6}{4a^2S^8} = \frac{16aS}{N}.$$

Thus, $S(T, p, N) = NT^3/16ap^2$, and an isobaric temperature increase by a factor of two will lead to an eightfold (2^3) increase in the entropy. Overall, the two processes result in an increase in the entropy by a factor of 32.

(e) A volume $V = 10$ ml at pressure $p = 2.0$ bar and temperature $T = 800$ K is adiabatically expanded to a volume $V = 40$ ml. How much work does W the system do during the expansion? What is the system's final temperature? [10 points]

In an adiabatic process, $W = -\Delta E$. In our case, $\Delta E = -\frac{15}{16} \frac{aS^4}{NV^2}$, where V is the initial volume. Now above in part (b) we found $p = 2aS^4/NV^3$, hence $W = -\Delta E = \frac{15}{32} pV = \frac{15}{16}$ J.

(3) Consider the equilibrium between a single component gas (assumed ideal and diatomic) and a solution of it in a liquid or solid solvent. Let μ_g denote the chemical potential of the gas molecules in the gas, and μ_s their chemical potential in solution.

(a) What are the conditions for thermal, mechanical, and chemical equilibrium of the gas and solute? [10 points]

Thermal equilibrium means T is constant throughout. Mechanical equilibrium means p/T is constant throughout. Chemical equilibrium means μ/T is constant throughout, where μ is the chemical potential of the solute.

- (b) Let $\psi(T, p)$ be the Gibbs free energy of a single solvent molecule in the liquid, *i.e.* without the entropy of mixing term. If the concentration of solute is x , what is the chemical potential $\mu_s(T, p)$, *i.e.* when the entropy of mixing term is included? You may assume $x \ll 1$. [10 points]

Let N_0 be the number of solvent molecules and N_s the number of solute molecules in the liquid. The entropy of mixing is

$$S_{\text{mix}} = -k_B \left[N_0 \ln \left(\frac{N_0}{N_0 + N_s} \right) + N_s \ln \left(\frac{N_s}{N_0 + N_s} \right) \right] \\ \approx -k_B N_s \ln \left(\frac{N_s}{e N_0} \right).$$

Thus, since $G = N_s \psi(T, p) - T S_{\text{mix}}$,

$$\mu_s(T, p) = \psi(T, p) - \frac{\partial}{\partial N_s} (T S_{\text{mix}}) \\ = \psi(T, p) + k_B T \ln x.$$

- (c) For an ideal gas, one has $\mu(T, p) = k_B T \left(\chi(p) - \left(\frac{1}{2}f + 1\right) \ln T \right)$, where f is the familiar number of relevant ‘degrees of freedom’ per molecule and $\chi(p)$ is a function of p alone. Determine $\chi(p)$. [10 points]

We have, using a Maxwell relation deriving from the exactness of dG ,

$$\left(\frac{\partial \mu}{\partial p} \right)_{T, N} = \left(\frac{\partial V}{\partial N} \right)_{T, p} = \frac{V}{N} = \frac{k_B T}{p}.$$

This says

$$\frac{\partial}{\partial p} \chi(p) = \frac{1}{p} \implies \chi(p) = \ln p + \chi_0,$$

where χ_0 is a constant.

- (d) In liquids, the dependence of $\psi(T, p)$ on p typically is weak. Assuming $\psi(T, p) = \psi(T)$, find an expression for $x(T, p)$ in equilibrium. [10 points]

Applying the condition of equilibrium between solute and vapor, we have

$$\chi_0 + \ln p - \left(\frac{1}{2}f + 1\right) \ln T = \frac{\psi(T)}{k_B T} + \ln x.$$

Exponentiating, we have

$$x(T, p) = A p T^{-\left(\frac{1}{2}f + 1\right)} e^{-\psi(T)/k_B T},$$

where $A = \exp(\chi_0)$ is a constant which also makes the units work out.

- (e) Suppose we further neglect the temperature dependence of ψ and write simply $\psi(T) = \psi_0$, where ψ_0 is a positive constant. Sketch $x(T, p)$ versus temperature at constant pressure. Be sure to identify any relevant features, such as maxima, minima, vanishings, etc. [10 points]

The $T^{-(\frac{1}{2}f+1)}$ factor diverges as $T \rightarrow 0$ and vanishes as $T \rightarrow \infty$. For $\psi(T) = \psi_0$ a constant, the quantity $e^{-\psi_0/k_B T}$ vanishes essentially at $T = 0$, and overwhelms the power law divergence of the prefactor. As $T \rightarrow \infty$, $e^{-\psi_0/k_B T} \rightarrow 1$. Thus, there is a maximum concentration, which, after differentiating $\ln x$, is found to occur at $k_B T^* = \psi_0 / (\frac{1}{2}f + 1) = \frac{2}{7}\psi_0$. See fig. 2 for a plot.

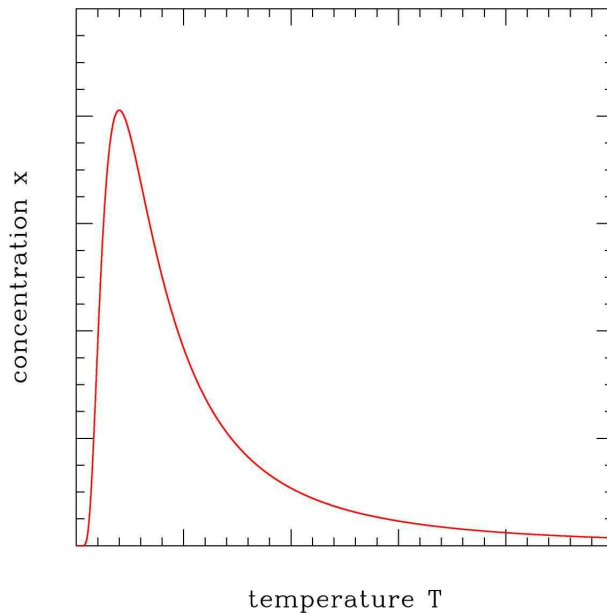


Figure 2: Concentration versus temperature for problem (3e).

PHYSICS 140A : STATISTICAL PHYSICS
PRACTICE FINAL EXAM
 105 POINTS TOTAL

(1) A pair of spins is described by the Hamiltonian

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

where S takes values $-1, 0$, or $+1$ (three possibilities) and σ takes values ± 1 but not 0 (two possibilities).

- (a) Find the partition function $Z(T, H)$. [10 points]
- (b) Find the magnetization $M(T, H)$. [10 points]
- (c) Find the zero field magnetic susceptibility, $\chi(T) = (\partial M / \partial H)_{H=0}$. [10 points]
- (d) Provide a physical interpretation of your result for $\chi(T)$ in the limits $J \rightarrow 0$ and $J \rightarrow \infty$. [5 points]

Solution : The partition function is

$$Z = \text{Tr} e^{-\beta \hat{h}} = \sum_S \sum_{\sigma} e^{-E(S, \sigma) / k_B T}. \quad (2)$$

It helps to make a little table of the energy values: From this we obtain

E	$S = +1$	$S = 0$	$S = -1$
$\sigma = +1$	$-J - 2\mu_0 H$	$-\mu_0 H$	J
$\sigma = -1$	J	$\mu_0 H$	$-J + 2\mu_0 H$

Table 1: Energy $E(S, \sigma)$ for the Hamiltonian of eqn. 1.

$$Z(T, H) = 2 e^{J/k_B T} \cosh\left(\frac{2\mu_0 H}{k_B T}\right) + 2 \cosh\left(\frac{\mu_0 H}{k_B T}\right) + 2 e^{-J/k_B T} \quad (3)$$

The magnetization is

$$\begin{aligned} M &= - \left(\frac{\partial F}{\partial H} \right)_T = \frac{k_B T}{Z} \frac{\partial Z}{\partial H} \\ &= \frac{2\mu_0 e^{J/k_B T} \sinh\left(\frac{2\mu_0 H}{k_B T}\right) + \mu_0 \sinh\left(\frac{\mu_0 H}{k_B T}\right)}{e^{J/k_B T} \cosh\left(\frac{2\mu_0 H}{k_B T}\right) + \cosh\left(\frac{\mu_0 H}{k_B T}\right) + e^{-J/k_B T}}. \end{aligned} \quad (4)$$

To find the zero field susceptibility, we first expand M to lowest order in the field H :

$$M(T, H) = \frac{\mu_0^2}{k_B T} \cdot \frac{4 e^{J/k_B T} + 1}{1 + e^{J/k_B T} + e^{-J/k_B T}} \cdot H + \mathcal{O}(H^2). \quad (5)$$

Thus,

$$\chi(T) = \left. \frac{\partial M}{\partial H} \right|_{H=0} = \frac{\mu_0^2}{k_B T} \cdot \frac{4 e^{J/k_B T} + 1}{1 + e^{J/k_B T} + e^{-J/k_B T}}. \quad (6)$$

We now examine some limits:

$$\chi(T) = \begin{cases} 4\mu_0^2/k_B T & J \rightarrow \infty \\ 5\mu_0^2/3k_B T & J \rightarrow 0 \\ \mu_0^2 e^{-|J|/k_B T}/k_B T & J \rightarrow -\infty. \end{cases} \quad (7)$$

In the case $J \rightarrow \infty$, the spins are ferromagnetically locked, and the only allowed configurations are $|S, \sigma\rangle = |1, 1\rangle$ and $|S, \sigma\rangle = |-1, -1\rangle$. The magnetization in these states is $M = \pm 2\mu_0$, respectively, hence the system acts as a single spin- $\frac{1}{2}$ object with effective magnetic moment $\tilde{\mu}_0 = 2\mu_0$. The Curie susceptibility is then $\tilde{\mu}_0^2/k_B T = 4\mu_0^2/k_B T$.

When $J = 0$, the S and σ spins are independent. The σ spin gives a contribution $\mu_0^2/k_B T$ to the susceptibility. The S spin's contribution is $2\mu_0^2/3k_B T$, because only $\frac{2}{3}$ of the states have a moment; the $S = 0$ state doesn't contribute to the susceptibility.

When $J \rightarrow -\infty$, the spins are locked antiferromagnetically, meaning the only allowed configurations are $|S, \sigma\rangle = |1, -1\rangle$ and $|S, \sigma\rangle = |-1, 1\rangle$, neither of which has a net magnetic moment. Thus, $\chi = 0$. If we consider large but finite $|J|$, then higher energy states contribute, with exponentially small Boltzmann weights, leading to an exponentially suppressed susceptibility, as we find by explicit calculation.

(2) A three-dimensional ($d = 3$) system has excitations with dispersion $\varepsilon(\mathbf{k}) = A|\mathbf{k}|^{4/3}$. There is no internal degeneracy ($g = 1$), and the excitations are noninteracting.

- (a) Find the density of states $g(\varepsilon)$ for this excitation branch. [15 points]
- (b) If the excitations obey photon statistics (*i.e.* $\mu = 0$), find $C_V(T)$. [10 points]
- (c) If the excitations obey Bose-Einstein statistics, show that the system undergoes Bose-Einstein condensation. Find the critical temperature $T_c(n)$, where n is the number density of the excitations. [10 points]

Solution : We have

$$g(\varepsilon) = \frac{g}{2\pi^2} \frac{k^2}{d\varepsilon/dk} = \frac{3}{8\pi^2 A} k^{5/3} = \frac{3}{8\pi^2} A^{-9/4} \varepsilon^{5/4} \Theta(\varepsilon). \quad (8)$$

If the particles obey photon statistics, the average energy is

$$E(T) = V \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \frac{\varepsilon}{e^{\varepsilon/k_B T} - 1}. \quad (9)$$

Substituting the expression for $g(\varepsilon)$ into this equation, we have

$$\begin{aligned} E(T) &= \frac{3V}{8\pi^2 A^{9/4}} \int_0^{\infty} d\varepsilon \frac{\varepsilon^{9/4}}{e^{\varepsilon/k_B T} - 1} \\ &= \frac{3V}{8\pi^2} \Gamma\left(\frac{13}{4}\right) \zeta\left(\frac{13}{4}\right) \frac{(k_B T)^{13/4}}{A^{9/4}}. \end{aligned} \quad (10)$$

Here, we've used the result

$$\int_0^{\infty} dt \frac{t^{\nu-1}}{e^t - 1} = \Gamma(\nu) \zeta(\nu). \quad (11)$$

We therefore have

$$C_V(T) = \left(\frac{\partial E}{\partial T} \right)_V = \frac{3V}{8\pi^2} \Gamma\left(\frac{17}{4}\right) \zeta\left(\frac{13}{4}\right) \left(\frac{k_B T}{A} \right)^{9/4}. \quad (12)$$

If the particles are bosons with $\mu \neq 0$, then we write

$$N(T, \mu) = V \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \frac{1}{z^{-1} e^{\varepsilon/k_B T} - 1}, \quad (13)$$

where $z = \exp(\mu/k_B T)$ is the fugacity. Condensation occurs when $z = 1$, hence

$$n = \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \frac{1}{e^{\varepsilon/k_B T_c} - 1} = \frac{3}{8\pi^2} \Gamma\left(\frac{9}{4}\right) \zeta\left(\frac{9}{4}\right) \left(\frac{k_B T_c}{A} \right)^{9/4}. \quad (14)$$

Thus,

$$T_c = \frac{A}{k_B} \left(\frac{8\pi^2 n}{3\Gamma\left(\frac{9}{4}\right) \zeta\left(\frac{9}{4}\right)} \right)^{4/9}. \quad (15)$$

(3) Consider a *two-dimensional* ($d = 2$) gas of relativistic particles with dispersion

$$\varepsilon(\mathbf{p}) = \sqrt{\mathbf{p}^2 c^2 + m^2 c^4}.$$

The particles are classical, *i.e.* they obey Maxwell-Boltzmann statistics.

- (a) Find the single particle partition function $\zeta(T, A)$ (A is the area of the system). You may find the substitution $p = mc \sinh \theta$ to be helpful at some stage. [10 points]

- (b) Find the entropy $S(T, A, N)$. [10 points]
- (c) Find the heat capacity (at constant area) per particle, $\tilde{c}(T) = C_A/N$. [10 points]
- (d) Which is the Dulong-Petit limit: $mc^2 \gg k_B T$ or $mc^2 \ll k_B T$, and why? Verify that your $\tilde{c}(T)$ has the correct asymptotic behavior. [5 points]

Solution : The single particle partition function for a system of area A is

$$\begin{aligned}\zeta(T, A) &= A \int \frac{d^2p}{h^2} e^{-\beta\sqrt{p^2c^2+m^2c^4}} = \frac{2\pi A}{h^2} \int_0^\infty dp p e^{-\beta\sqrt{p^2c^2+m^2c^4}} \\ &= \frac{A}{2\pi} \left(\frac{mc}{\hbar}\right)^2 \int_0^\infty d\theta \sinh(\theta) \cosh(\theta) e^{-\beta mc^2 \cosh(\theta)} \\ &= \frac{A}{2\pi} \left(\frac{mc}{\hbar}\right)^2 \int_1^\infty dx x e^{-\beta mc^2 x}\end{aligned}\tag{16}$$

$$= \frac{A}{2\pi} \left(\frac{mc}{\hbar}\right)^2 \left(\frac{k_B T}{mc^2}\right) \left(1 + \frac{k_B T}{mc^2}\right) e^{-mc^2/k_B T}.\tag{17}$$

Note that

$$\int_1^\infty dx x e^{-\alpha x} = -\frac{d}{d\alpha} \int_1^\infty dx e^{-\alpha x} = -\frac{d}{d\alpha} \left(\frac{e^{-\alpha}}{\alpha}\right) = \frac{1}{\alpha} \left(1 + \frac{1}{\alpha}\right) e^{-\alpha}.\tag{18}$$

The free energy for N indistinguishable classical particles is then

$$\begin{aligned}F(T, A, N) &= -k_B T \ln Z(T, A, N) = -k_B T \ln \left(\frac{\zeta^N}{N!}\right) = -Nk_B T \ln \left(\frac{\zeta}{N}\right) + Nk_B T \\ &= N(mc^2 + k_B T) - Nk_B T \ln \left[\frac{A}{2\pi N} \left(\frac{mc}{\hbar}\right)^2\right] \\ &\quad - Nk_B T \ln \left(\frac{k_B T}{mc^2}\right) - Nk_B T \ln \left(1 + \frac{k_B T}{mc^2}\right).\end{aligned}\tag{19}$$

Thus, the entropy is

$$\begin{aligned}S &= -\left(\frac{\partial F}{\partial T}\right)_{A,N} = Nk_B \ln \left(\frac{k_B T}{mc^2}\right) + Nk_B \ln \left(1 + \frac{k_B T}{mc^2}\right) \\ &\quad + Nk_B \cdot \frac{k_B T}{mc^2 + k_B T} + Nk_B \ln \left[\frac{A}{2\pi N} \left(\frac{mc}{\hbar}\right)^2\right].\end{aligned}\tag{20}$$

Accordingly, the specific heat is

$$\tilde{c}(T) = \frac{1}{N} \cdot T \left(\frac{\partial S}{\partial T}\right)_{A,N} = k_B + \frac{k_B^2 T}{mc^2 + k_B T} + \frac{mc^2 k_B^2 T}{(mc^2 + k_B T)^2}.\tag{21}$$

The Dulong-Petit limit is the nonrelativistic limit $mc^2 \gg k_B T$. In this case, $\tilde{c}(T) \rightarrow k_B$, corresponding to $\frac{1}{2}k_B$ per quadratic degree of freedom in the Hamiltonian, of which there are two: p_x and p_y . Note that the ultrarelativistic limit $mc^2 \ll k_B T$ results in $\tilde{c}(T) \rightarrow 2k_B$. This is also expected, because for a variable q which enters the energy as $\mathcal{C}|q|$, the contribution to the partition function is a factor $\int dq e^{-\mathcal{C}|q|/k_B T} = 2k_B T/\mathcal{C}$, resulting in a contribution of $\Delta F = -k_B T \ln(2k_B T/\mathcal{C})$ to the free energy and $-T \partial^2(\Delta F)/\partial T^2 = k_B$ to the heat capacity.

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

$$\hat{h} = \Delta S^2 - \mu_0 H S,$$

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,

$$\zeta = \text{Tr} e^{-\beta \hat{h}} = 1 + 2 e^{-\Delta/k_B T} \cosh\left(\frac{\mu_0 H}{k_B T}\right). \quad (1)$$

Thus,

$$(a) \quad F = -N k_B T \ln \zeta = -N k_B T \ln \left[1 + 2 e^{-\Delta/k_B T} \cosh\left(\frac{\mu_0 H}{k_B T}\right) \right] \quad (2)$$

The magnetization is

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

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

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

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

$$(d) \quad S = -\frac{\partial F}{\partial T} = N k_B \ln(1 + 2 e^{-\Delta/k_B T}) + \frac{N \Delta}{T} \cdot \frac{1}{2 + e^{\Delta/k_B T}} \quad (5)$$

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

$$\varepsilon_A(\mathbf{p}) = \frac{\mathbf{p}^2}{2m} \quad , \quad \varepsilon_B(\mathbf{p}) = \frac{\mathbf{p}^2}{4m} - \Delta .$$

In other words, $m_A = m$ and $m_B = 2m$, and there is an additional energy offset $-\Delta$ associated with the B species.

- (a) Find the grand potential $\Omega(T, V, \mu_A, \mu_B)$.
[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:

$$(a) \quad \boxed{\Omega = -Vk_B T \lambda_T^{-3} e^{\mu_A/k_B T} - 2^{3/2} V k_B T \lambda_T^{-3} e^{(\mu_B + \Delta)/k_B T}} \quad (6)$$

Here, we have defined the thermal wavelength for the A species as $\lambda_T \equiv \lambda_{T,A} = \sqrt{2\pi\hbar^2/mk_B T}$. 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

$$n_A = -\frac{1}{V} \cdot \frac{\partial \Omega}{\partial \mu_A} = V \lambda_T^{-3} e^{\mu_A/k_B T} \quad (7)$$

$$n_B = -\frac{1}{V} \cdot \frac{\partial \Omega}{\partial \mu_B} = 2^{3/2} V \lambda_T^{-3} e^{(\mu_B + \Delta)/k_B T} . \quad (8)$$

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

$$(b) \quad \boxed{n_A \lambda_T^3 = e^{\mu/k_B T}} \quad (9)$$

and

$$(b) \quad \boxed{n_B \lambda_T^3 = 2^{3/2} e^{(2\mu + \Delta)/k_B T}} \quad (10)$$

The relation we seek is therefore

$$(c) \quad n_B = 2^{3/2} (n_A \lambda_T^3)^2 e^{\Delta/k_B T} \quad (11)$$

If we initially have $n_A = n$ and $n_B = 0$, then in general we must have

$$n_A + 2n_B = n \quad \implies \quad n_B = \frac{1}{2}(n - n_A). \quad (12)$$

Thus, eliminating n_B , we have a quadratic equation,

$$2^{3/2} \lambda_T^3 e^{\Delta/k_B T} n_A^2 = \frac{1}{2}(n - n_A), \quad (13)$$

the solution of which is

$$(d) \quad n_A = \frac{-1 + \sqrt{1 + 16\sqrt{2} n \lambda_T^3 e^{\Delta/k_B T}}}{8\sqrt{2} \lambda_T^3 e^{\Delta/k_B T}} \quad (14)$$

(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, $g(\varepsilon)$. 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,

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

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

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

The energy is then

$$\begin{aligned}
 E &= V \int_0^{\infty} d\varepsilon g(\varepsilon) \frac{\varepsilon}{e^{\varepsilon/k_B T} - 1} \\
 &= \frac{3V}{4\pi^2} \Gamma\left(\frac{11}{2}\right) \zeta\left(\frac{11}{2}\right) \frac{(k_B T)^{11/2}}{A^{9/2}}.
 \end{aligned} \tag{17}$$

Thus,

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

The pressure is

$$\begin{aligned}
 p &= -\frac{\Omega}{V} = -k_B T \int_0^{\infty} d\varepsilon g(\varepsilon) \ln(1 - e^{-\varepsilon/k_B T}) \\
 &= -k_B T \int_0^{\infty} d\varepsilon \frac{3}{4\pi^2} \frac{\varepsilon^{7/2}}{A^{9/2}} \ln(1 - e^{-\varepsilon/k_B T}) \\
 &= -\frac{3}{4\pi^2} \frac{(k_B T)^{11/2}}{A^{9/2}} \int_0^{\infty} ds s^{7/2} \ln(1 - e^{-s}) \\
 &= \frac{3V}{4\pi^2} \Gamma\left(\frac{9}{2}\right) \zeta\left(\frac{11}{2}\right) \frac{(k_B T)^{11/2}}{A^{9/2}}.
 \end{aligned} \tag{19}$$

Thus,

$$\text{(c) } \boxed{\frac{E}{pV} = \frac{\Gamma\left(\frac{11}{2}\right)}{\Gamma\left(\frac{9}{2}\right)} = \frac{9}{2}} \tag{21}$$

To find T_c for BEC, we set $z = 1$ (i.e. $\mu = 0$) and $n_0 = 0$, and obtain

$$n = \int_0^{\infty} d\varepsilon g(\varepsilon) \frac{\varepsilon}{e^{\varepsilon/k_B T_c} - 1} \tag{22}$$

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

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

and therefore

$$\text{(d) } \boxed{T_c = \frac{A}{k_B} \left(\frac{4\pi^2 n}{3\Gamma\left(\frac{9}{2}\right) \zeta\left(\frac{9}{2}\right)}\right)^{2/9}} \tag{24}$$

(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 $\dot{\varphi} = \mathbf{X}(\varphi)$ this requires that the phase space divergence vanish: $\nabla \cdot \mathbf{X} = 0$.

(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

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

$$\langle f(\varphi) \rangle_S = \int d\mu \varrho(\varphi) f(\varphi), \quad (26)$$

where $\varrho(\varphi)$ is a phase space distribution. For the microcanonical ensemble,

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

(c) What is the microcanonical ensemble? [3 points]

The microcanonical ensemble is defined by the phase space probability distribution $\varrho(\varphi) = \delta(E - H(\varphi))$, 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 fermions is $\Omega_{\text{FD}}(L, N) = \binom{L}{N}$, so we have $\Omega = \binom{6}{3} = 20$.

(f) Explain how the Maxwell-Boltzmann limit results, starting from the expression for $\Omega_{\text{BE/FD}}(T, V, \mu)$. [3 points]

We have

$$\Omega_{\text{BE/FD}} = \pm k_B T \sum_{\alpha} \ln(1 \mp z e^{-\epsilon_{\alpha}/k_B T}). \quad (28)$$

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

$$\Omega_{\text{BE/FD}} \longrightarrow \Omega_{\text{MB}} = -k_B T \sum_{\alpha} e^{(\mu - \epsilon_{\alpha})/k_B T}, \quad (29)$$

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

- (g) For the Dieterici equation of state, $p(1 - bn) = nk_{\text{B}}T \exp(-an/k_{\text{B}}T)$, find the second virial coefficient $B_2(T)$. [3 points]

We must expand in powers of the density n :

$$\begin{aligned} p &= nk_{\text{B}}T \frac{e^{-an/k_{\text{B}}T}}{1 - bn} = nk_{\text{B}}T \left(1 - \frac{an}{k_{\text{B}}T} + \dots \right) (1 + bn + \dots) \\ &= nk_{\text{B}}T + (bk_{\text{B}}T - a)n^2 + \mathcal{O}(n^3). \end{aligned} \quad (30)$$

The virial expansion of the equation of state is

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

and so we identify

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

- (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 $g(\varepsilon) = C_{\text{E}} \delta(\varepsilon - \varepsilon_0)$, while for the Debye model one has $g(\varepsilon) = C_{\text{D}} \varepsilon^2 \Theta(\varepsilon_{\text{D}} - \varepsilon)$, where $C_{\text{E,D}}$ are constants, and ε_{D} is a cutoff known as the Debye energy. At high temperatures, both models yield a Dulong-Petit heat capacity of $3Nk_{\text{B}}$, 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.

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #1 SOLUTIONS

(1) Consider a two-dimensional gas of fermions which obey the dispersion relation

$$\varepsilon(\mathbf{k}) = \varepsilon_0 \left((k_x^2 + k_y^2) a^2 + \frac{1}{2} (k_x^4 + k_y^4) a^4 \right) .$$

Sketch, on the same plot, the Fermi surfaces for $\varepsilon_F = 0.1 \varepsilon_0$, $\varepsilon_F = \varepsilon_0$, and $\varepsilon_F = 10 \varepsilon_0$.

Solution : It is convenient to adimensionalize, writing

$$x \equiv k_x a \quad , \quad y \equiv k_y a \quad , \quad \nu \equiv \frac{\varepsilon}{\varepsilon_0} . \tag{1}$$

Then the equation for the Fermi surface becomes

$$x^2 + y^2 + \frac{1}{2} x^4 + \frac{1}{2} y^4 = \nu . \tag{2}$$

In other words, we are interested in the *level sets* of the function $\nu(x, y) \equiv x^2 + y^2 + \frac{1}{2} x^4 + \frac{1}{2} y^4$. When ν is small, we can ignore the quartic terms, and we have an isotropic dispersion, with $\nu = x^2 + y^2$. *I.e.* we can write $x = \nu^{1/2} \cos \theta$ and $y = \nu^{1/2} \sin \theta$. The quartic terms give a contribution of order ν^4 , which is vanishingly small compared with the quadratic term in the $\nu \rightarrow 0$ limit. When $\nu \sim \mathcal{O}(1)$, the quadratic and quartic terms in the dispersion are of the same order of magnitude, and the continuous $O(2)$ symmetry, namely the symmetry under rotation by any angle, is replaced by a discrete symmetry group, which is the group of the square, known as C_{4v} in group theory parlance. This group has eight elements:

$$\{ \mathbb{I} , R , R^2 , R^3 , \sigma , \sigma R , \sigma R^2 , \sigma R^3 \} \tag{3}$$

Here R is the operation of counterclockwise rotation by 90° , sending (x, y) to $(-y, x)$, and σ is reflection in the y -axis, which sends (x, y) to $(-x, y)$. One can check that the function $\nu(x, y)$ is invariant under any of these eight operations from C_{4v} .

Explicitly, we can set $y = 0$ and solve the resulting quadratic equation in x^2 to obtain the maximum value of x , which we call $a(\nu)$. One finds

$$\frac{1}{2} x^4 + x^2 - \nu = 0 \quad \implies \quad a = \sqrt{\sqrt{1 + 2\nu} - 1} . \tag{4}$$

So long as $x \in \{-a, a\}$, we can solve for $y(x)$:

$$y(x) = \pm \sqrt{\sqrt{1 + 2\nu - 2x^2 - x^4} - 1} . \tag{5}$$

A sketch of the level sets, showing the evolution from an isotropic (*i.e.* circular) Fermi surface at small ν , to surfaces with discrete symmetries, is shown in fig. 1.

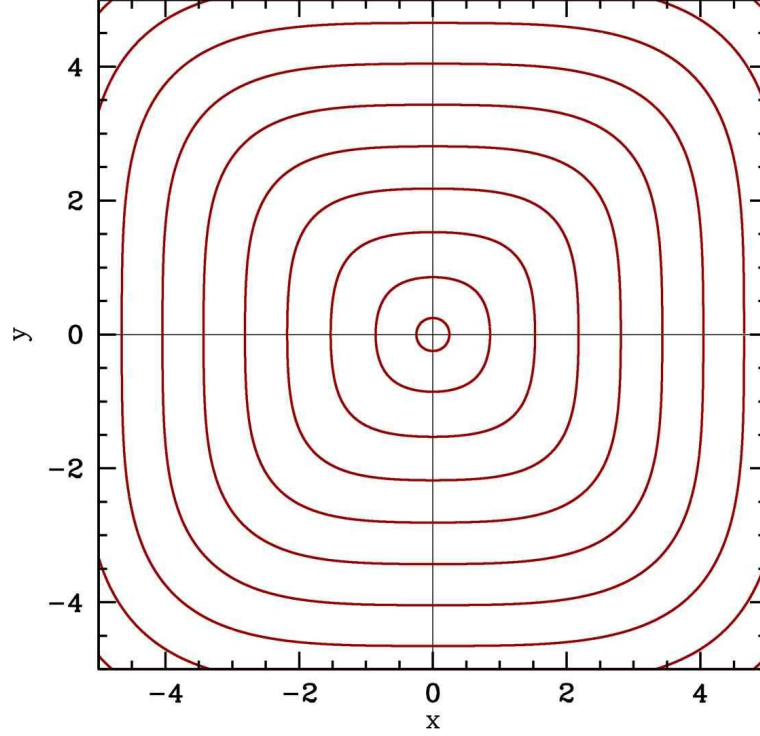


Figure 1: Level sets of the function $\nu(x, y) = x^2 + y^2 + \frac{1}{2}x^4 + \frac{1}{2}y^4$ for $\nu = (\frac{1}{2}n)^4$, with positive integer n .

(2) Using the Sommerfeld expansion, compute the heat capacity for a two-dimensional electron gas, to lowest nontrivial order in the temperature T .

Solution : In the notes, in section 4.7.6, we obtained the result

$$\frac{E}{V} = \int_{-\infty}^{\epsilon_F} d\epsilon g(\epsilon) \epsilon + \frac{\pi^2}{6} (k_B T)^2 g(\epsilon_F) + \mathcal{O}(T^4). \quad (6)$$

This entails a heat capacity of $C_{V,N} = V \cdot \frac{1}{3}\pi^2 k_B g(\epsilon_F) \cdot k_B T$. The density of states at the Fermi level, $g(\epsilon_F)$, is easily found to be

$$g(\epsilon_F) = \frac{d}{2} \cdot \frac{n}{\epsilon_F}. \quad (7)$$

Thus,

$$C_{V,N} = N \cdot \frac{d\pi^2}{6} k_B \cdot \left(\frac{k_B T}{\epsilon_F} \right), \quad (8)$$

a form which is valid in any spatial dimension d .

(3) ${}^3\text{He}$ atoms consist of an odd number of fermions (two electrons, two protons, and one neutron), and hence is itself a fermion. Consider a kilomole of ${}^3\text{He}$ atoms at standard temperature and pressure ($T = 293$, K, $p = 1$ atm).

- (a) What is the Fermi temperature of the gas?
- (b) Calculate $\mu/k_B T$ and $\exp(-\mu/k_B T)$.
- (c) Find the average occupancy $n(\varepsilon)$ of a single particle state with energy $\frac{3}{2}k_B T$.

Solution : Assuming the gas is essentially classical (this will be justified shortly), we find the gas density using the ideal gas law:

$$n = \frac{p}{k_B T} = \frac{1.013 \times 10^5 \text{ Pa}}{(1.38 \times 10^{-23} \text{ J/K})(293 \text{ K})} = 2.51 \times 10^{25} \text{ m}^{-3}. \quad (9)$$

It is convenient to compute the rest energy of a ${}^3\text{He}$ atom. The mass is 3.016 amu (look it up on Google), hence

$$m_3 c^2 = 3.016 \cdot (931.5 \text{ MeV}) = 2.809 \text{ GeV}. \quad (10)$$

For the conversion of amu to MeV/c^2 , again try googling. We'll then need $\hbar c = 1973 \text{ eV} \cdot \text{\AA}$. I remember 1973 because that was the summer I won third prize in an archery contest at Camp Mehakeno. Thus,

$$\begin{aligned} \varepsilon_F &= \frac{(\hbar c)^2}{2m_3 c^2} \cdot (3\pi^2 n)^{2/3} = \frac{(1973 \text{ eV} \cdot \text{\AA})^2}{2.809 \times 10^9 \text{ eV}} \cdot (3\pi^2 \cdot 2.51 \times 10^{25} \text{ m}^{-3})^{2/3} \\ &= 1.14 \times 10^{-5} \text{ eV}. \end{aligned} \quad (11)$$

Now with $k_B = 86.2 \mu\text{eV}/\text{K}$, we have $T_F = \varepsilon_F/k_B = 0.13 \text{ K}$.

Within the GCE, the fugacity is given by $z = n\lambda_T^3$. The thermal wavelength is

$$\lambda_T = \left(\frac{2\pi\hbar^2}{mk_B T} \right)^{1/2} = \left(\frac{2\pi \cdot (1973 \text{ eV} \cdot \text{\AA})^2}{(2.809 \times 10^9 \text{ eV}) \cdot (86.2 \times 10^{-6} \text{ eV/K}) \cdot (293 \text{ K})} \right)^{1/2} = 0.587 \text{\AA}, \quad (12)$$

hence

$$z = n\lambda_T^3 = (2.51 \times 10^{-5} \text{\AA}^{-3}) \cdot (0.587 \text{\AA})^3 = 5.08 \times 10^{-6}. \quad (13)$$

Thus,

$$\frac{\mu}{k_B T} = \ln z = -12.2, \quad e^{-\mu/k_B T} = z^{-1} = 1.97 \times 10^5. \quad (14)$$

To find the occupancy $f(\varepsilon - \mu)$, we note $\varepsilon - \mu = \left[\frac{3}{2} - (-12.2) \right] k_B T = 13.7 k_B T$, in which case

$$n(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} + 1} = \frac{1}{e^{13.7} + 1} = 1.12 \times 10^{-6}. \quad (15)$$

(4) For ideal Fermi gases in $d = 1, 2,$ and 3 dimensions, compute at $T = 0$ the average energy per particle E/N in terms of the Fermi energy ε_F .

Solution: The number of particles is

$$N = g V \int \frac{d^d k}{(2\pi)^d} \Theta(k_F - k) = V \cdot \frac{g \Omega_d}{(2\pi)^d} \frac{k_F^d}{d}, \quad (16)$$

where g is the internal degeneracy and Ω_d is the surface area of a sphere in d dimensions. The total energy is

$$E = g V \int \frac{d^d k}{(2\pi)^d} \frac{\hbar^2 k^2}{2m} \Theta(k_F - k) = V \cdot \frac{g \Omega_d}{(2\pi)^d} \frac{k_F^d}{d+2} \cdot \frac{\hbar^2 k_F^2}{2m}. \quad (17)$$

Therefore,

$$\frac{E}{N} = \frac{d}{d+2} \varepsilon_F. \quad (18)$$

(5) Obtain numerical estimates for the Fermi energy (in eV) and the Fermi temperature (in K) for the following systems:

- (a) conduction electrons in silver, lead, and aluminum
- (b) nucleons in a heavy nucleus, such as ^{200}Hg

Solution: The Fermi energy for ballistic dispersion is given by

$$\varepsilon_F = \frac{\hbar^2}{2m^*} (3\pi^2 n)^{2/3}, \quad (19)$$

where m^* is the effective mass, which one can assume is the electron mass $m = 9.11 \times 10^{-28}$ g. The electron density is given by the number of valence electrons of the atom divided by the volume of the unit cell. A typical unit cell volume is on the order of 30 \AA^3 , and if we assume one valence electron per atom we obtain a Fermi energy of $\varepsilon_F = 3.8 \text{ eV}$, and hence a Fermi temperature of $3.8 \text{ eV} / (86.2 \times 10^{-6} \text{ eV/K}) = 4.4 \times 10^4 \text{ K}$. This sets the overall scale. For detailed numbers, one can examine table 2.1 in *Solid State Physics* by Ashcroft and Mermin. One finds

$$T_F(\text{Ag}) = 6.38 \times 10^4 \text{ K} \quad ; \quad T_F(\text{Pb}) = 11.0 \times 10^4 \text{ K} \quad ; \quad T_F(\text{Al}) = 13.6 \times 10^4 \text{ K}. \quad (20)$$

Nuclear densities are of course much higher. In the literature one finds the relation $R \sim A^{1/3} r_0$, where R is the nuclear radius, A is the number of nucleons (*i.e.* the atomic mass number), and $r_0 \simeq 1.2 \text{ fm} = 1.2 \times 10^{-15} \text{ m}$. Under these conditions, the nuclear density is on the order of $n \sim 3A/4\pi R^3 = 3/4\pi r_0^3 = 1.4 \times 10^{44} \text{ m}^{-3}$. With the mass of the proton $m_p = 938 \text{ MeV}/c^2$ we find $\varepsilon_F \sim 30 \text{ MeV}$ for the nucleus, corresponding to a temperature of roughly $T_F \sim 3.5 \times 10^{11} \text{ K}$.

(6) Show that the chemical potential of a three-dimensional ideal nonrelativistic Fermi gas is given by

$$\mu(n, T) = \varepsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F} \right)^2 - \frac{\pi^4}{80} \left(\frac{k_B T}{\varepsilon_F} \right)^4 + \dots \right]$$

and the average energy per particle is

$$\frac{E}{N} = \frac{3}{5} \varepsilon_F \left[1 + \frac{5\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F} \right)^2 - \frac{\pi^4}{16} \left(\frac{k_B T}{\varepsilon_F} \right)^4 + \dots \right],$$

where $\mu_0(n)$ is the Fermi energy at $T = 0$. Compute the heat capacity $C_V(T)$ to terms of order T^3 . How does the T^3 contribution to the electronic heat capacity compare with the contribution from phonons?

Solution : From the Sommerfeld expansion we have

$$\int_{-\infty}^{\infty} d\varepsilon \phi(\varepsilon) f(\varepsilon - \mu) = \int_{-\infty}^{\mu} d\varepsilon \phi(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 \phi'(\mu) + \frac{7\pi^4}{360} (k_B T)^4 \phi'''(\mu) + \mathcal{O}(T^6) \quad (21)$$

$$= \left\{ 1 + \frac{\pi^2}{6} (k_B T)^2 \frac{d^2}{d\mu^2} + \frac{7\pi^4}{360} (k_B T)^2 \frac{d^4}{d\mu^4} + \mathcal{O}(T^6) \right\} H(\mu), \quad (22)$$

where $\phi(\varepsilon) = H'(\varepsilon)$. Let's work this out to second order in T^2 for the case $\phi(\varepsilon) = g(\varepsilon)$. The integral then gives the overall density n . We write $\mu = \varepsilon_F + \delta\mu$ and expand the RHS to second order in $\delta\mu$. Thus yields

$$\begin{aligned} n &= \int_{-\infty}^{\varepsilon_F} d\varepsilon g(\varepsilon) + g(\varepsilon_F) \delta\mu + \frac{1}{2} g'(\varepsilon_F) (\delta\mu)^2 + \dots \\ &+ \frac{\pi^2}{6} (k_B T)^2 g'(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 g''(\varepsilon_F) \delta\mu + \dots \\ &+ \frac{7\pi^4}{360} (k_B T)^4 g'''(\varepsilon_F) + \dots \end{aligned} \quad (23)$$

RHS of the first line above comes from expanding the integral in the first term on the RHS of the previous equation to second order in $\delta\mu$. The subsequent lines come from the expansions of the second and third terms on the RHS of the previous equation, respectively. We expand out to the necessary order in each case. From this equation we thus obtain

$$\delta\mu = -\frac{\pi^2}{6} (k_B T)^2 \frac{g'(\varepsilon_F)}{g(\varepsilon_F)} - \frac{\pi^4}{36} (k_B T)^4 \cdot \left[\frac{1}{2} \left(\frac{g'(\varepsilon_F)}{g(\varepsilon_F)} \right)^3 - \frac{g'(\varepsilon_F) g''(\varepsilon_F)}{g^2(\varepsilon_F)} + \frac{7}{10} \frac{g'''(\varepsilon_F)}{g(\varepsilon_F)} \right] + \dots \quad (24)$$

If we assume that $g(\varepsilon)$ is a homogeneous function with $g(\varepsilon) \propto \varepsilon^\alpha$, then find

$$\delta\mu = -\frac{\alpha \pi^2}{6} \frac{(k_B T)^2}{\varepsilon_F} - \alpha(\alpha - 2)(2\alpha - 7) \frac{\pi^4}{360} \frac{(k_B T)^4}{\varepsilon_F^3} + \mathcal{O}(T^6). \quad (25)$$

Substituting $\alpha = \frac{1}{2}$, as is appropriate for three-dimensional ballistic fermions, we obtain

$$\delta\mu = -\frac{\pi^2}{12} \frac{(k_B T)^2}{\varepsilon_F} - \frac{\pi^4}{80} \frac{(k_B T)^4}{\varepsilon_F^3} + \mathcal{O}(T^6), \quad (26)$$

which is the desired result.

The result for the energy is tedious to carry out by hand, but is rather straightforward using a symbolic manipulation program such as Mathematica or Maple. We assume the density of states is of the form $g(\varepsilon) = C\varepsilon^\alpha$. Then from the Sommerfeld expansion we have

$$\frac{E}{V} = \frac{C\mu^{\alpha+2}}{\alpha+2} \left\{ 1 + \alpha(\alpha+1) \frac{\pi^2}{6} \left(\frac{k_B T}{\mu} \right)^2 + (\alpha-2)(\alpha-1)\alpha(\alpha+1) \frac{7\pi^4}{360} \left(\frac{k_B T}{\mu} \right)^4 + \dots \right\} \quad (27)$$

$$\frac{N}{V} = \frac{C\mu^{\alpha+1}}{\alpha+2} \left\{ 1 + (\alpha-1)\alpha \frac{\pi^2}{6} \left(\frac{k_B T}{\mu} \right)^2 + (\alpha-3)(\alpha-2)(\alpha-1)\alpha \frac{7\pi^4}{360} \left(\frac{k_B T}{\mu} \right)^4 + \dots \right\} \quad (28)$$

Carefully taking the ratio and evaluating to order T^4 , we find

$$\frac{E}{N} = \left(\frac{\alpha+1}{\alpha+2} \right) \mu \cdot \left\{ 1 + (\alpha+1) \frac{\pi^2}{3} \left(\frac{k_B T}{\mu} \right)^2 + \alpha(\alpha+1)(\alpha-6) \frac{\pi^4}{45} \left(\frac{k_B T}{\mu} \right)^4 + \dots \right\}. \quad (29)$$

Unfortunately we're not quite done, since we now must expand μ in a power series in T , invoking our previous result. Working this out (by hand!), I obtain

$$\frac{E}{N} = \left(\frac{\alpha+1}{\alpha+2} \right) \varepsilon_F \cdot \left\{ 1 + (\alpha+2) \frac{\pi^2}{6} \left(\frac{k_B T}{\varepsilon_F} \right)^2 + \alpha(\alpha+2)(2\alpha-7) \frac{\pi^4}{120} \left(\frac{k_B T}{\varepsilon_F} \right)^4 + \mathcal{O}(T^6) \right\}. \quad (30)$$

Setting $\alpha = \frac{1}{2}$ we have $\frac{1}{6}(\alpha+2) = \frac{5}{12}$ and $\frac{1}{120}\alpha(\alpha+2)(2\alpha-7) = -\frac{1}{16}$, as indicated in the statement of the problem. Our formula holds for general α , so we can find the result for $d = 2$ by setting $\alpha = 0$.

The heat capacity is

$$\begin{aligned} C_{V,N} &= \left(\frac{\partial E}{\partial T} \right)_{V,N} \\ &= Nk_B \left\{ (\alpha+1) \frac{\pi^2}{3} \left(\frac{k_B T}{\varepsilon_F} \right) + \alpha(\alpha+1)(2\alpha-7) \frac{\pi^4}{30} \left(\frac{k_B T}{\varepsilon_F} \right)^3 + \mathcal{O}(T^5) \right\}. \end{aligned} \quad (31)$$

In $d = 3$, with $\alpha = \frac{1}{2}$, the order T^3 term is $-\frac{3}{20}\pi^4(k_B T/\varepsilon_F)^3 Nk_B$. The low temperature phonon contribution is $C_V^{(\text{phonon})} = \frac{12}{5}\pi^4 (T/\Theta_D)^3 Nk_B$, where Θ_D is the Debye temperature. The ratio is

$$\frac{\Delta C_V^{(\text{elec})}}{C_V^{(\text{phonon})}} = -\frac{1}{16} \left(\frac{\Theta_D}{T_F} \right)^3. \quad (32)$$

Since Θ_D is typically hundreds of K while T_F is tens of thousands of K, this ratio is on the order of 10^{-7} .

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #2 SOLUTIONS

(1) Consider a model in which there are three possible states per site, which we can denote by A, B, and V. The states A and B are for our purposes identical. The energies of A-A, A-B, and B-B links are all identical and equal to W . The state V represents a vacancy, and any link containing a vacancy, meaning A-V, B-V, or V-V, has energy 0.

- (a) Suppose we write $\sigma = +1$ for A, $\sigma = -1$ for B, and $\sigma = 0$ for V. How would you write a Hamiltonian for this system? Your result should be of the form

$$\hat{H} = \sum_{\langle ij \rangle} E(\sigma_i, \sigma_j).$$

Find a simple and explicit function $E(\sigma, \sigma')$ which yields the correct energy for each possible bond configuration.

Solution: The quantity σ_i^2 is 1 if site i is in state A or B and is 0 in state V. Therefore we have

$$\hat{H} = W \sum_{\langle ij \rangle} \sigma_i^2 \sigma_j^2.$$

- (b) Consider a triangle of three sites. Find the average total energy at temperature T . There are $3^3 = 27$ states for the triangle. You can just enumerate them all and find the energies.

Solution: Of the 27 states, eight have zero vacancies – each site has two possible states A and B – with energy $E = 3W$. There are 12 states with one vacancy, since there are three possible locations for the vacancy and then four possibilities for the remaining two sites (each can be either A or B). Each of these 12 single vacancy states has energy $E = W$. There are 6 states with two vacancies and 1 state with three vacancies, all of which have energy $E = 0$. The partition function is therefore

$$Z = 8e^{-3\beta W} + 12e^{-\beta W} + 7.$$

Note that $Z(\beta = 0) = \text{Tr } 1 = 27$ is the total number of ‘microstates’. The average energy is then

$$E = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = \left(\frac{24e^{-3\beta W} + 12e^{-\beta W}}{8e^{-3\beta W} + 12e^{-\beta W} + 7} \right) W$$

- (c) For a one-dimensional ring of N sites, find the 3×3 transfer matrix R . Find the free energy per site $F(T, N)/N$ and the ground state entropy per site $S(T, N)/N$ in the $N \rightarrow \infty$ limit for the cases $W < 0$ and $W > 0$. Interpret your results. The eigenvalue equation for R factorizes, so you only have to solve a quadratic equation.

Solution: The transfer matrix is

$$R_{\sigma\sigma'} = e^{-\beta W \sigma^2 \sigma'^2} = \begin{pmatrix} e^{-\beta W} & e^{-\beta W} & 1 \\ e^{-\beta W} & e^{-\beta W} & 1 \\ 1 & 1 & 1 \end{pmatrix},$$

where the row and column indices are A (1), B (2), and V (3), respectively. The partition function on a ring of N sites is

$$Z = \lambda_1^N + \lambda_2^N + \lambda_3^N,$$

where $\lambda_{1,2,3}$ are the three eigenvalues of R . Generally the eigenvalue equation for a 3×3 matrix is cubic, but we can see immediately that $\det R = 0$ because the first two rows are identical. Thus, $\lambda = 0$ is a solution to the characteristic equation $P(\lambda) = \det(\lambda \mathbb{I} - R) = 0$, and the cubic polynomial $P(\lambda)$ factors into the product of λ and a quadratic. The latter is easily solved. One finds

$$P(\lambda) = \lambda^3 - (2x + 1)\lambda^2 + (2x - 2)\lambda,$$

where $x = e^{-\beta W}$. The roots are $\lambda = 0$ and

$$\lambda_{\pm} = x + \frac{1}{2} \pm \sqrt{x^2 - x + \frac{9}{4}}.$$

The largest of the three eigenvalues is λ_+ , hence, in the thermodynamic limit,

$$F = -k_B T \ln Z = -N k_B T \ln \left(e^{-W/k_B T} + \frac{1}{2} + \sqrt{e^{-2W/k_B T} - e^{-W/k_B T} + \frac{9}{4}} \right).$$

The entropy is $S = -\frac{\partial F}{\partial T}$. In the limit $T \rightarrow 0$ with $W < 0$, we have

$$\lambda_+(T \rightarrow 0, W < 0) = 2e^{|W|/k_B T} + e^{-|W|/k_B T} + \mathcal{O}(e^{-2|W|/k_B T}).$$

Thus

$$\begin{aligned} F(T \rightarrow 0, W < 0) &= -N |W| - N k_B T \ln 2 + \dots \\ S(T \rightarrow 0, W < 0) &= N \ln 2. \end{aligned}$$

When $W > 0$, we have

$$\lambda_+(T \rightarrow 0, W > 0) = 2 + \frac{2}{3} e^{-W/k_B T} + \mathcal{O}(e^{-2W/k_B T}).$$

Then

$$\begin{aligned} F(T \rightarrow 0, W > 0) &= -N k_B T \ln 2 - \frac{1}{3} N k_B T e^{-W/k_B T} + \dots \\ S(T \rightarrow 0, W > 0) &= N \ln 2. \end{aligned}$$

Thus, the ground state entropies are the same, even though the allowed microstates are very different. For $W < 0$, there are no vacancies. For $W > 0$, every link must contain at least one vacancy.

(2) Consider a two-state Ising model on a one-dimensional ring, where each site supports a spin $\sigma_n = \pm 1$. The Hamiltonian is

$$\hat{H} = -J \sum_n \left(\frac{1 + \sigma_{n-1} \sigma_n}{2} \right) \left(\frac{1 + \sigma_n \sigma_{n+1}}{2} \right).$$

(a) Show explicitly that $P_{\sigma\sigma'} = \frac{1}{2}(1 + \sigma\sigma')$ is zero if $\sigma \neq \sigma'$ and is unity if $\sigma = \sigma'$.

Solution : Well this is pretty obvious. Since each Ising variable is ± 1 , we have $\sigma\sigma' = +1$ when $\sigma = \sigma'$ and $\sigma\sigma' = -1$ when $\sigma \neq \sigma'$. Thus, $P_{\sigma\sigma'} = \frac{1}{2}(1 + \sigma\sigma')$ registers a 1 when $\sigma = \sigma'$ and 0 when $\sigma \neq \sigma'$.

(b) Show that \hat{H} is proportional to the number of consecutive *triples* of sites $(n-1, n, n+1)$ for which $\sigma_{n-1} = \sigma_n = \sigma_{n+1}$.

Solution : Clearly $P_{\sigma\sigma'} P_{\sigma'\sigma''} = 1$ if and only if $\sigma = \sigma' = \sigma''$. So the above Hamiltonian counts the number of consecutive triples where $\sigma_{n-1} = \sigma_n = \sigma_{n+1}$.

(c) Calculate the partition function for a ring of $N = 4$ sites. There are $2^4 = 16$ states of the ring, so you can attack the problem by direct enumeration of all the possibilities. Remember that the system is a ring.

Solution : On an $N = 4$ site ring, there are two states with energy $E = -4J$, corresponding to all spins \uparrow and all spins \downarrow . There are eight states with energy $E = -J$, corresponding to four configurations with one \uparrow spin (and three \downarrow spins) and four configurations with one \downarrow spin (and three \uparrow spins). The remaining $\binom{4}{2} = 6$ configurations have two \uparrow and two \downarrow spins, and have energy $E = 0$. Thus,

$$Z = 2e^{4\beta J} + 8e^{\beta J} + 6.$$

Note that $Z(\beta = 0) = \text{Tr } 1 = 16$.

(3) For the Mayer cluster expansion, write down all possible unlabeled connected subgraphs γ which contain four vertices. For your favorite of these animals, identify its symmetry factor s_γ , and write down the corresponding expression for the cluster integral b_γ . For example, for the \square diagram with four vertices the symmetry factor is $s_\square = 8$ and the cluster integral is

$$\begin{aligned} b_\square &= \frac{1}{8V} \int d^d r_1 \int d^d r_2 \int d^d r_3 \int d^d r_4 f(r_{12}) f(r_{23}) f(r_{34}) f(r_{14}) \\ &= \frac{1}{8} \int d^d r_1 \int d^d r_2 \int d^d r_3 f(r_{12}) f(r_{23}) f(r_1) f(r_3). \end{aligned}$$

(You'll have to choose a favorite other than \square .) If you're really energetic, compute s_γ and b_γ for all of the animals with four vertices.

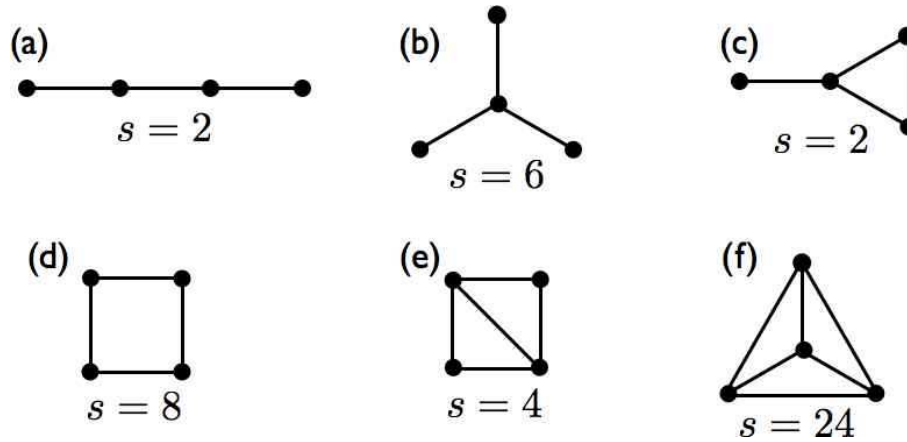


Figure 1: Connected clusters with $n_\gamma = 4$ sites.

Solution: The animals and their symmetry factors are shown in fig. 1.

$$\begin{aligned}
 b_a &= \frac{1}{2} \int d^d r_1 \int d^d r_2 \int d^d r_3 f(r_1) f(r_{12}) f(r_{23}) \\
 b_b &= \frac{1}{6} \int d^d r_1 \int d^d r_2 \int d^d r_3 f(r_1) f(r_2) f(r_3) \\
 b_c &= \frac{1}{2} \int d^d r_1 \int d^d r_2 \int d^d r_3 f(r_1) f(r_{12}) f(r_{13}) f(r_{23}) \\
 b_d &= \frac{1}{8} \int d^d r_1 \int d^d r_2 \int d^d r_3 f(r_1) f(r_2) f(r_{13}) f(r_{23}) \\
 b_e &= \frac{1}{4} \int d^d r_1 \int d^d r_2 \int d^d r_3 f(r_1) f(r_2) f(r_{12}) f(r_{13}) f(r_{23}) \\
 b_f &= \frac{1}{24} \int d^d r_1 \int d^d r_2 \int d^d r_3 f(r_1) f(r_2) f(r_3) f(r_{12}) f(r_{13}) f(r_{23}) .
 \end{aligned}$$

(4) Explain physically, using pictures and/or drawing analogies to other common knowledge (of upper division physics majors) why the pair distribution function $g(r)$ should have the features it does in fig. 5.7 of the notes.

Solution: The radial distribution function,

$$g(r) = \frac{1}{V n^2} \left\langle \sum_{i \neq j} \delta(\mathbf{r} - \mathbf{x}_i + \mathbf{x}_j) \right\rangle ,$$

tells us how likely it is to find a pair of particles with separation r . For particles which behave as hard spheres at distances larger than some diameter a , we therefore expect $g(r) \rightarrow 0$ for $r < a$. Beyond $r = a$ the distribution function exhibits a damped oscillation on a length scale $\sim a$, since the relative absence of pairs at a particular radial separation r

leads to a relative abundance of pairs at radial separation $r + a$. See the figures in chapter 5 of the notes.

(5) An ionic solution of dielectric constant ϵ and mean ionic density n fills a grounded conducting sphere of radius R . A charge Q lies at the center of the sphere. Calculate the ionic charge density as a function of the radial coordinate r , assuming $Q/r \ll k_B T$.

Solution: Debye-Hückel theory tells us that

$$n_{\pm}(\mathbf{r}) = \frac{1}{2}n_{\infty} e^{\mp e\phi(\mathbf{r})/k_B T}$$

and

$$\nabla^2 \phi = -\frac{4\pi e}{\epsilon} (n_+ - n_-) - \frac{4\pi}{\epsilon} \rho_{\text{ext}},$$

where ϵ is the dielectric constant. Assuming $\phi \ll k_B T$, we have $\nabla^2 \phi = \kappa_D^2 \phi - 4\pi\epsilon^{-1}\rho_{\text{ext}}$, with

$$\kappa_D = \sqrt{\frac{4\pi n_{\infty} e^2}{\epsilon k_B T}}.$$

Assuming a spherically symmetric solution, with a point charge Q at the origin, we solve

$$\left(-\frac{1}{r} \frac{\partial^2}{\partial r^2} r + \kappa_D^2 \right) \phi = \frac{4\pi Q}{\epsilon} \delta(\mathbf{r}).$$

The solution is then of the form $\phi(r) = \frac{1}{r} u(r)$, with $u'' = \kappa_D^2 u$ for $r > 0$. Thus,

$$\phi(r) = A \frac{\cosh(\kappa_D r)}{r} + B \frac{\sinh(\kappa_D r)}{r}.$$

As $r \rightarrow 0$ we must have an unscreened charge Q , hence $A = Q/\epsilon$. The boundary condition on the conducting sphere is $\phi(R) = 0$, hence $B = -A \operatorname{ctnh}(\kappa_D R)$. Thus,

$$\phi(\mathbf{r}) = \frac{Q \cosh(\kappa_D r)}{\epsilon r} \cdot \left(1 - \frac{\tanh(\kappa_D r)}{\tanh(\kappa_D R)} \right).$$

We stress that this solution is valid only where $e\phi(\mathbf{r}) \ll k_B T$.

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #3 SOLUTIONS

(1) Consider an Ising ferromagnet where the nearest neighbor exchange temperature is $J_{\text{NN}}/k_{\text{B}} = 50 \text{ K}$ and the next nearest neighbor exchange temperature is $J_{\text{NNN}}/k_{\text{B}} = 10 \text{ K}$. What is the mean field transition temperature T_{c} if the lattice is:

- (a) square
- (b) honeycomb
- (c) triangular
- (d) simple cubic
- (e) body centered cubic

Hint : As an intermediate step, you might want to show that the mean field transition temperature is given by

$$k_{\text{B}}T_{\text{c}}^{\text{MF}} = z_1 J_{\text{NN}} + z_2 J_{\text{NNN}} ,$$

where z_1 and z_2 are the number of nearest neighbors and next-nearest neighbors of a given lattice site, respectively.

Solution : The mean field transition temperature is given by $k_{\text{B}}T_{\text{c}}^{\text{MF}} = \hat{J}(0)$. With only nearest and next-nearest neighbors, we have

$$k_{\text{B}}T_{\text{c}}^{\text{MF}} = \sum_{\mathbf{R}} J(\mathbf{R}) = z_1 J_{\text{NN}} + z_2 J_{\text{NNN}} ,$$

where J_{NN} and J_{NNN} are the nearest neighbor and next nearest neighbor exchange interaction energies. According to sketches in fig. 1, we have

- (a) square lattice : $z_1 = 4$ and $z_2 = 4$. Thus, $T_{\text{c}}^{\text{MF}} = 240 \text{ K}$.
- (b) honeycomb lattice : $z_1 = 3$ and $z_2 = 6$. Thus, $T_{\text{c}}^{\text{MF}} = 210 \text{ K}$.
- (c) triangular lattice : $z_1 = 6$ and $z_2 = 6$. Thus, $T_{\text{c}}^{\text{MF}} = 360 \text{ K}$.
- (d) simple cubic lattice : $z_1 = 6$ and $z_2 = 12$. Thus, $T_{\text{c}}^{\text{MF}} = 420 \text{ K}$.
- (e) body-centered cubic lattice : $z_1 = 8$ and $z_2 = 6$. Thus, $T_{\text{c}}^{\text{MF}} = 460 \text{ K}$.

(2) Consider a three state Ising model,

$$\hat{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i ,$$

where $S_i \in \{-1, 0, +1\}$.

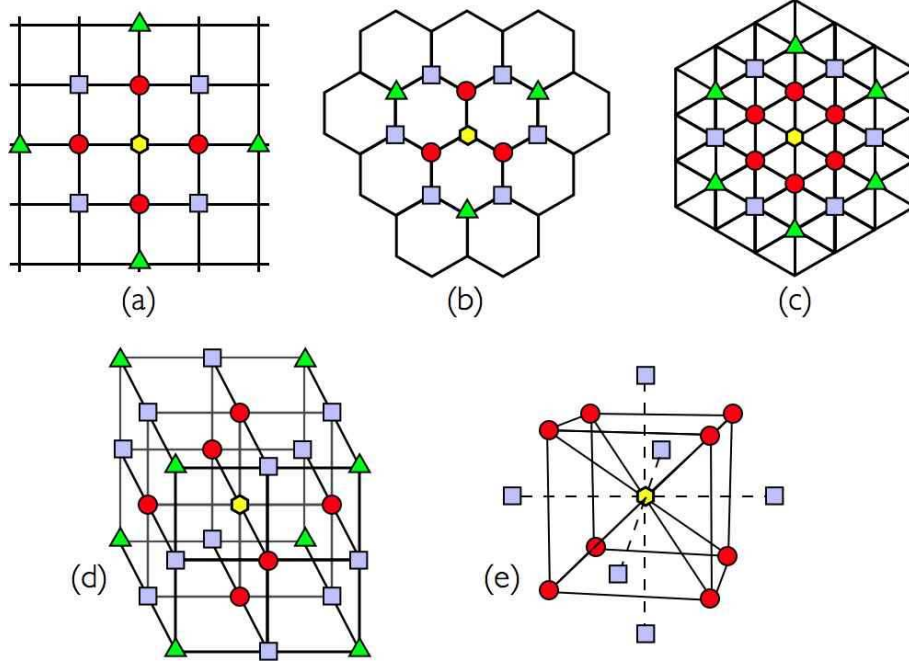


Figure 1: Nearest neighbors (red circles), next nearest neighbors (light blue squares), and some third nearest neighbors (green triangles) for five common lattices. (a) square, (b) honeycomb, (c) triangular, (d) simple cubic, and (e) body centered cubic.

- (a) Writing $S_i = m + \delta S_i$ and ignoring terms quadratic in the fluctuations, derive the mean field Hamiltonian H_{MF} .

Solution: We have

$$\begin{aligned}
 S_i S_j &= (m + \delta S_i)(m + \delta S_j) \\
 &= m^2 + m(\delta S_i + \delta S_j) + \delta S_i \delta S_j \\
 &= -m^2 + m(S_i + S_j) + \delta S_i \delta S_j .
 \end{aligned}$$

We ignore the fluctuation term, resulting in the mean field Hamiltonian

$$H_{\text{MF}} = \frac{1}{2} N z J m^2 - (z J m + H) \sum_i S_i .$$

- (b) Find the dimensionless mean field free energy density, $f = F_{\text{MF}}/NzJ$, where z is the lattice coordination number. You should define the dimensionless temperature $\theta \equiv k_{\text{B}}T/zJ$ and the dimensionless field $h \equiv H/zJ$.

Solution: The effective field is $H_{\text{eff}} = zJm + H$. Note that

$$\sum_S e^{H_{\text{eff}} S/k_{\text{B}}T} = 1 + 2 \cosh\left(\frac{zJm + H}{k_{\text{B}}T}\right) .$$

It is convenient to adimensionalize, writing $f = /NzJ$, $\theta = k_B T / zJ$, and $h = H / zJ$. Then we have

$$f(m, \theta, h) = \frac{1}{2}m^2 - \theta \ln \left(1 + 2 \cosh \left(\frac{m+h}{\theta} \right) \right).$$

- (c) Find the self-consistency equation for $m = \langle S_i \rangle$ and show that this agrees with the condition $\partial f / \partial m = 0$.

Solution: Extremizing the free energy $f(m)$ with respect to m , we obtain the mean field equation:

$$\frac{\partial f}{\partial m} = 0 \quad \implies \quad m = \frac{2 \sinh \left(\frac{m+h}{\theta} \right)}{1 + 2 \cosh \left(\frac{m+h}{\theta} \right)}.$$

The self consistency condition is the same:

$$m = \frac{\sum_S S e^{(m+h)S/\theta}}{\sum_S e^{(m+h)S/\theta}} = \frac{2 \sinh \left(\frac{m+h}{\theta} \right)}{1 + 2 \cosh \left(\frac{m+h}{\theta} \right)}.$$

- (d) Expand $f(m)$ to fourth order in m and first order in h .

Solution: We have

$$\begin{aligned} f(m) &= \frac{1}{2}m^2 - \theta \ln \left(3 + \frac{(h+m)^2}{\theta^2} + \frac{(h+m)^4}{12\theta^4} + \dots \right) \\ &= -\theta \ln 3 + \frac{1}{2} \left(1 - \frac{2}{3\theta} \right) m^2 + \frac{m^4}{36\theta^3} - \frac{2hm}{3\theta} + \dots \end{aligned}$$

- (e) Find the critical temperature θ_c .

Solution: The critical temperature is identified as the value of θ where the coefficient of the m^2 term in the free energy vanishes. Thus, $\theta_c = \frac{2}{3}$.

- (f) Find $m(\theta_c, h)$.

Solution: Setting $\theta = \theta_c = \frac{2}{3}$, we extremize $f(m)$ and obtain the equation

$$f'(m, \theta_c, h) = 0 = \frac{m^3}{9\theta_c^3} - \frac{2h}{3\theta_c} \quad \implies \quad m(\theta_c, h) = (6\theta_c^2 h)^{1/3} = \left(\frac{8}{3}h \right)^{1/3}.$$

- (3) For the O(3) Heisenberg ferromagnet,

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\Omega}_i \cdot \hat{\Omega}_j,$$

find the mean field transition temperature T_c^{MF} . Here, each $\hat{\Omega}_i$ is a three-dimensional unit vector, which can be parameterized using the usual polar and azimuthal angles:

$$\hat{\Omega}_i = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i).$$

The thermodynamic trace is defined as

$$\text{Tr} A(\hat{\Omega}_1, \dots, \hat{\Omega}_N) = \int \prod_{i=1}^N \frac{d\Omega_i}{4\pi} A(\hat{\Omega}_1, \dots, \hat{\Omega}_N),$$

where

$$d\Omega_i = \sin \theta_i d\theta_i d\phi_i.$$

Hint: Your mean field Ansatz will look like $\hat{\Omega}_i = \mathbf{m} + \delta\Omega_i$, where $\mathbf{m} = \langle \Omega_i \rangle$. You'll want to ignore terms in the Hamiltonian which are quadratic in fluctuations, i.e. $\delta\Omega_i \cdot \delta\Omega_j$. You can, without loss of generality, assume \mathbf{m} to lie in the \hat{z} direction.

Solution: Writing $\hat{\Omega}_i = \mathbf{m} + \delta\Omega_i$ and neglecting the fluctuations, we arrive at the mean field Hamiltonian

$$H_{\text{MF}} = \frac{1}{2} N z J m^2 - z J \mathbf{m} \cdot \sum_i \hat{\Omega}_i,$$

where $\mathbf{m} = \langle \hat{\Omega}_i \rangle$ is assumed to be independent of the site index i . The partition function is

$$Z = e^{-\frac{1}{2} N \beta z J m^2} \left(\int \frac{d\Omega}{4\pi} e^{\beta z J \mathbf{m} \cdot \hat{\Omega}} \right)^N.$$

We once again adimensionalize, writing $f = F/NzJ$ and $\theta = k_B T/zJ$. We then find

$$\begin{aligned} f(\mathbf{m}, \theta) &= \frac{1}{2} m^2 - \theta \ln \int \frac{d\Omega}{4\pi} e^{\mathbf{m} \cdot \hat{\Omega} / \theta} \\ &= \frac{1}{2} m^2 - \theta \ln \left(\frac{\sinh(m/\theta)}{m/\theta} \right) \\ &= \frac{1}{2} m^2 - \theta \ln \left(1 + \frac{m^2}{6\theta^2} + \frac{m^4}{120\theta^4} + \dots \right) \\ &= \frac{1}{2} \left(1 - \frac{1}{3\theta} \right) m^2 + \frac{m^4}{180\theta^3} + \dots \end{aligned}$$

Setting the coefficient of the quadratic term to zero, we obtain $\theta_c = \frac{1}{3}$.

(4) A system is described by the Hamiltonian

$$\hat{H} = -J \sum_{\langle ij \rangle} \mathcal{I}(\mu_i, \mu_j) - H \sum_i \delta_{\mu_i, A},$$

where on each site i there are four possible choices for μ_i : $\mu_i \in \{A, B, C, D\}$. The interaction matrix $\mathcal{I}(\mu, \mu')$ is given in the following table:

\mathcal{I}	A	B	C	D
A	+1	-1	-1	0
B	-1	+1	0	-1
C	-1	0	+1	-1
D	0	-1	-1	+1

(a) Write a trial density matrix

$$\begin{aligned}\varrho_N(\mu_1, \dots, \mu_N) &= \prod_{i=1}^N \varrho(\mu_i) \\ \varrho(\mu) &= x \delta_{\mu,A} + y (\delta_{\mu,B} + \delta_{\mu,C} + \delta_{\mu,D}).\end{aligned}$$

What is the relationship between x and y ? Henceforth use this relationship to eliminate y in terms of x .

Solution: The density matrix ϱ must be normalized, hence

$$\text{Tr } \varrho = x + 3y \equiv 1 \quad \implies \quad y = \frac{1}{3}(1 - x).$$

(b) What is the variational energy per site, $E(x)/N$?

Solution: The energy per site is

$$\begin{aligned}\frac{E}{N} &= -\frac{1}{2}zJ \text{Tr} \left(\varrho(\mu) \varrho(\mu') \mathcal{I}(\mu, \mu') \right) - H \text{Tr} \left(\varrho(\mu) \delta_{\mu,A} \right) \\ &= -\frac{1}{2}zJ \left\{ x^2 + 3y^2 - 4xy - 4y^2 \right\} - Hx \\ &= -\frac{1}{2}zJ \left(x^2 + \frac{1}{3}(1-x)^2 - \frac{4}{3}x(1-x) - \frac{4}{9}(1-x)^2 \right) - Hx \\ &= \frac{1}{18}zJ \left(1 + 10x - 20x^2 \right) - Hx.\end{aligned}$$

(c) What is the variational entropy per site, $S(x)/N$?

Solution: The entropy per site is

$$\begin{aligned}\frac{S}{N} &= -k_B T \text{Tr} \left(\varrho \ln \varrho \right) \\ &= -k_B \left(x \ln x + 3y \ln y \right) \\ &= -k_B \left\{ x \ln x + (1-x) \ln \left(\frac{1-x}{3} \right) \right\}.\end{aligned}$$

(d) What is the mean field equation for x ?

Solution: The free energy per site is

$$f \equiv \frac{E - TS}{NzJ} \\ = \frac{1}{18} (1 + 10x - 20x^2) - hx + \theta \left\{ x \ln x + (1-x) \ln \left(\frac{1-x}{3} \right) \right\},$$

where $h = H/zJ$ and $\theta = k_B T/zJ$ are the dimensionless field and temperature, respectively. The mean field equation is obtained by extremizing $f(x, \theta, h)$:

$$\frac{\partial f}{\partial x} = 0 = \frac{5}{9}(1 - 4x) - h + \theta \ln \left(\frac{3x}{1-x} \right).$$

(e) What value x^* does x take when the system is disordered?

Solution: Clearly $x = y = \frac{1}{4}$ in the disordered phase, since each state is then equally probable. The global symmetry of the problem, which is \mathbb{Z}_4 , is then unbroken.

(f) Write $x = x^* + \frac{3}{4}\varepsilon$ and expand the free energy to fourth order in ε . The factor $\frac{3}{4}$ should generate manageable coefficients in the Taylor series expansion. You may want to use a symbolic manipulator like Mathematica here.

Solution: We write $x = \frac{1}{4} + \frac{3}{4}\varepsilon$, in which case

$$f = \frac{5}{9}(1 - 4x) - h + \theta \ln \left(\frac{3x}{1-x} \right) \\ = -\theta \ln 4 - \frac{3}{4}h\varepsilon + \frac{3}{2} \left(\theta - \frac{5}{12} \right) \varepsilon^2 - \theta \varepsilon^3 + \frac{7}{4} \theta \varepsilon^4 + \mathcal{O}(\varepsilon^5).$$

(g) Sketch ε as a function of T for $H = 0$ and find T_c . Is the transition first order or second order?

Solution: The transition in zero field is first order, but you'd have had to read ahead a little in the notes to understand this. The point is that whenever a Landau expansion of the free energy has a cubic term, e.g. for

$$f(\varepsilon) = f_0 + \frac{1}{2} a \varepsilon^2 - \frac{1}{3} u \varepsilon^3 + \frac{1}{4} b \varepsilon^4 + \dots,$$

the second order transition we would expect occurs at $a = 0$ is preempted by a first order transition that occurs at some positive value of a , i.e. before the curvature at $\varepsilon = 0$ goes negative. To see this, we differentiate, obtaining

$$f'(\varepsilon) = 0 = (a - u\varepsilon + b\varepsilon^2) \varepsilon.$$

The first order transition occurs when the local minimum of $f(\varepsilon)$ at $\varepsilon > 0$ crosses the value $f(0)$. Thus, in addition to the mean field equation above, we have the condition

$$f(\varepsilon) = f(0) \quad \implies \quad \frac{1}{2} a \varepsilon^2 - \frac{1}{3} u \varepsilon^3 + \frac{1}{4} b \varepsilon^4 = 0.$$

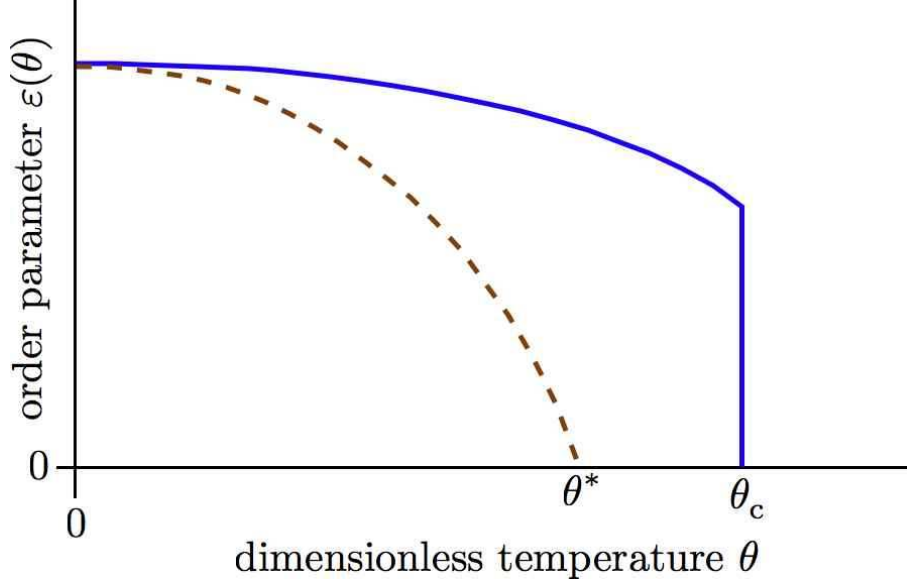


Figure 2: Order parameter *versus* temperature for a free energy $f = \frac{1}{2} a \varepsilon^2 - \frac{1}{3} u \varepsilon^3 + \frac{1}{4} b \varepsilon^4$. When $b > 0$, the usual second order transition at $a(\theta^*) = 0$ is *preempted* by a first order transition at $a(\theta_c) = 2u^2/9b$. The cubic term stabilizes the ordered phase for temperatures between θ^* and θ_c . The dashed curve is what $\varepsilon(\theta)$ would resemble in the absence of the cubic term, *i.e.* when $u = 0$.

Thus, we have the following two quadratic equations to solve simultaneously:

$$\begin{aligned} a - u\varepsilon + b\varepsilon^2 &= 0 \\ \frac{1}{2}a - \frac{1}{3}u\varepsilon + \frac{1}{4}b\varepsilon^2 &= 0. \end{aligned}$$

Eliminating the quadratic term, we obtain $\varepsilon = 3a/u$ at the first order transition, and inserting this into either of the above equations we obtain the relation $u^2 = \frac{9}{2}ab$. For our specific model, we have $a = 3(\theta - \frac{5}{12})$, $u = 3\theta$, and $b = 7\theta$. Thus, the first order transition occurs at a critical temperature

$$\theta_c = \frac{35}{76}.$$

Note that the sign of the quadratic term in $f(\varepsilon)$ is still positive at this point, and remains so down to a temperature $\theta^* = \frac{5}{12}$. If there were no cubic term, we would expect a second order transition at this latter temperature, but as we see it is preempted by the first order transition.

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #5 SOLUTIONS

(1) Find in the scientific literature two examples of phase transitions, one first order and one second order. Describe the systems and identify the order parameter in each case. Reproduce a plot of the order parameter *versus* temperature showing how the transition is discontinuous (first order) or continuous (second order). If the transition is first order, is a latent heat reported? If second order, are any critical exponents reported? Some examples of phase transitions, which might help you in your searches: liquid-gas transitions, Curie transitions, order-disorder transitions, structural phase transitions, normal fluid to superfluid transitions (^3He and ^4He are two examples), metal-superconductor transitions, crystallization transitions, *etc.* An excellent search engine for scholarly publications is available at scholar.google.com.

Solution : For an example of a system which exhibits both a second-order and a first-order transition as a function of temperature, see fig. 1, which shows the cubic lattice constant $a(T)$ *versus* temperature for the solid material C_{60} . The C_{60} molecule is one of a class known as fullerenes, after the architect and futurist Buckminster Fuller, the inventor of the geodesic dome. At a temperature $T_c^{\text{II}} = 260 \text{ K}$, there is a discontinuity in the $a(T)$ curve, signaling a first order phase transition. This is akin to the density discontinuity in water when it boils or freezes. For $T > T_c^{\text{II}} = 260 \text{ K}$, the C_{60} molecules form a face centered cubic lattice, while below this temperature the lattice is simple cubic. For $T \in [T_c^{\text{I}}, T_c^{\text{II}}]$, with $T_c^{\text{I}} = 90 \text{ K}$, the individual C_{60} molecules are in one of two *orientational* states. There is long-ranged orientational order in this phase – both orientational states are not equally probable – however as T approaches T_c^{I} from above, the distribution of molecular orientations approaches a nearly fixed distribution and varies very little for $T < T_c^{\text{I}}$.

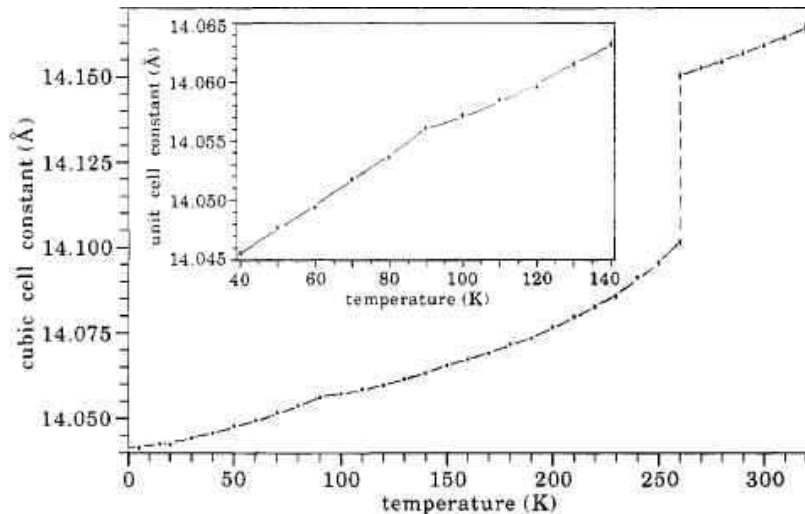


Figure 1: Temperature variation of the cubic lattice constant $a(T)$ of C_{60} as a function of temperature, from W. I. F. David *et al.*, *Europhys. Lett.* **18**, 219 (1992).

(2) Consider a two-state Ising model, with an added dash of flavor from what you have learned in your Physics 130 (Quantum Mechanics) sequence. You are invited to investigate the *transverse Ising model*, whose Hamiltonian is written

$$\hat{H} = -\frac{1}{2} \sum_{i,j} J_{ij} \sigma_i^x \sigma_j^x - H \sum_i \sigma_i^z,$$

where the σ_i^α are Pauli matrices:

$$\sigma_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_i, \quad \sigma_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_i.$$

You may find the material in §6.15 of the notes useful to study before attempting this problem.

(a) Using the trial density matrix,

$$\rho_i = \frac{1}{2} + \frac{1}{2} m_x \sigma_i^x + \frac{1}{2} m_z \sigma_i^z$$

compute the mean field free energy $F/N\hat{J}(0) \equiv f(\theta, h, m_x, m_z)$, where $\theta = k_B T/\hat{J}(0)$, and $h = H/\hat{J}(0)$. *Hint: Work in an eigenbasis when computing $\text{Tr}(\rho \ln \rho)$.*

Solution: We have $\text{Tr}(\rho \sigma^x) = m_x$ and $\text{Tr}(\rho \sigma^z) = m_z$. The eigenvalues of ρ are $\frac{1}{2}(1 \pm m)$, where $m = (m_x^2 + m_z^2)^{1/2}$. Thus,

$$f(\theta, h, m_x, m_z) = -\frac{1}{2} m_x^2 - h m_z + \theta \left[\frac{1+m}{2} \ln \left(\frac{1+m}{2} \right) + \frac{1-m}{2} \ln \left(\frac{1-m}{2} \right) \right].$$

(b) Derive the mean field equations for m_x and m_z .

Solution: Differentiating with respect to m_x and m_z yields

$$\begin{aligned} \frac{\partial f}{\partial m_x} = 0 &= -m_x + \frac{\theta}{2} \ln \left(\frac{1+m}{1-m} \right) \cdot \frac{m_x}{m} \\ \frac{\partial f}{\partial m_z} = 0 &= -h + \frac{\theta}{2} \ln \left(\frac{1+m}{1-m} \right) \cdot \frac{m_z}{m}. \end{aligned}$$

Note that we have used the result

$$\frac{\partial m}{\partial m_\mu} = \frac{m_\mu}{m}$$

where m_α is any component of the vector \mathbf{m} .

(c) Show that there is always a solution with $m_x = 0$, although it may not be the solution with the lowest free energy. What is $m_z(\theta, h)$ when $m_x = 0$?

Solution : If we set $m_x = 0$, the first mean field equation is satisfied. We then have $m_z = m \operatorname{sgn}(h)$, and the second mean field equation yields $m_z = \tanh(h/\theta)$. Thus, in this phase we have

$$m_x = 0 \quad , \quad m_z = \tanh(h/\theta) .$$

- (d) Show that $m_z = h$ for all solutions with $m_x \neq 0$.

Solution : When $m_x \neq 0$, we divide the first mean field equation by m_x to obtain the result

$$m = \frac{\theta}{2} \ln \left(\frac{1+m}{1-m} \right) ,$$

which is equivalent to $m = \tanh(m/\theta)$. Plugging this into the second mean field equation, we find $m_z = h$. Thus, when $m_x \neq 0$,

$$m_z = h \quad , \quad m_x = \sqrt{m^2 - h^2} \quad , \quad m = \tanh(m/\theta) .$$

Note that the length of the magnetization vector, m , is purely a function of the temperature θ in this phase and thus does not change as h is varied when θ is kept fixed. What does change is the canting angle of \mathbf{m} , which is $\alpha = \tan^{-1}(h/m)$ with respect to the \hat{z} axis.

- (e) Show that for $\theta \leq 1$ there is a curve $h = h^*(\theta)$ below which $m_x \neq 0$, and along which m_x vanishes. That is, sketch the mean field phase diagram in the (θ, h) plane. Is the transition at $h = h^*(\theta)$ first order or second order?

Solution : The two solutions coincide when $m = h$, hence

$$h = \tanh(h/\theta) \quad \implies \quad \theta^*(h) = \frac{2h}{\ln \left(\frac{1+h}{1-h} \right)} .$$

Inverting the above transcendental equation yields $h^*(\theta)$. The component m_x , which serves as the order parameter for this system, vanishes smoothly at $\theta = \theta_c(h)$. The transition is therefore second order.

- (f) Sketch, on the same plot, the behavior of $m_x(\theta, h)$ and $m_z(\theta, h)$ as functions of the field h for fixed θ . Do this for $\theta = 0$, $\theta = \frac{1}{2}$, and $\theta = 1$.

Solution : See fig. 2.

- (3) Consider the U(1) Ginsburg-Landau theory with

$$F = \int d^d \tilde{\mathbf{x}} \left[\frac{1}{2} a |\Psi|^2 + \frac{1}{4} b |\Psi|^4 + \frac{1}{2} \kappa |\tilde{\nabla} \Psi|^2 \right] .$$

Here $\Psi(\tilde{\mathbf{x}})$ is a complex-valued field, and both b and κ are positive. This theory is appropriate for describing the transition to superfluidity. The order parameter is $\langle \Psi(\tilde{\mathbf{x}}) \rangle$. Note that the free energy is a functional of the two independent fields $\Psi(\tilde{\mathbf{x}})$ and $\Psi^*(\tilde{\mathbf{x}})$, where Ψ^* is the complex conjugate of Ψ . Alternatively, one can consider F a functional of the real and imaginary parts of Ψ .

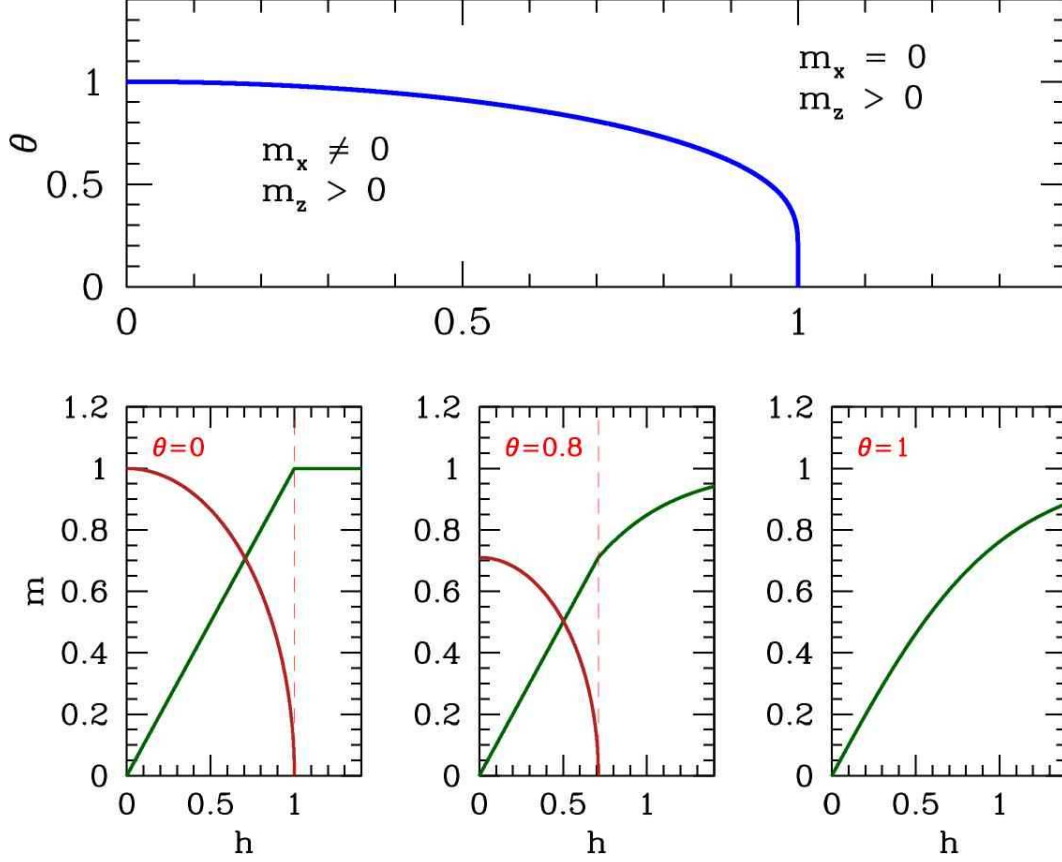


Figure 2: Solution to the mean field equations for problem 2. Top panel: phase diagram. The region within the thick blue line is a canted phase, where $m_x \neq 0$ and $m_z = h > 0$; outside this region the moment is aligned along \hat{z} and $m_x = 0$ with $m_z = \tanh(h/\theta)$.

- (a) Show that one can rescale the field Ψ and the coordinates \tilde{x} so that the free energy can be written in the form

$$F = \varepsilon_0 \int d^d x \left[\pm \frac{1}{2} |\psi|^2 + \frac{1}{4} |\psi|^4 + \frac{1}{2} |\nabla \psi|^2 \right],$$

where ψ and x are dimensionless, ε_0 has dimensions of energy, and where the sign on the first term on the RHS is $\text{sgn}(a)$. Find ε_0 and the relations between Ψ and ψ and between \tilde{x} and x .

Solution: Taking the ratio of the second and first terms in the free energy density, we learn that Ψ has units of $A \equiv (|a|/b)^{1/2}$. Taking the ratio of the third to the first terms yields a length scale $\xi = (\kappa/|a|)^{1/2}$. We therefore write $\Psi = A\psi$ and $\tilde{x} = \xi x$ to obtain the desired form of the free energy, with

$$\varepsilon_0 = A^2 \xi^d |a| = |a|^{2-\frac{1}{2}d} b^{-1} \kappa^{\frac{1}{2}d}.$$

- (b) By extremizing the functional $F[\psi, \psi^*]$ with respect to ψ^* , find a partial differential equation describing the behavior of the order parameter field $\psi(\mathbf{x})$.

Solution: We extremize with respect to the field ψ^* . Writing $F = \varepsilon_0 \int d^3x \mathcal{F}$, with $\mathcal{F} = \pm \frac{1}{2} |\psi|^2 + \frac{1}{4} |\psi|^4 + \frac{1}{2} |\nabla \psi|^2$,

$$\frac{\delta(F/\varepsilon_0)}{\delta\psi^*(\mathbf{x})} = \frac{\partial \mathcal{F}}{\partial \psi^*} - \nabla \cdot \frac{\partial \mathcal{F}}{\partial \nabla \psi^*} = \pm \frac{1}{2} \psi + \frac{1}{2} |\psi|^2 \psi - \frac{1}{2} \nabla^2 \psi.$$

Thus, the desired PDE is

$$-\nabla^2 \psi \pm \psi + |\psi|^2 \psi = 0,$$

which is known as the time-independent nonlinear Schrödinger equation.

- (c) Consider a two-dimensional system ($d = 2$) and let $a < 0$ (i.e. $T < T_c$). Consider the case where $\psi(\mathbf{x})$ describe a *vortex* configuration: $\psi(\mathbf{x}) = f(r) e^{i\phi}$, where (r, ϕ) are two-dimensional polar coordinates. Find the ordinary differential equation for $f(r)$ which extremizes F .

Solution: In two dimensions,

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2}.$$

Plugging in $\psi = f(r) e^{i\phi}$ into $\nabla^2 \psi + \psi - |\psi|^2 \psi = 0$, we obtain

$$\frac{d^2 f}{dr^2} + \frac{1}{r} \frac{df}{dr} - \frac{f}{r^2} + f - f^3 = 0.$$

- (d) Show that the free energy, up to a constant, may be written as

$$F = 2\pi\varepsilon_0 \int_0^R dr r \left[\frac{1}{2} (f')^2 + \frac{f^2}{2r^2} + \frac{1}{4} (1 - f^2)^2 \right],$$

where R is the radius of the system, which we presume is confined to a disk. Consider a *trial solution* for $f(r)$ of the form

$$f(r) = \frac{r}{\sqrt{r^2 + a^2}},$$

where a is the variational parameter. Compute $F(a, R)$ in the limit $R \rightarrow \infty$ and extremize with respect to a to find the optimum value of a within this variational class of functions.

Solution: Plugging $\nabla \psi = \hat{r} f'(r) + \frac{i}{r} f(r) \hat{\phi}$ into our expression for F , we have

$$\begin{aligned} \mathcal{F} &= \frac{1}{2} |\nabla \psi|^2 - \frac{1}{2} |\psi|^2 + \frac{1}{4} |\psi|^4 \\ &= \frac{1}{2} (f')^2 + \frac{f^2}{2r^2} + \frac{1}{4} (1 - f^2)^2 - \frac{1}{4}, \end{aligned}$$

which, up to a constant, is the desired form of the free energy. It is a good exercise to show that the Euler-Lagrange equations,

$$\frac{\partial (r\mathcal{F})}{\partial f} - \frac{d}{dr} \left(\frac{\partial (r\mathcal{F})}{\partial f'} \right) = 0$$

results in the same ODE we obtained for f in part (c). We now insert the trial form for $f(r)$ into F . The resulting integrals are elementary, and we obtain

$$F(a, R) = \frac{1}{4}\pi\epsilon_0 \left\{ 1 - \frac{a^4}{(R^2 + a^2)^2} + 2 \ln \left(\frac{R^2}{a^2} + 1 \right) + \frac{R^2 a^2}{R^2 + a^2} \right\}.$$

Taking the limit $R \rightarrow \infty$, we have

$$F(a, R \rightarrow \infty) = 2 \ln \left(\frac{R^2}{a^2} \right) + a^2.$$

We now extremize with respect to a , which yields $a = \sqrt{2}$. Note that the energy in the vortex state is logarithmically infinite. In order to have a finite total free energy (relative to the ground state), we need to introduce an *antivortex* somewhere in the system. An antivortex has a phase winding which is opposite to that of the vortex, *i.e.* $\psi = f e^{-i\phi}$. If the vortex and antivortex separation is r , the energy is

$$V(r) = \frac{1}{2}\pi\epsilon_0 \ln \left(\frac{r^2}{a^2} + 1 \right).$$

This tends to $V(r) = \pi\epsilon_0 \ln(d/a)$ for $d \gg a$ and smoothly approaches $V(0) = 0$, since when $r = 0$ the vortex and antivortex annihilate leaving the ground state condensate. Recall that two-dimensional point charges also interact via a logarithmic potential, according to Maxwell's equations. Indeed, there is a rather extensive analogy between the physics of two-dimensional models with $O(2)$ symmetry and $(2 + 1)$ -dimensional electrodynamics.

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #6 SOLUTIONS

(1) Consider the situation in §7.6.2 of the notes, where a temperature gradient is applied at constant pressure. Show that there is no resulting particle current: $\mathbf{j} = 0$.

Solution : We have

$$\begin{aligned} \mathbf{j} &= - \int \frac{d^3p}{h^3} \frac{\tau(\varepsilon - h)}{k_B T^2} f^0(\mathbf{v} \cdot \nabla T) \mathbf{v} \\ &= - \frac{2\tau}{3mk_B T^2} \nabla T \cdot \frac{2}{\sqrt{\pi}} (k_B T)^{-3/2} \int_0^\infty d\varepsilon \varepsilon^{1/2} e^{-\varepsilon/k_B T} \cdot \varepsilon(\varepsilon - h) \end{aligned} \quad (1)$$

Now we have that

$$\langle \varepsilon^s \rangle \equiv \frac{2}{\sqrt{\pi}} (k_B T)^{-3/2} \int_0^\infty d\varepsilon \varepsilon^{s+1/2} e^{-\varepsilon/k_B T} = \frac{\Gamma(\frac{3}{2} + s)}{\Gamma(\frac{3}{2})} (k_B T)^s. \quad (2)$$

Thus,

$$\langle \varepsilon^2 \rangle = \frac{3}{2} \cdot \frac{5}{2} (k_B T)^2 = \langle \varepsilon \rangle h, \quad (3)$$

since $h = \frac{5}{2} k_B T$. Thus, $\mathbf{j} = 0$.

(2) Consider a nonequilibrium distribution of the form

$$f(\mathbf{r}, \mathbf{p}, t = 0) = n\lambda_T^3 e^{-\mathbf{p}^2/2mk_B T} \left(1 + \frac{\alpha \mathbf{p}^2}{2mk_B T} \right)$$

and investigate its relaxation to the equilibrium distribution $f^0(\mathbf{p}) = n\lambda_T^3 e^{-\mathbf{p}^2/2mk_B T}$ using the Boltzmann equation in the relaxation time approximation, with no external forces. Find $f(\mathbf{r}, \mathbf{p}, t)$. Then find $N(t)$ and $E(t)$, the time-dependent values for the total particle number and total energy. You may abbreviate $N_0 \equiv nV$, where V is the system volume and N_0 is the number of particles at equilibrium. Then, drawing upon your understanding of collisional invariants, explain why your calculation is complete BS. What has gone wrong?

Solution : It is convenient to express everything in terms of the single particle energy $\varepsilon = \mathbf{p}^2/2m$:

$$f(\mathbf{p}, t = 0) = n\lambda_T^3 e^{-\beta\varepsilon} (1 + \alpha \cdot \beta\varepsilon) = f^0 (1 + \alpha \cdot \beta\varepsilon), \quad (4)$$

where $\beta = 1/k_B T$ as usual. In the absence of temperature or velocity gradients, and with no external forces, the Boltzmann equation takes the form

$$\frac{\partial \delta f}{\partial t} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}. \quad (5)$$

Within the relaxation time approximation, then,

$$\frac{\partial \delta f}{\partial t} = -\frac{\delta f}{\tau} \Rightarrow \delta f(\mathbf{p}, t) = \delta f(\mathbf{p}, 0) e^{-t/\tau} . \quad (6)$$

So we have

$$f(\mathbf{p}, t) = f^0 + \alpha \beta \varepsilon f^0 e^{-t/\tau} . \quad (7)$$

Recall further that we may write

$$\frac{d^3 p}{h^3} f^0(\mathbf{p}) = \frac{2}{\sqrt{\pi}} (k_B T)^{-3} d\varepsilon e^{1/2} e^{-\beta\varepsilon} \equiv n P_{\text{MB}}(\varepsilon) d\varepsilon , \quad (8)$$

with

$$\langle \varepsilon^s \rangle = \int_0^\infty d\varepsilon P_{\text{MB}}(\varepsilon) \varepsilon^s = \frac{\Gamma(\frac{3}{2} + s)}{\Gamma(\frac{3}{2})} (k_B T)^s . \quad (9)$$

Thus, we find

$$N(t) = N_0 \left(1 + \frac{3}{2} \alpha e^{-t/\tau} \right) \quad (10)$$

$$E(t) = \frac{3}{2} N_0 k_B T \left(1 + \frac{15}{4} \alpha e^{-t/\tau} \right) , \quad (11)$$

where $N_0 = nV$. We see that neither particle number nor total energy are conserved, which is clearly wrong. This is a defect of the relaxation time approximation. In general, the collision integral must annihilate the five *collisional invariants*, which are total particle number, total energy, and the three components of the total momentum. These quantities are all conserved by the collisions. Every quantity other than these should relax on some microscopic time scale, but the collisional invariants don't relax at all, and the relaxation time approximation (RTA) is too crude to distinguish between the collisional invariants and other quantities – everything relaxes at the same rate within the RTA.

Incidentally, there is a minor modification to the relaxation time approximation collision integral which results in number conservation, although it does not yield energy conservation. This is the so-called BGK collision integral, named for P. L. Bhatnagar, E. P. Gross, and M. Krook, *Phys. Rev.* **94**, 511 (1954). BGK took

$$\left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = -\frac{f(\mathbf{r}, \mathbf{p}, t)}{\tau} + \frac{n(\mathbf{r}, t)}{n_0(\mathbf{r})} \frac{f^0(\mathbf{r}, \mathbf{p})}{\tau} , \quad (12)$$

where

$$n(\mathbf{r}, t) = \int \frac{d^3 p}{h^3} f(\mathbf{r}, \mathbf{p}, t) \quad (13)$$

$$n_0(\mathbf{r}) = \int \frac{d^3 p}{h^3} f^0(\mathbf{r}, \mathbf{p}) . \quad (14)$$

Note then that

$$\int \frac{d^3 p}{h^3} \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = 0 , \quad (15)$$

and there is local number conservation by collisions¹. The nice thing about the BTG collision integral is that it is still linear in f .

(3) Consider a classical gas of charged particles in the presence of a magnetic field \mathbf{B} . The Boltzmann equation is then given by

$$\frac{\varepsilon - h}{k_B T^2} f^0 \mathbf{v} \cdot \nabla T - \frac{e}{mc} \mathbf{v} \times \mathbf{B} \cdot \frac{\partial \delta f}{\partial \mathbf{v}} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}.$$

Consider the case where $T = T(x)$ and $\mathbf{B} = B\hat{\mathbf{z}}$. Making the relaxation time approximation, show that a solution to the above equation exists in the form $\delta f = \mathbf{v} \cdot \mathbf{A}(\varepsilon)$, where $\mathbf{A}(\varepsilon)$ is a vector-valued function of $\varepsilon(\mathbf{v}) = \frac{1}{2}m\mathbf{v}^2$ which lies in the (x, y) plane. Find the energy current \mathbf{j}_ε . Interpret your result physically.

Solution : We'll use index notation and the Einstein summation convention for ease of presentation. Recall that the curl is given by $(\mathbf{A} \times \mathbf{B})_\mu = \epsilon_{\mu\nu\lambda} A_\nu B_\lambda$. We write $\delta f = v_\mu A_\mu(\varepsilon)$, and compute

$$\frac{\partial \delta f}{\partial v_\lambda} = A_\lambda + v_\alpha \frac{\partial A_\alpha}{\partial v_\lambda} \quad (16)$$

$$= A_\lambda + v_\lambda v_\alpha \frac{\partial A_\alpha}{\partial \varepsilon}. \quad (17)$$

Thus,

$$\begin{aligned} \mathbf{v} \times \mathbf{B} \cdot \frac{\partial \delta f}{\partial \mathbf{v}} &= \epsilon_{\mu\nu\lambda} v_\mu B_\nu \frac{\partial \delta f}{\partial v_\lambda} \\ &= \epsilon_{\mu\nu\lambda} v_\mu B_\nu \left(A_\lambda + v_\lambda v_\alpha \frac{\partial A_\alpha}{\partial \varepsilon} \right) \\ &= \epsilon_{\mu\nu\lambda} v_\mu B_\nu A_\lambda. \end{aligned} \quad (18)$$

We then have

$$\frac{\varepsilon - h}{k_B T^2} f^0 v_\mu \partial_\mu T = \frac{e}{mc} \epsilon_{\mu\nu\lambda} v_\mu B_\nu A_\lambda - \frac{v_\mu A_\mu}{\tau}. \quad (19)$$

Since this must be true for all \mathbf{v} , we have

$$A_\mu - \frac{eB\tau}{mc} \epsilon_{\mu\nu\lambda} n_\nu A_\lambda = -\frac{(\varepsilon - h)\tau}{k_B T^2} f^0 \partial_\mu T, \quad (20)$$

where $\mathbf{B} \equiv B\hat{\mathbf{n}}$. It is conventional to define the *cyclotron frequency*, $\omega_c = eB/mc$, in which case

$$(\delta_{\mu\nu} + \omega_c \tau \epsilon_{\mu\nu\lambda} n_\lambda) A_\nu = X_\mu, \quad (21)$$

where $\mathbf{X} = -(\varepsilon - h)\tau f^0 \nabla T / k_B T^2$. So we must invert the matrix

$$M_{\mu\nu} = \delta_{\mu\nu} + \omega_c \tau \epsilon_{\mu\nu\lambda} n_\lambda. \quad (22)$$

¹The BGK collision integral also can be used in the presence of streaming terms.

To do so, we make the *Ansatz*,

$$M_{\nu\sigma}^{-1} = A \delta_{\nu\sigma} + B n_\nu n_\sigma + C \epsilon_{\nu\sigma\rho} n_\rho, \quad (23)$$

and we determine the constants A , B , and C by demanding

$$\begin{aligned} M_{\mu\nu} M_{\nu\sigma}^{-1} &= (\delta_{\mu\nu} + \omega_c \tau \epsilon_{\mu\nu\lambda} n_\lambda) (A \delta_{\nu\sigma} + B n_\nu n_\sigma + C \epsilon_{\nu\sigma\rho} n_\rho) \\ &= (A - C \omega_c \tau) \delta_{\mu\sigma} + (B + C \omega_c \tau) n_\mu n_\sigma + (C + A \omega_c \tau) \epsilon_{\mu\sigma\rho} n_\rho \\ &\equiv \delta_{\mu\sigma}. \end{aligned} \quad (24)$$

Here we have used the result

$$\epsilon_{\mu\nu\lambda} \epsilon_{\nu\sigma\rho} = \epsilon_{\nu\lambda\mu} \epsilon_{\nu\sigma\rho} = \delta_{\lambda\sigma} \delta_{\mu\rho} - \delta_{\lambda\rho} \delta_{\mu\sigma}, \quad (25)$$

as well as the fact that \hat{n} is a unit vector: $n_\mu n_\mu = 1$. We can now read off the results:

$$A - C \omega_c \tau = 1, \quad B + C \omega_c \tau = 0, \quad C + A \omega_c \tau = 0, \quad (26)$$

which entail

$$A = \frac{1}{1 + \omega_c^2 \tau^2}, \quad B = \frac{\omega_c^2 \tau^2}{1 + \omega_c^2 \tau^2}, \quad C = -\frac{\omega_c \tau}{1 + \omega_c^2 \tau^2}. \quad (27)$$

So we can now write

$$A_\mu = M_{\mu\nu}^{-1} X_\nu = \frac{\delta_{\mu\nu} + \omega_c^2 \tau^2 n_\mu n_\nu - \omega_c \tau \epsilon_{\mu\nu\lambda} n_\lambda}{1 + \omega_c^2 \tau^2} X_\nu. \quad (28)$$

The α -component of the energy current is

$$j_\varepsilon^\alpha = \int \frac{d^3p}{h^3} v_\alpha \varepsilon_\alpha v_\mu A_\mu(\varepsilon) = \frac{2}{3m} \int \frac{d^3p}{h^3} \varepsilon^2 A_\alpha(\varepsilon), \quad (29)$$

where we have replaced $v_\alpha v_\mu \rightarrow \frac{2}{3m} \varepsilon \delta_{\alpha\mu}$. Next, we use

$$\frac{2}{3m} \int \frac{d^3p}{h^3} \varepsilon^2 X_\nu = -\frac{5\tau}{3m} k_B^2 T \frac{\partial T}{\partial x_\nu}, \quad (30)$$

hence

$$j_\varepsilon = -\frac{5\tau}{3m} \frac{k_B^2 T}{1 + \omega_c^2 \tau^2} \left(\nabla T + \omega_c^2 \tau^2 \hat{n} (\hat{n} \cdot \nabla T) + \omega_c \tau \hat{n} \times \nabla T \right). \quad (31)$$

We are given that $\hat{n} = \hat{z}$ and $\nabla T = T'(x) \hat{x}$. We see that the energy current j_ε is flowing both along $-\hat{x}$ and along $-\hat{y}$. Why does heat flow along \hat{y} ? It is because the particles are charged, and as they individually flow along $-\hat{x}$, there is a Lorentz force in the $-\hat{y}$ direction, so the energy flows along $-\hat{y}$ as well.

(4) Consider one dimensional motion according to the equation

$$\dot{p} + \gamma p = \eta(t),$$

and compute the average $\langle p^4(t) \rangle$. You should assume that

$$\langle \eta(s_1) \eta(s_2) \eta(s_3) \eta(s_4) \rangle = \phi(s_1 - s_2) \phi(s_3 - s_4) + \phi(s_1 - s_3) \phi(s_2 - s_4) + \phi(s_1 - s_4) \phi(s_2 - s_3)$$

where $\phi(s) = \Gamma \delta(s)$. You may further assume that $p(0) = 0$.

Solution: Integrating the Langevin equation, we have

$$p(t) = \int_0^t dt_1 e^{-\gamma(t-t_1)} \eta(t_1). \quad (32)$$

Raising this to the fourth power and taking the average, we have

$$\begin{aligned} \langle p^4(t) \rangle &= \int_0^t dt_1 e^{-\gamma(t-t_1)} \int_0^t dt_2 e^{-\gamma(t-t_2)} \int_0^t dt_3 e^{-\gamma(t-t_3)} \int_0^t dt_4 e^{-\gamma(t-t_4)} \langle \eta(t_1) \eta(t_2) \eta(t_3) \eta(t_4) \rangle \\ &= 3\Gamma^2 \int_0^t dt_1 e^{-2\gamma(t-t_1)} \int_0^t dt_2 e^{-2\gamma(t-t_2)} = \frac{3\Gamma^2}{4\gamma^2} (1 - e^{-2\gamma t})^2. \end{aligned} \quad (33)$$

We have here used the fact that the three contributions to the average of the product of the four η 's each contribute the same amount to $\langle p^4(t) \rangle$. Recall $\Gamma = 2M\gamma k_B T$, where M is the mass of the particle. Note that

$$\langle p^4(t) \rangle = 3 \langle p^2(t) \rangle^2. \quad (34)$$

(5) *For the brave only!* Due to quantum coherence effects in the backscattering from impurities, one-dimensional wires don't obey Ohm's law (in the limit where the 'inelastic mean free path' is greater than the sample dimensions, which you may assume). Rather, let $\mathcal{R}(L) = R(L)/(h/e^2)$ be the dimensionless resistance of a quantum wire of length L , in units of $h/e^2 = 25.813 \text{ k}\Omega$. Then the dimensionless resistance of a quantum wire of length $L + \delta L$ is given by

$$\begin{aligned} \mathcal{R}(L + \delta L) &= \mathcal{R}(L) + \mathcal{R}(\delta L) + 2\mathcal{R}(L)\mathcal{R}(\delta L) \\ &\quad + 2\cos\alpha \sqrt{\mathcal{R}(L)[1 + \mathcal{R}(L)]\mathcal{R}(\delta L)[1 + \mathcal{R}(\delta L)]}, \end{aligned}$$

where α is a *random phase* uniformly distributed over the interval $[0, 2\pi)$. Here,

$$\mathcal{R}(\delta L) = \frac{\delta L}{2\ell},$$

is the dimensionless resistance of a small segment of wire, of length $\delta L \lesssim \ell$, where ℓ is the 'elastic mean free path'. (Using the Boltzmann equation, we would obtain $\ell = 2\pi\hbar n\tau/m$.)

Show that the distribution function $P(\mathcal{R}, L)$ for resistances of a quantum wire obeys the equation

$$\frac{\partial P}{\partial L} = \frac{1}{2\ell} \frac{\partial}{\partial \mathcal{R}} \left\{ \mathcal{R}(1 + \mathcal{R}) \frac{\partial P}{\partial \mathcal{R}} \right\}.$$

Show that this equation may be solved in the limits $\mathcal{R} \ll 1$ and $\mathcal{R} \gg 1$, with

$$P(\mathcal{R}, z) = \frac{1}{z} e^{-\mathcal{R}/z}$$

for $\mathcal{R} \ll 1$, and

$$P(\mathcal{R}, z) = (4\pi z)^{-1/2} \frac{1}{\mathcal{R}} e^{-(\ln \mathcal{R} - z)^2/4z}$$

for $\mathcal{R} \gg 1$, where $z = L/2\ell$ is the dimensionless length of the wire. Compute $\langle \mathcal{R} \rangle$ in the former case, and $\langle \ln \mathcal{R} \rangle$ in the latter case.

Solution: From the composition rule for series quantum resistances, we derive the phase averages

$$\langle \delta \mathcal{R} \rangle = \left(1 + 2 \mathcal{R}(L)\right) \frac{\delta L}{2\ell} \quad (35)$$

$$\langle (\delta \mathcal{R})^2 \rangle = \left(1 + 2 \mathcal{R}(L)\right)^2 \left(\frac{\delta L}{2\ell}\right)^2 + 2 \mathcal{R}(L) \left(1 + \mathcal{R}(L)\right) \frac{\delta L}{2\ell} \left(1 + \frac{\delta L}{2\ell}\right) \quad (36)$$

$$= 2 \mathcal{R}(L) \left(1 + \mathcal{R}(L)\right) \frac{\delta L}{2\ell} + \mathcal{O}((\delta L)^2), \quad (37)$$

whence we obtain the drift and diffusion terms

$$F_1(\mathcal{R}) = \frac{2 \mathcal{R} + 1}{2\ell}, \quad F_2(\mathcal{R}) = \frac{\mathcal{R}(1 + \mathcal{R})}{2\ell}. \quad (38)$$

Note that $F_1(\mathcal{R}) = dF_2/d\mathcal{R}$, which allows us to write the Fokker-Planck equation as

$$\frac{\partial P}{\partial L} = \frac{\partial}{\partial \mathcal{R}} \left\{ \frac{\mathcal{R}(1 + \mathcal{R})}{2\ell} \frac{\partial P}{\partial \mathcal{R}} \right\}. \quad (39)$$

Defining the dimensionless length $z = L/2\ell$, we have

$$\frac{\partial P}{\partial z} = \frac{\partial}{\partial \mathcal{R}} \left\{ \mathcal{R}(1 + \mathcal{R}) \frac{\partial P}{\partial \mathcal{R}} \right\}. \quad (40)$$

In the limit $\mathcal{R} \ll 1$, this reduces to

$$\frac{\partial P}{\partial z} = \mathcal{R} \frac{\partial^2 P}{\partial \mathcal{R}^2} + \frac{\partial P}{\partial \mathcal{R}}, \quad (41)$$

which is satisfied by $P(\mathcal{R}, z) = z^{-1} \exp(-\mathcal{R}/z)$. For this distribution one has $\langle \mathcal{R} \rangle = z$.

In the opposite limit, $\mathcal{R} \gg 1$, we have

$$\frac{\partial P}{\partial z} = \mathcal{R}^2 \frac{\partial^2 P}{\partial \mathcal{R}^2} + 2 \mathcal{R} \frac{\partial P}{\partial \mathcal{R}} \quad (42)$$

$$= \frac{\partial^2 P}{\partial \nu^2} + \frac{\partial P}{\partial \nu}, \quad (43)$$

where $\nu \equiv \ln \mathcal{R}$. This is solved by the log-normal distribution,

$$P(\mathcal{R}, z) = (4\pi z)^{-1/2} e^{-(\nu+z)^2/4z} . \quad (44)$$

Note that

$$P(\mathcal{R}, z) d\mathcal{R} = (4\pi z)^{-1/2} \exp \left\{ -\frac{(\ln \mathcal{R} - z)^2}{4z} \right\} d \ln \mathcal{R} . \quad (45)$$

One then obtains $\langle \ln \mathcal{R} \rangle = z$.

**PHYSICS 140B : STATISTICAL PHYSICS
PRACTICE MIDTERM SOLUTIONS**

Consider a four-state ferromagnetic Ising model with the Hamiltonian

$$\hat{H} = -J_1 \sum_{\langle ij \rangle} S_i S_j - J_2 \sum_{\langle\langle ij \rangle\rangle} S_i S_j - H \sum_i S_i,$$

where the first sum is over all nearest neighbor pairs and the second sum is over all next nearest neighbor pairs. The spin variables S_i take values in the set $\{-\frac{3}{2}, -\frac{1}{2}, +\frac{1}{2}, +\frac{3}{2}\}$.

- (a) Making the mean field *Ansatz* $S_i = m + (S_i - m)$, where $m = \langle S_i \rangle$ is presumed independent of i , derive the mean field Hamiltonian \hat{H}_{MF} . You may denote z_1 as the number of nearest neighbors and z_2 as the number of next nearest neighbors of any site on the lattice.

[15 points]

Solution: As usual, we neglect fluctuations and obtain

$$\hat{H}_{\text{MF}} = \frac{1}{2} N \hat{J}(0) m^2 - (\hat{J}(0) m + H) \sum_i S_i,$$

where

$$\hat{J}(0) = \sum_{\mathbf{R}} J(\mathbf{R}) = z_1 J_1 + z_2 J_2.$$

- (b) Find the mean field free energy $F(m, T, H)$.

[15 points]

Solution: The free energy is obtained from the partition function,

$$\begin{aligned} Z &= e^{-\beta F} = e^{-\frac{1}{2} N \beta \hat{J}(0) m^2} \left(\text{Tr}_S e^{\beta (\hat{J}(0) m + H) S} \right)^N \\ &= e^{-\frac{1}{2} N \beta \hat{J}(0) m^2} \left[2 \cosh \left(\frac{\hat{J}(0) m + H}{2 k_B T} \right) + 2 \cosh \left(\frac{3(\hat{J}(0) m + H)}{2 k_B T} \right) \right]^N. \end{aligned}$$

Thus,

$$F(m, T, H) = \frac{1}{2} N \hat{J}(0) m^2 - N k_B T \ln \left[2 \cosh \left(\frac{\hat{J}(0) m + H}{2 k_B T} \right) + 2 \cosh \left(\frac{3(\hat{J}(0) m + H)}{2 k_B T} \right) \right].$$

- (c) Adimensionalize, writing $\theta = k_B T / \hat{J}(0)$ and $h = H / \hat{J}(0)$. Find the dimensionless free energy per site $f = F / N \hat{J}(0)$.

[15 points]

Solution: We have

$$f(m, \theta, h) = \frac{1}{2} m^2 - \theta \ln \left[2 \cosh \left(\frac{m + h}{2\theta} \right) + 2 \cosh \left(\frac{3(m + h)}{2\theta} \right) \right].$$

(d) What is the self-consistent mean field equation for m ?

[15 points]

Solution: Setting $\frac{\partial f}{\partial m} = 0$ we obtain the mean field equation

$$m = \frac{\sinh\left(\frac{m+h}{2\theta}\right) + 3 \sinh\left(\frac{3(m+h)}{2\theta}\right)}{2 \cosh\left(\frac{m+h}{2\theta}\right) + 2 \cosh\left(\frac{3(m+h)}{2\theta}\right)}.$$

(e) Find the critical temperature θ_c .

[15 points]

Solution: We set $h = 0$ and expand the RHS of the above equation to lowest order in m . This yields

$$\begin{aligned} m &= \frac{\sinh\left(\frac{m}{2\theta}\right) + 3 \sinh\left(\frac{3m}{2\theta}\right)}{2 \cosh\left(\frac{m}{2\theta}\right) + 2 \cosh\left(\frac{3m}{2\theta}\right)} \\ &= \frac{5m}{4\theta} + \mathcal{O}(m^3). \end{aligned}$$

The critical temperature occurs when the slope of the RHS matches the slope of the LHS, which occurs at $\theta_c = \frac{5}{4}$.

(f) For $\theta > \theta_c$, find $m(h, \theta)$ assuming $|h| \ll 1$.

[15 points]

Solution: For $\theta > \theta_c$, if $|h| \ll 1$ then $|m| \ll 1$ and we can again expand, obtaining
Thus,

$$m \simeq \frac{5(m+h)}{4\theta} \quad \implies \quad m(h) = \frac{5h}{4\theta - 5}.$$

(g) What is the mean field result for $\langle |S_i| \rangle$? Interpret your result in the $\theta \rightarrow \infty$ and $\theta \rightarrow 0$ limits. *Hint: We don't neglect fluctuations from the same site.*

[10 points]

Solution: We have

$$\begin{aligned} \langle |S| \rangle &= \frac{\frac{3}{2} \cdot e^{-3(m+h)2/\theta} + \frac{3}{2} \cdot e^{3(m+h)2/\theta} + \frac{1}{2} \cdot e^{-(m+h)2/\theta} + \frac{1}{2} \cdot e^{(m+h)2/\theta}}{2 \cosh\left(\frac{m+h}{2\theta}\right) + 2 \cosh\left(\frac{3(m+h)}{2\theta}\right)} \\ &= \frac{\cosh\left(\frac{m+h}{2\theta}\right) + 3 \cosh\left(\frac{3(m+h)}{2\theta}\right)}{2 \cosh\left(\frac{m+h}{2\theta}\right) + 2 \cosh\left(\frac{3(m+h)}{2\theta}\right)}. \end{aligned}$$

Note that as $\theta \rightarrow \infty$ we have $\langle |S| \rangle \rightarrow 1$, since all four states are equally probable and two of them have $|S| = \frac{1}{2}$ and the other two have $|S| = \frac{3}{2}$. As $\theta \rightarrow 0$ the ground state configurations are selected. These are two completely polarized states, one with $S_i = +\frac{3}{2} \forall i$ and the other with $S_i = -\frac{3}{2} \forall i$. Thus $\langle |S| \rangle \rightarrow \frac{3}{2}$ in this limit.

**PHYSICS 140B : STATISTICAL PHYSICS
MIDTERM EXAM SOLUTIONS**

Consider a four-state ferromagnetic Ising model with the Hamiltonian

$$\hat{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i,$$

where the first sum is over all links of a lattice of coordination number z . The spin variables S_i take values in the set $\{-1, 0, 0, +1\}$. Note that there are two distinct states, each with $S_i = 0$, and a total of four possible states on each site. Taking the trace for a single site means we sum over the four independent states, one with $S = +1$, two with $S = 0$, and one with $S = -1$.

- (a) Making the mean field *Ansatz* $S_i = m + (S_i - m)$, where $m = \langle S_i \rangle$ is presumed independent of i , derive the mean field Hamiltonian \hat{H}_{MF} .
[15 points]

Solution: As usual, we neglect fluctuations and obtain

$$\hat{H}_{\text{MF}} = \frac{1}{2} N z J m^2 - (z J m + H) \sum_i S_i.$$

- (b) Find the mean field free energy $F(m, T, H)$.
[15 points]

Solution: The free energy is obtained from the partition function,

$$\begin{aligned} Z &= e^{-\beta F} = e^{-\frac{1}{2} N z \beta J m^2} \left(\text{Tr}_S e^{\beta (z J m + H) S} \right)^N \\ &= e^{-\frac{1}{2} N z \beta J m^2} \left[2 + 2 \cosh \left(\frac{z J m + H}{k_B T} \right) \right]^N. \end{aligned}$$

Thus,

$$F(m, T, H) = \frac{1}{2} N z J m^2 - N k_B T \ln \left[2 + 2 \cosh \left(\frac{z J m + H}{k_B T} \right) \right].$$

- (c) Adimensionalize, writing $\theta = k_B T / z J$ and $h = H / z J$. Find the dimensionless free energy per site $f = F / N z J$.
[15 points]

Solution: We have

$$\begin{aligned} f(m, \theta, h) &= \frac{1}{2} m^2 - \theta \ln \left[2 + 2 \cosh \left(\frac{m + h}{\theta} \right) \right] \\ &= \frac{1}{2} m^2 - 2\theta \ln \left[2 \cosh \left(\frac{m + h}{2\theta} \right) \right]. \end{aligned}$$

(d) What is the self-consistent mean field equation for m ?

[15 points]

Solution: Setting $\frac{\partial f}{\partial m} = 0$ we obtain the mean field equation

$$m = \tanh\left(\frac{m+h}{2\theta}\right).$$

(e) Find the critical temperature θ_c . Show that when $h = 0$ the graphical solution to the mean field equation depends on whether $\theta < \theta_c$ or $\theta > \theta_c$.

[15 points]

Solution: We set $h = 0$ and ask when the RHS of the above equation has slope unity. This occurs for $\theta = \theta_c$, where $\theta_c = \frac{1}{2}$. The graphical solution is depicted in fig 6.4 of the lecture notes.

(f) For $\theta > \theta_c$, find $m(h, \theta)$ assuming $|h| \ll 1$.

[15 points]

Solution: For $\theta > \theta_c$, if $|h| \ll 1$ then $|m| \ll 1$ and we can replace the tanh function by the first term in its Taylor series. Thus,

$$m \simeq \frac{m+h}{2\theta} \quad \implies \quad m(h) = \frac{h}{2\theta - 1}.$$

(g) What is the mean field result for $\langle S_i^2 \rangle$?

Hint: We don't neglect fluctuations from the same site.

[10 points]

Solution: We have

$$\begin{aligned} \langle S^2 \rangle &= \frac{(-1)^2 \cdot e^{-(m+h)/\theta} + 2 \cdot (0)^2 \cdot e^0 + (+1)^2 \cdot e^{(m+h)/\theta}}{e^{-(m+h)/\theta} + 2 \cdot e^0 + e^{(m+h)/\theta}} \\ &= \frac{\cosh\left(\frac{m+h}{\theta}\right)}{1 + \cosh\left(\frac{m+h}{\theta}\right)}. \end{aligned}$$

Note that as $\theta \rightarrow \infty$ we have $\langle S^2 \rangle \rightarrow \frac{1}{2}$, since all four states are equally probable and two of them have $S^2 = +1$ and the other two have $S^2 = 0$. As $\theta \rightarrow 0$ the ground state configurations are selected. These are two completely polarized states, one with $S_i = +1 \forall i$ and the other with $S_i = -1 \forall i$. Thus $\langle S^2 \rangle \rightarrow 1$ in this limit.

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

(1) Consider a spin-2 Ising model with Hamiltonian

$$\hat{H} = -\frac{1}{2} \sum_{i,j} J_{ij} S_i S_j - H \sum_i S_i$$

where $S_i \in \{-2, -1, 0, 1, 2\}$. The system is on a simple cubic lattice, with nearest neighbor coupling $J_1/k_B = 40$ K and next-nearest neighbor coupling $J_2/k_B = 10$ K.

- (a) Find the mean field free energy per site $f(\theta, h, m)$, where $\theta = k_B T / \hat{J}(0)$, $h = H / \hat{J}(0)$, $m = \langle S_i \rangle$, and $f = F / N \hat{J}(0)$.
 [5 points]
- (b) Find the mean field equation for m .
 [5 points]
- (c) Setting $h = 0$, find θ_c . What is T_c ?
 [5 points]
- (d) Find the linear magnetic susceptibility $\chi(\theta)$ for $\theta > \theta_c$.
 [5 points]
- (e) For $0 < \theta_c - \theta \ll 1$ and $h = 0$, the magnetization is of the form $m = A(\theta_c - \theta)^{1/2}$. Find the coefficient A .
 [5 points]

Solution : The mean field Hamiltonian is

$$\hat{H}_{\text{MF}} = \frac{1}{2} N \hat{J}(0) m^2 - (H + \hat{J}(0) m) \sum_i S_i. \quad (1)$$

Here

$$\hat{J}(0)/k_B = z_1 J_1/k_B + z_2 J_2/k_B = 360 \text{ K}, \quad (2)$$

since $z_1 = 6$ and $z_2 = 12$ on the simple cubic lattice. We'll need this number in part (c). Computing the partition function $Z_{\text{MF}} = \text{Tr} \exp(-\beta \hat{H}_{\text{MF}})$, taking the logarithm, and dividing by $N \hat{J}(0)$, we find

$$(a) \quad f = \frac{1}{2} m^2 - \theta \ln \left(1 + 2 \cosh \left(\frac{m+h}{\theta} \right) + 2 \cosh \left(\frac{2m+2h}{\theta} \right) \right) \quad (3)$$

The mean field equation is obtained by setting $\frac{\partial f}{\partial m} = 0$. Thus,

$$(b) \quad m = \frac{2 \sinh \left(\frac{m+h}{\theta} \right) + 4 \sinh \left(\frac{2m+2h}{\theta} \right)}{1 + 2 \cosh \left(\frac{m+h}{\theta} \right) + 2 \cosh \left(\frac{2m+2h}{\theta} \right)} \quad (4)$$

To find θ_c , we set $h = 0$ and equate the slopes of the LHS and RHS of the above equation. This yields

$$(c) \quad \boxed{\theta_c = 2 \Rightarrow T_c = \hat{J}(0) \theta_c = 720 \text{ K}} \quad (5)$$

To find the zero field susceptibility, we assume that m and h are both small and expand the RHS of the self-consistency equation, yielding

$$(d) \quad \boxed{m(h, \theta) = \frac{2h}{\theta - 2} \Rightarrow \chi(\theta) = \frac{2}{\theta - 2}} \quad (6)$$

When $\theta < \theta_c$, we need to expand the RHS of the self-consistency equation to order m^3 . Equivalently, we can work from f , and using $\cosh x = 1 + \frac{x^2}{2} + \frac{x^4}{24} + \dots$, we have

$$\begin{aligned} f &= \frac{1}{2}m^2 - \theta \ln \left(5 + \frac{m^2}{\theta^2} + \frac{m^4}{12\theta^4} + \dots + \frac{4m^2}{\theta^2} + \frac{4m^4}{3\theta^4} + \dots \right) \\ &= -\theta \ln 5 + \frac{1}{2}m^2 - \theta \ln \left(1 + \frac{m^2}{\theta^2} + \frac{17m^4}{60\theta^4} + \dots \right) \\ &= -\theta \ln 5 + \frac{\theta - 2}{2\theta} m^2 + \frac{13m^4}{60\theta^3} + \dots, \end{aligned} \quad (7)$$

since $\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots$. We can directly differentiate this with respect to m^2 and obtain

$$(e) \quad \boxed{m^2 = \frac{15}{13} \theta^2 (2 - \theta) \simeq \frac{60}{13} (2 - \theta) \Rightarrow A = 2\sqrt{\frac{15}{13}}} \quad (8)$$

In deriving the above result we have assumed $\theta \approx \theta_c = 2$ and worked only to lowest order in the difference $\theta_c - \theta$.

(2) The Landau free energy of a crystalline magnet is given by the expression

$$f = \frac{1}{2}\alpha t (m_x^2 + m_y^2) + \frac{1}{4}b_1 (m_x^4 + m_y^4) + \frac{1}{2}b_2 m_x^2 m_y^2,$$

where the constants α and b_1 are both positive, and where t is the dimensionless reduced temperature, $t = (T - T_c)/T_c$.

(a) Rescale, so that f is of the form

$$f = \varepsilon_0 \left\{ \frac{1}{2}t (\phi_x^2 + \phi_y^2) + \frac{1}{4}(\phi_x^4 + \phi_y^4 + 2\lambda \phi_x^2 \phi_y^2) \right\},$$

where $m_{x,y} = s \phi_{x,y}$, where s is a scale factor. Find the appropriate scale factor and find expressions for the energy scale ε_0 and the dimensionless parameter λ in terms of α , b_1 , and b_2 .

[5 points]

(b) For what values of λ is the free energy unbounded from below?

[5 points]

- (c) Find the equations which minimize f as a function of $\phi_{x,y}$.
[5 points]
- (d) Show that there are three distinct phases: one in which $\phi_x = \phi_y = 0$ (phase I), another in which one of $\phi_{x,y}$ vanishes but the other is finite (phase II) and one in which both of $\phi_{x,y}$ are finite (phase III). Find f in each of these phases, and be clear to identify any constraints on the parameters t and λ .
[5 points]
- (e) Sketch the phase diagram for this theory in the (t, λ) plane, clearly identifying the unphysical region where f is unbounded, and indicating the phase boundaries for all phase transitions. Make sure to label the phase transitions according to whether they are first or second order.
[5 points]

Solution : It is a simple matter to find

$$(a) \quad m_{x,y} = \sqrt{\frac{\alpha}{b_1}} \phi_{x,y} \quad , \quad \varepsilon_0 = \frac{\alpha^2}{b_1} \quad , \quad \lambda = \frac{b_2}{b_1} \quad (9)$$

Note that

$$f = \frac{1}{4} \varepsilon_0 \begin{pmatrix} \phi_x^2 & \phi_y^2 \end{pmatrix} \begin{pmatrix} 1 & \lambda \\ \lambda & 1 \end{pmatrix} \begin{pmatrix} \phi_x^2 \\ \phi_y^2 \end{pmatrix} + \frac{1}{2} \varepsilon_0 \begin{pmatrix} \phi_x^2 & \phi_y^2 \end{pmatrix} \begin{pmatrix} t \\ t \end{pmatrix} \quad (10)$$

We need to make sure that the quartic term goes to positive infinity when the fields $\phi_{x,y}$ tend to infinity. Else the free energy will not be bounded from below and the model is unphysical. Clearly the matrix in the first term on the RHS has eigenvalues $1 \pm \lambda$ and corresponding (unnormalized) eigenvectors $\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$. Since $\phi_{x,y}^2$ cannot be negative, we only need worry about the eigenvalue $1 + \lambda$. This is negative for $\lambda < -1$. Thus,

$$(b) \quad \lambda \leq -1 \text{ is unphysical} \quad (11)$$

Differentiating with respect to $\phi_{x,y}$ yields the equations

$$(c1) \quad \frac{\partial f}{\partial \phi_x} = (t + \phi_x^2 + \lambda \phi_y^2) \phi_x = 0 \quad , \quad (c2) \quad \frac{\partial f}{\partial \phi_y} = (t + \phi_y^2 + \lambda \phi_x^2) \phi_y = 0 \quad (12)$$

Clearly phase I with $\phi_x = \phi_y = 0$ is a solution to these equations. In phase II, we set one of the fields to zero, $\phi_y = 0$ and solve for $\phi_x = \sqrt{-t}$, which requires $t < 0$. A corresponding solution exists if we exchange $\phi_x \leftrightarrow \phi_y$. In phase III, we solve

$$\begin{pmatrix} 1 & \lambda \\ \lambda & 1 \end{pmatrix} \begin{pmatrix} \phi_x^2 \\ \phi_y^2 \end{pmatrix} = - \begin{pmatrix} t \\ t \end{pmatrix} \quad \Rightarrow \quad \phi_x^2 = \phi_y^2 = -\frac{t}{1 + \lambda} \quad (13)$$

This phase also exists only for $t < 0$, and $\lambda > -1$ as well, which is required if the free energy is to be bounded from below. Thus, we find

$$(d1) \quad (\phi_{x,I}, \phi_{y,I}) = (0, 0) \quad , \quad f_I = 0 \quad (14)$$

$$(d2) \quad (\phi_{x,II}, \phi_{y,II}) = (\pm\sqrt{-t}, 0) \text{ or } (0, \pm\sqrt{-t}) \quad , \quad f_{II} = -\frac{1}{4}\varepsilon_0 t^2 \quad (15)$$

$$(d3) \quad (\phi_{x,III}, \phi_{y,III}) = \pm\sqrt{\frac{-t}{1+\lambda}} (1, 1) \text{ or } \pm\sqrt{\frac{-t}{1+\lambda}} (1, -1) \quad , \quad f_{III} = -\frac{\varepsilon_0 t^2}{2(1+\lambda)} \quad (16)$$

To find the phase diagram, we note that phase I has the lowest free energy for $t > 0$. For $t < 0$ we find

$$f_{III} - f_{II} = \frac{1}{4}\varepsilon_0 t^2 \frac{\lambda - 1}{\lambda + 1} \quad , \quad (17)$$

which is negative for $|\lambda| < 1$. Thus, the phase diagram is as depicted in fig. 1.

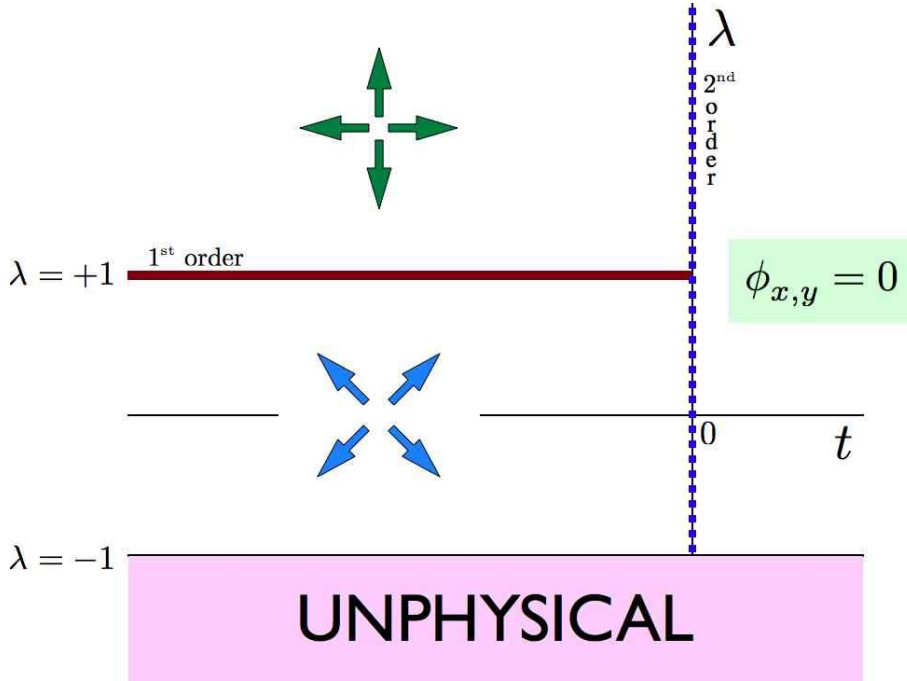


Figure 1: (e) Phase diagram for problem (2).

(3) A photon gas in equilibrium is described by the distribution function

$$f^0(\mathbf{p}) = \frac{2}{e^{cp/k_B T} - 1} \quad ,$$

where the factor of 2 comes from summing over the two independent polarization states.

- (a) Consider a photon gas (in three dimensions) slightly out of equilibrium, but in steady state under the influence of a temperature gradient ∇T . Write $f = f^0 + \delta f$ and write the Boltzmann equation in the relaxation time approximation. Remember that $\varepsilon(\mathbf{p}) = cp$ and $\mathbf{v} = \frac{\partial \varepsilon}{\partial \mathbf{p}} = c\hat{\mathbf{p}}$, so the speed is always c .
[10 points]

- (b) What is the formal expression for the energy current, expressed as an integral of something times the distribution f ?
[5 points]
- (c) Compute the thermal conductivity κ . It is OK for your expression to involve *dimensionless* integrals.
[10 points]

Solution : We have

$$df^0 = -\frac{2cp e^{\beta cp}}{(e^{\beta cp} - 1)^2} d\beta = \frac{2cp e^{\beta cp}}{(e^{\beta cp} - 1)^2} \frac{dT}{k_B T^2}. \quad (18)$$

The steady state Boltzmann equation is $\mathbf{v} \cdot \frac{\partial f^0}{\partial \mathbf{r}} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}$, hence with $\mathbf{v} = c\hat{\mathbf{p}}$,

$$(a) \quad \boxed{-\frac{2c^2 e^{cp/k_B T}}{(e^{cp/k_B T} - 1)^2} \frac{1}{k_B T^2} \mathbf{p} \cdot \nabla T = -\frac{\delta f}{\tau}} \quad (19)$$

The energy current is given by

$$(b) \quad \boxed{\mathbf{j}_\varepsilon(\mathbf{r}) = \int \frac{d^3 p}{h^3} c^2 \mathbf{p} f(\mathbf{p}, \mathbf{r})} \quad (20)$$

Integrating, we find

$$\begin{aligned} \kappa &= \frac{2c^4 \tau}{3h^3 k_B T^2} \int d^3 p \frac{p^2 e^{cp/k_B T}}{(e^{cp/k_B T} - 1)^2} \\ &= \frac{8\pi k_B \tau}{3c} \left(\frac{k_B T}{c} \right)^3 \int_0^\infty ds \frac{s^4 e^s}{(e^s - 1)^2} \\ &= \frac{4k_B \tau}{3\pi^2 c} \left(\frac{k_B T}{c} \right)^3 \int_0^\infty ds \frac{s^3}{e^s - 1}, \end{aligned} \quad (21)$$

where we simplified the integrand somewhat using integration by parts. The integral may be computed in closed form:

$$\mathcal{I}_n = \int_0^\infty ds \frac{s^n}{e^s - 1} = \Gamma(n+1) \zeta(n+1) \quad \Rightarrow \quad \mathcal{I}_3 = \frac{\pi^4}{15}, \quad (22)$$

and therefore

$$(c) \quad \boxed{\kappa = \frac{\pi^2 k_B \tau}{45 c} \left(\frac{k_B T}{c} \right)^3} \quad (23)$$

(4) At the surface of every metal a dipolar layer develops which lowers the potential energy for electrons inside the metal. Some electrons near the surface escape to the outside, leaving a positively charged layer behind, while overall there is charge neutrality. The situation is depicted in fig. 2. The electron density outside the metal is very low and Maxwell-Boltzmann statistics are appropriate.

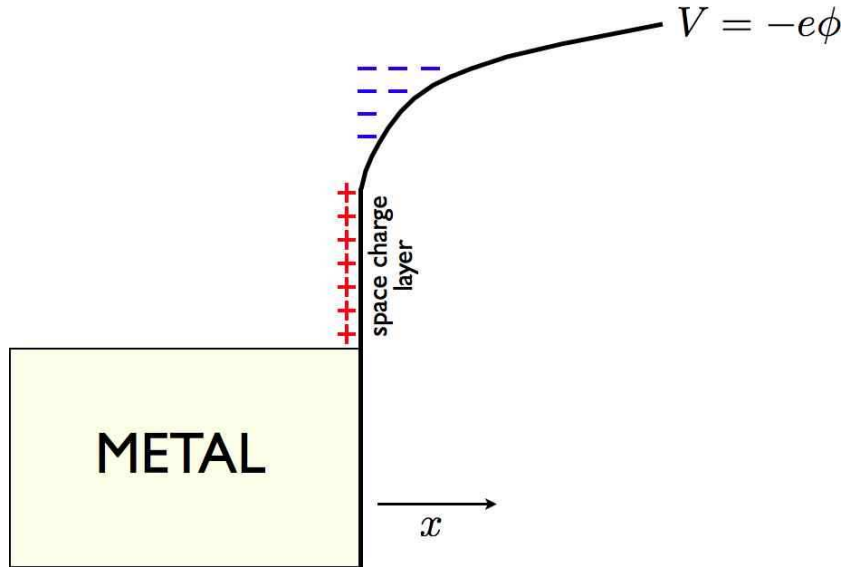


Figure 2: Electron distribution in the vicinity of the surface of a metal.

- (a) Consider a flat metallic surface, normal to \hat{x} , located at $x = 0$. Assume for $x > 0$ an electronic distribution $n(x) = n_0 \exp(e\phi/k_B T)$, where ϕ is the electric potential. For $x > 0$ there are only electrons; all the positive charges are located within the metal. Write down the self-consistent equation for the potential $\phi(x)$.
[5 points]
- (b) Having found the self-consistent equation for $\phi(x)$, show that, multiplying by $\phi'(x)$, the equation can be integrated once, analogous to the conservation of energy for mechanical systems (with ϕ playing the role of the coordinate and x playing the role of time). Show that the equation can be integrated once again to yield $\phi(x)$, with the constant determined by the requirement that $n(x = 0) = n_0$.
[15 points]
- (c) Find $n(x)$.
[5 points]

Solution : The self-consistent equation is Poisson's equation,

$$(a) \quad \nabla^2 \phi = -4\pi\rho = 4\pi en_0 e^{e\phi/k_B T} \quad (24)$$

Since the only variation is along x , we have

$$\frac{d^2\phi}{dx^2} = 4\pi en_0 e^{e\phi/k_B T}. \quad (25)$$

Multiplying each side by $\frac{d\phi}{dx}$, we have

$$\frac{d}{dx}\left(\frac{1}{2}\phi'^2\right) = \frac{d}{dx}\left(4\pi n_0 k_B T e^{e\phi/k_B T}\right), \quad (26)$$

and integrating this equation from x to ∞ we obtain

$$\frac{d\phi}{dx} = -(8\pi n_0 k_B T)^{1/2} e^{e\phi/2k_B T}. \quad (27)$$

Note also the choice of sign here, due to the fact that the potential $-e\phi$ for electrons must increase with x . The boundary term at $x = \infty$ must vanish since $n(\infty) = 0$, which requires $e^{e\phi(\infty)/k_B T} = 0$.

Integrating once more, we have

$$e^{-e\phi(x)/2k_B T} = \left(\frac{2\pi n_0 e^2}{k_B T}\right)^{1/2} (x + a), \quad (28)$$

where a is a constant of integration. Since $n(x = 0) \equiv n_0$, we must have $\phi(0) = 0$, and hence

$$a = \left(\frac{k_B T}{2\pi n_0 e^2}\right)^{1/2}. \quad (29)$$

Thus,

$$(b) \quad \boxed{\phi(x) = -\frac{2k_B T}{e} \ln\left(\frac{x+a}{a}\right)} \quad \text{with} \quad \boxed{a = \left(\frac{k_B T}{2\pi n_0 e^2}\right)^{1/2}} \quad (30)$$

The electron number distribution is then

$$(c) \quad \boxed{n(x) = n_0 \left(\frac{a}{x+a}\right)^2} \quad (31)$$