

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #1 SOLUTIONS

(1) Consider the contraption in Fig. 1. At each of k steps, a particle can fork to either the left ($n_j = 1$) or to the right ($n_j = 0$). The final location is then a k -digit binary number.

- (a) Assume the probability for moving to the left is p and the probability for moving to the right is $q \equiv 1 - p$ at each fork, independent of what happens at any of the other forks. *I.e.* all the forks are uncorrelated. Compute $\langle X_k \rangle$. *Hint:* X_k can be represented as a k -digit binary number, *i.e.* $X_k = n_{k-1}n_{k-2} \cdots n_1n_0 = \sum_{j=0}^{k-1} 2^j n_j$.
- (b) Compute $\langle X_k^2 \rangle$ and the variance $\langle X_k^2 \rangle - \langle X_k \rangle^2$.
- (c) X_k may be written as the sum of k random numbers. Does X_k satisfy the central limit theorem as $k \rightarrow \infty$? Why or why not?

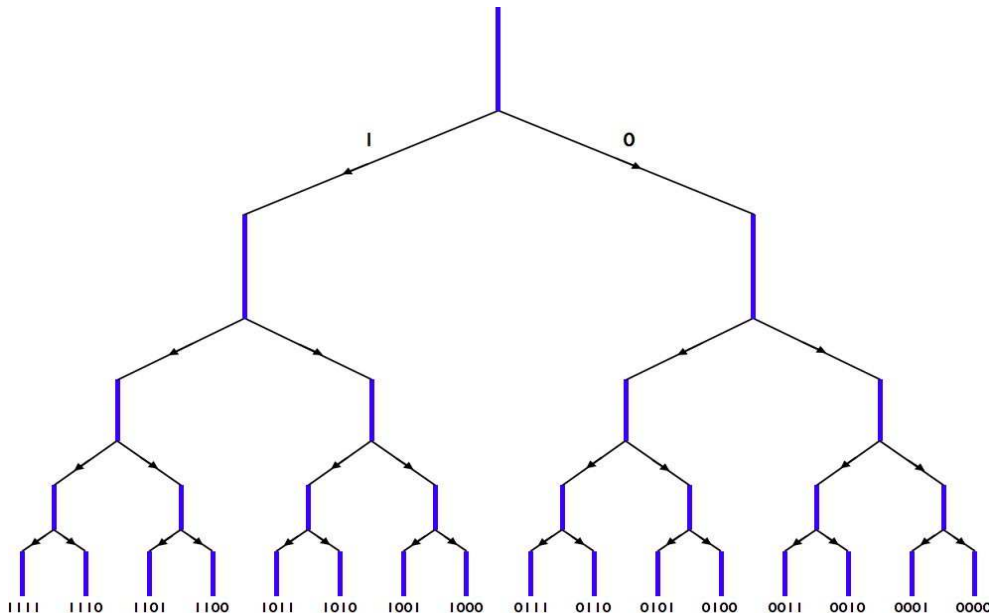


Figure 1: Generator for a k -digit random binary number ($k = 4$ shown).

Solution :

(a) The position after k forks can be written as a k -digit binary number: $n_{k-1}n_{k-2} \cdots n_1n_0$. Thus,

$$X_k = \sum_{j=0}^{k-1} 2^j n_j ,$$

where $n_j = 0$ or 1 according to $P_n = p \delta_{n,1} + q \delta_{n,0}$. Now it is clear that $\langle n_j \rangle = p$, and

therefore

$$\langle X_k \rangle = p \sum_{j=0}^{k-1} 2^j = p \cdot (2^k - 1).$$

(b) The variance in X_k is

$$\begin{aligned} \text{Var}(X_k) &= \langle X_k^2 \rangle - \langle X_k \rangle^2 = \sum_{j=0}^{k-1} \sum_{j'=0}^{k-1} 2^{j+j'} \left(\langle n_j n_{j'} \rangle - \langle n_j \rangle \langle n_{j'} \rangle \right) \\ &= p(1-p) \sum_{j=0}^{k-1} 4^j = p(1-p) \cdot \frac{1}{3} (4^k - 1), \end{aligned}$$

since $\langle n_j n_{j'} \rangle - \langle n_j \rangle \langle n_{j'} \rangle = p(1-p) \delta_{jj'}$.

(c) Clearly the distribution of X_k does not obey the CLT, since $\langle X_k \rangle$ scales exponentially with k . Also note

$$\lim_{k \rightarrow \infty} \frac{\sqrt{\text{Var}(X_k)}}{\langle X_k \rangle} = \sqrt{\frac{1-p}{3p}},$$

which is a constant. For distributions obeying the CLT, the ratio of the rms fluctuations to the mean scales as the inverse square root of the number of trials. The reason that this distribution does not obey the CLT is that the variance of the individual terms is increasing with j .

(2) Let $P(x) = (2\pi\sigma^2)^{-1/2} e^{-(x-\mu)^2/2\sigma^2}$. Compute the following integrals:

(a) $I = \int_{-\infty}^{\infty} dx P(x) x^3.$

(b) $I = \int_{-\infty}^{\infty} dx P(x) \cos(Qx).$

(c) $I = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy P(x) P(y) e^{xy}.$ You may set $\mu = 0$ to make this somewhat simpler.

Under what conditions does this expression converge?

Solution :

(a) Write

$$x^3 = (x - \mu + \mu)^3 = (x - \mu)^3 + 3(x - \mu)^2\mu + 3(x - \mu)\mu^2 + \mu^3,$$

so that

$$\langle x^3 \rangle = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} dt e^{-t^2/2\sigma^2} \left\{ t^3 + 3t^2\mu + 3t\mu^2 + \mu^3 \right\}.$$

Since $\exp(-t^2/2\sigma^2)$ is an even function of t , odd powers of t integrate to zero. We have $\langle t^2 \rangle = \sigma^2$, so

$$\langle x^3 \rangle = \mu^3 + 3\mu\sigma^2 .$$

A nice trick for evaluating $\langle t^{2k} \rangle$:

$$\begin{aligned} \langle t^{2k} \rangle &= \frac{\int_{-\infty}^{\infty} dt e^{-\lambda t^2} t^{2k}}{\int_{-\infty}^{\infty} dt e^{-\lambda t^2}} = \frac{(-1)^k \frac{d^k}{d\lambda^k} \int_{-\infty}^{\infty} dt e^{-\lambda t^2}}{\int_{-\infty}^{\infty} dt e^{-\lambda t^2}} = \frac{(-1)^k}{\sqrt{\lambda}} \frac{d^k \sqrt{\lambda}}{d\lambda^k} \Big|_{\lambda=1/2\sigma^2} \\ &= \frac{1}{2} \cdot \frac{3}{2} \dots \frac{(2k-1)}{2} \lambda^{-k} \Big|_{\lambda=1/2\sigma^2} = \frac{(2k)!}{2^k k!} \sigma^{2k} . \end{aligned}$$

(b) We have

$$\begin{aligned} \langle \cos(Qx) \rangle &= \text{Re} \langle e^{iQx} \rangle = \text{Re} \left[\frac{e^{iQ\mu}}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} dt e^{-t^2/2\sigma^2} e^{iQt} \right] \\ &= \text{Re} \left[e^{iQ\mu} e^{-Q^2\sigma^2/2} \right] = \cos(Q\mu) e^{-Q^2\sigma^2/2} . \end{aligned}$$

Here we have used the result

$$\frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} dt e^{-\alpha t^2 - \beta t} = \sqrt{\frac{\pi}{\alpha}} e^{\beta^2/4\alpha}$$

with $\alpha = 1/2\sigma^2$ and $\beta = -iQ$. Another way to do it is to use the general result derive above in part (a) for $\langle t^{2k} \rangle$ and do the sum:

$$\begin{aligned} \langle \cos(Qx) \rangle &= \text{Re} \langle e^{iQx} \rangle = \text{Re} \left[\frac{e^{iQ\mu}}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} dt e^{-t^2/2\sigma^2} e^{iQt} \right] \\ &= \cos(Q\mu) \sum_{k=0}^{\infty} \frac{(-Q^2)^k}{(2k)!} \langle t^{2k} \rangle = \cos(Q\mu) \sum_{k=0}^{\infty} \frac{1}{k!} \left(-\frac{1}{2}Q^2\sigma^2\right)^k \\ &= \cos(Q\mu) e^{-Q^2\sigma^2/2} . \end{aligned}$$

(c) We have

$$I = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy P(x) P(y) e^{\kappa^2 xy} = \frac{e^{-\mu^2/2\sigma^2}}{2\pi\sigma^2} \int d^2x e^{-\frac{1}{2}A_{ij} x_i x_j} e^{b_i x_i} ,$$

where $\mathbf{x} = (x, y)$,

$$A = \begin{pmatrix} \sigma^2 & -\kappa^2 \\ -\kappa^2 & \sigma^2 \end{pmatrix} , \quad \mathbf{b} = \begin{pmatrix} \mu/\sigma^2 \\ \mu/\sigma^2 \end{pmatrix} .$$

Using the general formula for the Gaussian integral,

$$\int d^n x e^{-\frac{1}{2} A_{ij} x_i x_j} e^{b_i x_i} = \frac{(2\pi)^{n/2}}{\sqrt{\det(A)}} \exp\left(\frac{1}{2} A_{ij}^{-1} b_i b_j\right),$$

we obtain

$$I = \frac{1}{\sqrt{1 - \kappa^4 \sigma^4}} \exp\left(\frac{\mu^2 \kappa^2}{1 - \kappa^2 \sigma^2}\right).$$

Convergence requires $\kappa^2 \sigma^2 < 1$.

(3) The binomial distribution,

$$B_N(n, p) = \binom{N}{n} p^n (1-p)^{N-n},$$

tells us the probability for n successes in N trials if the individual trial success probability is p . The average number of successes is $\nu = \sum_{n=0}^N n B_N(n, p) = Np$. Consider the limit $N \rightarrow \infty$.

- (a) Show that the probability of n successes becomes a function of n and ν alone. That is, evaluate

$$P_\nu(n) = \lim_{N \rightarrow \infty} B_N(n, \nu/N).$$

This is the *Poisson distribution*.

- (b) Show that the moments of the Poisson distribution are given by

$$\langle n^k \rangle = e^{-\nu} \left(\nu \frac{\partial}{\partial \nu} \right)^k e^\nu.$$

- (c) Evaluate the mean and variance of the Poisson distribution.

The Poisson distribution is also known as the *law of rare events* since $p = \nu/N \rightarrow 0$ in the $N \rightarrow \infty$ limit. See http://en.wikipedia.org/wiki/Poisson_distribution#Occurrence for some amusing applications of the Poisson distribution.

Solution :

(a) We have

$$P_\nu(n) = \lim_{N \rightarrow \infty} \frac{N!}{n!(N-n)!} \left(\frac{\nu}{N}\right)^n \left(1 - \frac{\nu}{N}\right)^{N-n}.$$

Note that

$$(N-n)! \simeq (N-n)^{N-n} e^{n-N} = N^{N-n} \left(1 - \frac{n}{N}\right)^N e^{n-N} \rightarrow N^{N-n} e^N,$$

where we have used the result $\lim_{N \rightarrow \infty} \left(1 + \frac{x}{N}\right)^N = e^x$. Thus, we find

$$P_\nu(n) = \frac{1}{n!} \nu^n e^{-\nu},$$

the Poisson distribution. Note that $\sum_{n=0}^{\infty} P_n(\nu) = 1$ for any ν .

(b) We have

$$\begin{aligned} \langle n^k \rangle &= \sum_{n=0}^{\infty} P_\nu(n) n^k = \sum_{n=0}^{\infty} \frac{1}{n!} n^k \nu^n e^{-\nu} \\ &= e^{-\nu} \left(\nu \frac{d}{d\nu} \right)^k \sum_{n=0}^{\infty} \frac{\nu^n}{n!} = e^{-\nu} \left(\nu \frac{\partial}{\partial \nu} \right)^k e^\nu. \end{aligned}$$

(c) Using the result from (b), we have $\langle n \rangle = \nu$ and $\langle n^2 \rangle = \nu + \nu^2$, hence $\text{Var}(n) = \nu$.

(4) Consider a D -dimensional *random walk* on a hypercubic lattice. The position of a particle after N steps is given by

$$\mathbf{R}_N = \sum_{j=1}^N \hat{\mathbf{n}}_j,$$

where $\hat{\mathbf{n}}_j$ can take on one of $2D$ possible values: $\hat{\mathbf{n}}_j \in \{\pm \hat{\mathbf{e}}_1, \dots, \pm \hat{\mathbf{e}}_D\}$, where $\hat{\mathbf{e}}_\mu$ is the unit vector along the positive x_μ axis. Each of these possible values occurs with probability $1/2D$, and each step is statistically independent from all other steps.

(a) Consider the *generating function* $S_N(\mathbf{k}) = \langle e^{i\mathbf{k} \cdot \mathbf{R}_N} \rangle$. Show that

$$\langle R_N^{\alpha_1} \dots R_N^{\alpha_J} \rangle = \frac{1}{i} \frac{\partial}{\partial k_{\alpha_1}} \dots \frac{1}{i} \frac{\partial}{\partial k_{\alpha_J}} \Big|_{\mathbf{k}=0} S_N(\mathbf{k}).$$

For example, $\langle R_N^\alpha R_N^\beta \rangle = -(\partial^2 S_N(\mathbf{k}) / \partial k_\alpha \partial k_\beta)_{\mathbf{k}=0}$.

(b) Evaluate $S_N(\mathbf{k})$ for the case $D = 3$ and compute the quantities $\langle X_N^4 \rangle$ and $\langle X_N^2 Y_N^2 \rangle$.

Solution :

(a) The result follows immediately from

$$\begin{aligned} \frac{1}{i} \frac{\partial}{\partial k_\alpha} e^{i\mathbf{k} \cdot \mathbf{R}} &= R_\alpha e^{i\mathbf{k} \cdot \mathbf{R}} \\ \frac{1}{i} \frac{\partial}{\partial k_\alpha} \frac{1}{i} \frac{\partial}{\partial k_\beta} e^{i\mathbf{k} \cdot \mathbf{R}} &= R_\alpha R_\beta e^{i\mathbf{k} \cdot \mathbf{R}}, \end{aligned}$$

et cetera. Keep differentiating with respect to the various components of \mathbf{k} .

(b) For $D = 3$, there are six possibilities for $\hat{n}_j : \pm\hat{x}, \pm\hat{y},$ and $\pm\hat{z}$. Each occurs with a probability $\frac{1}{6}$, independent of all the other $\hat{n}_{j'}$ with $j' \neq j$. Thus,

$$\begin{aligned} S_N(\mathbf{k}) &= \prod_{j=1}^N \langle e^{i\mathbf{k} \cdot \hat{n}_j} \rangle = \left[\frac{1}{6} \left(e^{ik_x} + e^{-ik_x} + e^{ik_y} + e^{-ik_y} + e^{ik_z} + e^{-ik_z} \right) \right]^N \\ &= \left(\frac{\cos k_x + \cos k_y + \cos k_z}{3} \right)^N. \end{aligned}$$

We have

$$\begin{aligned} \langle X_N^4 \rangle &= \left. \frac{\partial^4 S(\mathbf{k})}{\partial k_x^4} \right|_{\mathbf{k}=0} = \left. \frac{\partial^4}{\partial k_x^4} \right|_{k_x=0} \left(1 - \frac{1}{6} k_x^2 + \frac{1}{72} k_x^4 + \dots \right)^N \\ &= \left. \frac{\partial^4}{\partial k_x^4} \right|_{k_x=0} \left[1 + N \left(-\frac{1}{6} k_x^2 + \frac{1}{72} k_x^4 + \dots \right) + \frac{1}{2} N(N-1) \left(-\frac{1}{6} k_x^2 + \frac{1}{72} k_x^4 + \dots \right)^2 + \dots \right] \\ &= \left. \frac{\partial^4}{\partial k_x^4} \right|_{k_x=0} \left[1 - \frac{1}{6} N k_x^2 + \frac{1}{72} N^2 k_x^4 + \dots \right] = \frac{1}{3} N^2. \end{aligned}$$

Similarly, we have

$$\begin{aligned} \langle X_N^2 Y_N^2 \rangle &= \left. \frac{\partial^4 S(\mathbf{k})}{\partial k_x^2 \partial k_y^2} \right|_{\mathbf{k}=0} = \left. \frac{\partial^4}{\partial k_x^2 \partial k_y^2} \right|_{k_x=k_y=0} \left(1 - \frac{1}{6} (k_x^2 + k_y^2) + \frac{1}{72} (k_x^4 + k_y^4) + \dots \right)^N \\ &= \left. \frac{\partial^4}{\partial k_x^2 \partial k_y^2} \right|_{k_x=k_y=0} \left[1 + N \left(-\frac{1}{6} (k_x^2 + k_y^2) + \frac{1}{72} (k_x^4 + k_y^4) + \dots \right) + \frac{1}{2} N(N-1) \left(-\frac{1}{6} (k_x^2 + k_y^2) + \dots \right)^2 + \dots \right] \\ &= \left. \frac{\partial^4}{\partial k_x^2 \partial k_y^2} \right|_{k_x=k_y=0} \left[1 - \frac{1}{6} N (k_x^2 + k_y^2) + \frac{1}{72} N^2 (k_x^4 + k_y^4) + \frac{1}{36} k_x^2 k_y^2 + \dots \right] = \frac{1}{9} N(N-1). \end{aligned}$$

(5) A rare disease is known to occur in $f = 0.02\%$ of the general population. Doctors have designed a test for the disease with $\nu = 99.90\%$ sensitivity and $\rho = 99.95\%$ specificity.

- What is the probability that someone who tests positive for the disease is actually sick?
- Suppose the test is administered twice, and the results of the two tests are independent. If a random individual tests positive both times, what are the chances he or she actually has the disease?
- For a binary partition of events, find an expression for $P(X|A \cap B)$ in terms of $P(A|X)$, $P(B|X)$, $P(A|\neg X)$, $P(B|\neg X)$, and the priors $P(X)$ and $P(\neg X) = 1 - P(X)$. You should assume A and B are independent, so $P(A \cap B|X) = P(A|X) \cdot P(B|X)$.

Solution :

(a) Let X indicate that a person is infected, and A indicate that a person has tested positive. We then have $\nu = P(A|X) = 0.9990$ is the sensitivity and $\rho = P(\neg A|\neg X) = 0.9995$ is the specificity. From Bayes' theorem, we have

$$P(X|A) = \frac{P(A|X) \cdot P(X)}{P(A|X) \cdot P(X) + P(A|\neg X) \cdot P(\neg X)} = \frac{\nu f}{\nu f + (1 - \rho)(1 - f)},$$

where $P(A|\neg X) = 1 - P(\neg A|\neg X) = 1 - \rho$ and $P(X) = f$ is the fraction of infected individuals in the general population. With $f = 0.0002$, we find $P(X|A) = 0.2856$.

(b) We now need

$$P(X|A^2) = \frac{P(A^2|X) \cdot P(X)}{P(A^2|X) \cdot P(X) + P(A^2|\neg X) \cdot P(\neg X)} = \frac{\nu^2 f}{\nu^2 f + (1 - \rho)^2(1 - f)},$$

where A^2 indicates two successive, independent tests. We find $P(X|A^2) = 0.9987$.

(c) Assuming A and B are independent, we have

$$\begin{aligned} P(X|A \cap B) &= \frac{P(A \cap B|X) \cdot P(X)}{P(A \cap B|X) \cdot P(X) + P(A \cap B|\neg X) \cdot P(\neg X)} \\ &= \frac{P(A|X) \cdot P(B|X) \cdot P(X)}{P(A|X) \cdot P(B|X) \cdot P(X) + P(A|\neg X) \cdot P(B|\neg X) \cdot P(\neg X)}. \end{aligned}$$

This is exactly the formula used in part (b).

(6) Compute the entropy of the F08 Physics 140A grade distribution (in bits). The distribution is available from <http://physics.ucsd.edu/students/courses/fall2008/physics140>. Assume 11 possible grades: A+, A, A-, B+, B, B-, C+, C, C-, D, F.

$\sum_n N_n = 38$	A+	A	A-	B+	B	B-	C+	C	C-	D	F
N_n	2	9	7	3	9	3	1	2	0	2	0
$-p_n \log_2 p_n$	0.224	0.492	0.450	0.289	0.492	0.289	0.138	0.224	0	0.224	0

Table 1: F08 Physics 140A final grade distribution.

Solution :

Assuming the only possible grades are A+, A, A-, B+, B, B-, C+, C, C-, D, F (11 possibilities), then from the chart we produce the entries in Tab. 1. We then find

$$S = - \sum_{n=1}^{11} p_n \log_2 p_n = 2.82 \text{ bits}$$

For maximum information, set $p_n = \frac{1}{11}$ for all n , whence $S_{\max} = \log_2 11 = 3.46$ bits.

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #2 SOLUTIONS

(1) Consider the matrix

$$M = \begin{pmatrix} 4 & 4 \\ -1 & 9 \end{pmatrix} .$$

- (a) Find the characteristic polynomial $P(\lambda) = \det(\lambda\mathbb{I} - M)$ and the eigenvalues.
 (b) For each eigenvalue λ_α , find the associated right eigenvector R_i^α and left eigenvector L_i^α . Normalize your eigenvectors so that $\langle L^\alpha | R^\beta \rangle = \delta_{\alpha\beta}$.
 (c) Show explicitly that $M_{ij} = \sum_\alpha \lambda_\alpha R_i^\alpha L_j^\alpha$.

Solution :

(a) The characteristic polynomial is

$$P(\lambda) = \det \begin{pmatrix} \lambda - 4 & -4 \\ 1 & \lambda - 9 \end{pmatrix} = \lambda^2 - 13\lambda + 40 = (\lambda - 5)(\lambda - 8) ,$$

so the two eigenvalues are $\lambda_1 = 5$ and $\lambda_2 = 8$.

(b) Let us write the right eigenvectors as $\vec{R}^\alpha = \begin{pmatrix} R_1^\alpha \\ R_2^\alpha \end{pmatrix}$ and the left eigenvectors as $\vec{L}^\alpha = (L_1^\alpha \ L_2^\alpha)$. Having found the eigenvalues, we only need to solve four equations:

$$4R_1^1 + 4R_2^1 = 5R_1^1 \quad , \quad 4R_1^2 + 4R_2^2 = 8R_1^2 \quad , \quad 4L_1^1 - L_2^1 = 5L_1^1 \quad , \quad 4L_1^2 - L_2^2 = 8L_1^2 .$$

We are free to choose $R_1^\alpha = 1$ when possible. We must also satisfy the normalizations $\langle L^\alpha | R^\beta \rangle = L_i^\alpha R_i^\beta = \delta^{\alpha\beta}$. We then find

$$\vec{R}^1 = \begin{pmatrix} 1 \\ \frac{1}{4} \end{pmatrix} \quad , \quad \vec{R}^2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad , \quad \vec{L}^1 = \left(\frac{4}{3} \quad -\frac{4}{3}\right) \quad , \quad \vec{L}^2 = \left(-\frac{1}{3} \quad \frac{4}{3}\right) .$$

(c) The projectors onto the two eigendirections are

$$P_1 = |R^1\rangle\langle L^1| = \begin{pmatrix} \frac{4}{3} & -\frac{4}{3} \\ \frac{1}{3} & -\frac{1}{3} \end{pmatrix} \quad , \quad P_2 = |R^2\rangle\langle L^2| = \begin{pmatrix} -\frac{1}{3} & \frac{4}{3} \\ -\frac{1}{3} & \frac{4}{3} \end{pmatrix} .$$

Note that $P_1 + P_2 = \mathbb{I}$. Now construct

$$\lambda_1 P_1 + \lambda_2 P_2 = \begin{pmatrix} 4 & 4 \\ -1 & 9 \end{pmatrix} ,$$

as expected.

(2) A *Markov chain* is a probabilistic process which describes the transitions of discrete stochastic variables in time. Let $P_i(t)$ be the probability that the system is in state i at time t . The time evolution equation for the probabilities is

$$P_i(t+1) = \sum_j Y_{ij} P_j(t).$$

Thus, we can think of $Y_{ij} = P(i, t+1 | j, t)$ as the *conditional probability* that the system is in state i at time $t+1$ given that it was in state j at time t . Y is called the *transition matrix*. It must satisfy $\sum_i Y_{ij} = 1$ so that the total probability $\sum_i P_i(t)$ is conserved.

Suppose I have two bags of coins. Initially bag A contains two quarters and bag B contains five dimes. Now I do an experiment. Every minute I exchange a random coin chosen from each of the bags. Thus the number of coins in each bag does not fluctuate, but their values do fluctuate.

- Label all possible states of this system, consistent with the initial conditions. (I.e. there are always two quarters and five dimes shared among the two bags.)
- Construct the transition matrix Y_{ij} .
- Show that the total probability is conserved is $\sum_i Y_{ij} = 1$, and verify this is the case for your transition matrix Y . This establishes that $(1, 1, \dots, 1)$ is a left eigenvector of Y corresponding to eigenvalue $\lambda = 1$.
- Find the eigenvalues of Y .
- Show that as $t \rightarrow \infty$, the probability $P_i(t)$ converges to an equilibrium distribution P_i^{eq} which is given by the right eigenvector of i corresponding to eigenvalue $\lambda = 1$. Find P_i^{eq} , and find the long time averages for the value of the coins in each of the bags.

Solution :

(a) There are three possible states consistent with the initial conditions. In state $|1\rangle$, bag A contains two quarters and bag B contains five dimes. In state $|2\rangle$, bag A contains a quarter and a dime while bag B contains a quarter and five dimes. In state $|3\rangle$, bag A contains two dimes while bag B contains three dimes and two quarters. We list these states in the table below, along with their degeneracies. The degeneracy of a state is the number of configurations consistent with the state label. Thus, in state $|2\rangle$ the first coin in bag A could be a quarter and the second a dime, or the first could be a dime and the second a quarter. For bag B, any of the five coins could be the quarter.

(b) To construct Y_{ij} , note that transitions out of state $|1\rangle$, i.e. the elements Y_{i1} , are particularly simple. With probability 1, state $|1\rangle$ always evolves to state $|2\rangle$. Thus, $Y_{21} = 1$ and $Y_{11} = Y_{31} = 0$. Now consider transitions out of state $|2\rangle$. To get to state $|1\rangle$, we need to choose the D from bag A (probability $\frac{1}{2}$) and the Q from bag B (probability $\frac{1}{5}$). Thus,

$Y_{12} = \frac{1}{2} \times \frac{1}{5} = \frac{1}{10}$. For transitions back to state $|2\rangle$, we could choose the Q from bag A (probability $\frac{1}{2}$) if we also chose the Q from bag B (probability $\frac{1}{5}$). Or we could choose the D from bag A (probability $\frac{1}{2}$) and one of the D's from bag B (probability $\frac{4}{5}$). Thus, $Y_{22} = \frac{1}{2} \times \frac{1}{5} + \frac{1}{2} \times \frac{4}{5} = \frac{1}{2}$. Reasoning thusly, one obtains the transition matrix,

$$Y = \begin{pmatrix} 0 & \frac{1}{10} & 0 \\ 1 & \frac{1}{2} & \frac{2}{5} \\ 0 & \frac{2}{5} & \frac{3}{5} \end{pmatrix}.$$

Note that $\sum_i Y_{ij} = 1$.

$ j\rangle$	bag A	bag B	g_j^A	g_j^B	g_j^{TOT}
$ 1\rangle$	QQ	DDDDD	1	1	1
$ 2\rangle$	QD	DDDDQ	2	5	10
$ 3\rangle$	DD	DDDQQ	1	10	10

Table 1: States and their degeneracies.

(c) Our explicit form for Y confirms the sum rule $\sum_i Y_{ij} = 1$ for all j . Thus, $\vec{L}^1 = (1 \ 1 \ 1)$ is a left eigenvector of Y with eigenvalue $\lambda = 1$.

(d) To find the other eigenvalues, we compute the characteristic polynomial of Y and find, easily,

$$P(\lambda) = \det(\lambda \mathbb{I} - Y) = \lambda^3 - \frac{11}{10} \lambda^2 + \frac{1}{25} \lambda + \frac{3}{50}.$$

This is a cubic, however we already know a root, *i.e.* $\lambda = 1$, and we can explicitly verify $P(\lambda = 1) = 0$. Thus, we can divide $P(\lambda)$ by the monomial $\lambda - 1$ to get a quadratic function, which we can factor. One finds after a small bit of work,

$$\frac{P(\lambda)}{\lambda - 1} = \lambda^2 - \frac{3}{10} \lambda - \frac{3}{50} = \left(\lambda - \frac{3}{10}\right) \left(\lambda + \frac{1}{5}\right).$$

Thus, the eigenspectrum of Y is $\lambda_1 = 1$, $\lambda_2 = \frac{3}{10}$, and $\lambda_3 = -\frac{1}{5}$.

(e) We can decompose Y into its eigenvalues and eigenvectors, like we did in problem (1). Write

$$Y_{ij} = \sum_{\alpha=1}^3 \lambda_{\alpha} R_i^{\alpha} L_j^{\alpha}.$$

Now let us start with initial conditions $P_i(0)$ for the three configurations. We can always decompose this vector in the right eigenbasis for Y , *viz.*

$$P_i(t) = \sum_{\alpha=1}^3 C_{\alpha}(t) R_i^{\alpha},$$

The initial conditions are $C_\alpha(0) = \sum_i L_i^\alpha P_i(0)$. But now using our eigendecomposition of Y , we find that the equations for the discrete time evolution for each of the C_α decouple:

$$C_\alpha(t+1) = \lambda_\alpha C_\alpha(t).$$

Clearly as $t \rightarrow \infty$, the contributions from $\alpha = 2$ and $\alpha = 3$ get smaller and smaller, since $C_\alpha(t) = \lambda_\alpha^t C_\alpha(0)$, and both λ_2 and λ_3 are smaller than unity in magnitude. Thus, as $t \rightarrow \infty$ we have $C_1(t) \rightarrow C_1(0)$, and $C_{2,3}(t) \rightarrow 0$. Note $C_1(0) = \sum_i L_i^1 P_i(0) = \sum_i P_i(0) = 1$, since $\vec{L}^1 = (1 \ 1 \ 1)$. Thus, we obtain $P_i(t \rightarrow \infty) \rightarrow R_i^1$, the components of the eigenvector \vec{R}^1 . It is not too hard to explicitly compute the eigenvectors:

$$\begin{aligned} \vec{L}^1 &= (1 \ 1 \ 1) & \vec{L}^2 &= (10 \ 3 \ -4) & \vec{L}^3 &= (10 \ -2 \ 1) \\ \vec{R}^1 &= \frac{1}{21} \begin{pmatrix} 1 \\ 10 \\ 10 \end{pmatrix} & \vec{R}^2 &= \frac{1}{35} \begin{pmatrix} 1 \\ 3 \\ -4 \end{pmatrix} & \vec{R}^3 &= \frac{1}{15} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}. \end{aligned}$$

Thus, the equilibrium distribution $P_i^{\text{eq}} = \lim_{t \rightarrow \infty} P_i(t)$ satisfies detailed balance:

$$P_j^{\text{eq}} = \frac{g_j^{\text{TOT}}}{\sum_l g_l^{\text{TOT}}}.$$

Working out the average coin value in bags A and B under equilibrium conditions, one finds $A = \frac{200}{7}$ and $B = \frac{500}{7}$ (centa), and B/A is simply the ratio of the number of coins in bag B to the number in bag A. Note $A + B = 100$ cents, as the total coin value is conserved.

(3) Poincaré recurrence is guaranteed for phase space dynamics that are *invertible*, *volume preserving*, and acting on a *bounded phase space*.

- Give an example of a map which is volume preserving on a bounded phase space, but which is not invertible and not recurrent.
- Give an example of a map which is invertible on a bounded phase space, but which is not volume preserving and not recurrent.
- Give an example of a map which is invertible and volume preserving, but on an unbounded phase space and not recurrent.

Solution :

(a) Consider the map $f(x) = \text{frac}(x)$, where $\text{frac}(x) = x - \text{gint}(x)$ is the fractional part of x , obtained by subtracting from x the greatest integer less than x . Acting on any set of width less than unity, this map is volume-preserving. However it is many-to-one hence not invertible. For example, $f(\pi) = f(\pi - 1) = f(\pi - 2) = \pi - 3$. For sufficiently small ϵ , the interval $[\pi - \epsilon, \pi + \epsilon]$ gets mapped onto the interval $[\pi - 3 - \epsilon, \pi - 3 + \epsilon]$, never to return to the original interval.

(b) Any dissipative dynamical system will do. For example, consider $\dot{x} = p/m, \dot{p} = -\gamma p$, on some finite region of (x, p) space which contains the origin.

(c) Consider $\dot{x} = p/m, \dot{p} = 0$ on the infinite phase space $(x, p) \in \mathbb{R}^2$. If $p \neq 0$ the x -motion is monotonically increasing or decreasing (*i.e.* either to the right or to the left along the real line).

(4) Consider a toroidal phase space $(x, p) \in \mathbb{T}^2$. You can describe the torus as a square $[0, 1] \times [0, 1]$ with opposite sides identified. Design your own modified Arnold cat map acting on this phase space, *i.e.* a 2×2 matrix with integer coefficients and determinant 1.

(a) Start with an initial distribution localized around the center – say a disc centered at $(\frac{1}{2}, \frac{1}{2})$. Show how these initial conditions evolve under your map. Can you tell whether your dynamics are mixing?

(b) Now take a pixelated image. For reasons discussed in the lecture notes, this image should exhibit Poincaré recurrence. Can you see this happening?

Solution :

(a) Any map

$$\begin{pmatrix} x' \\ p' \end{pmatrix} = \overbrace{\begin{pmatrix} a & b \\ c & d \end{pmatrix}}^M \begin{pmatrix} x \\ p \end{pmatrix},$$

will do, provided $\det M = ad - bc = 1$. Arnold's cat map has $M = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$. Consider the generalized cat map with $M = \begin{pmatrix} 1 & 1 \\ p & p+1 \end{pmatrix}$. Starting from an initial square distribution, we iterate the map up to three times and show the results in Figs. 1, 3, and 5. The numerical results are consistent with a mixing flow. (With just a few further iterations, almost the entire torus is covered.)

(c) A pixelated image exhibits Poincaré recurrence, as we see in Figs. 2, 4, and 6.

(5) Consider a spin singlet formed by two $S = \frac{1}{2}$ particles, $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow_A \downarrow_B\rangle - |\downarrow_A \uparrow_B\rangle)$. Find the reduced density matrix, $\rho_A = \text{Tr}_B |\Psi\rangle\langle\Psi|$.

Solution :

We have

$$|\Psi\rangle\langle\Psi| = \frac{1}{2} |\uparrow_A \downarrow_B\rangle\langle\uparrow_A \downarrow_B| + \frac{1}{2} |\downarrow_A \uparrow_B\rangle\langle\downarrow_A \uparrow_B| - \frac{1}{2} |\uparrow_A \downarrow_B\rangle\langle\downarrow_A \uparrow_B| - \frac{1}{2} |\downarrow_A \uparrow_B\rangle\langle\uparrow_A \downarrow_B|.$$

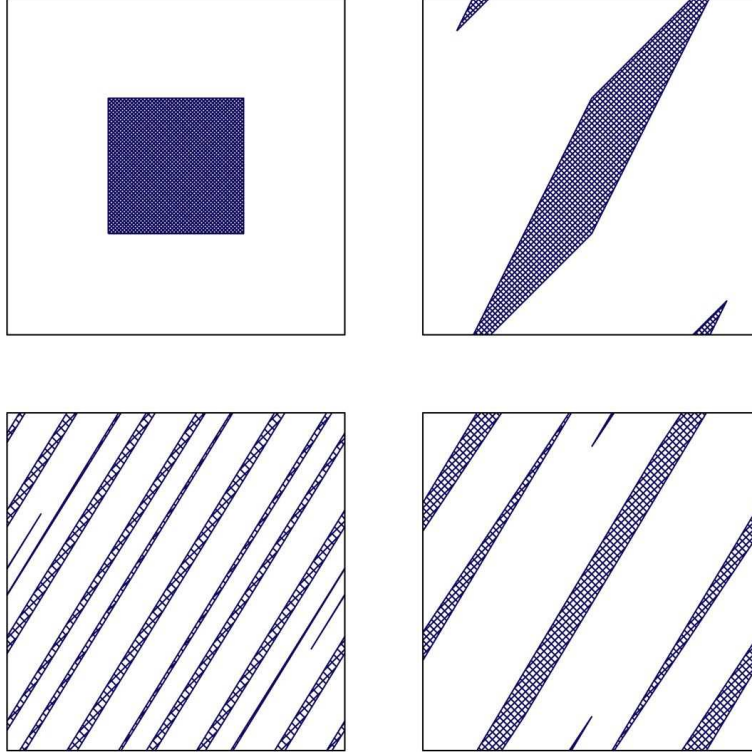


Figure 1: Zeroth, first, second, and third iterates of the generalized cat map with $p = 1$ (i.e. Arnold's cat map), acting on an initial square distribution (clockwise from upper left).



Figure 2: Evolution of a pixelated blobfish under the Arnold cat map.

Now take the trace over the spin degrees of freedom on site B. Only the first two terms contribute, resulting in the reduced density matrix

$$\rho_A = \text{Tr}_B |\Psi\rangle\langle\Psi| = \frac{1}{2} |\uparrow_A\rangle\langle\uparrow_A| + \frac{1}{2} |\downarrow_A\rangle\langle\downarrow_A|.$$

Note that $\text{Tr} \rho_A = 1$, but whereas the full density matrix $\rho = \text{Tr}_B |\Psi\rangle\langle\Psi|$ had one eigenvalue of 1, corresponding to eigenvector $|\Psi\rangle$, and three eigenvalues of 0 (any state or-

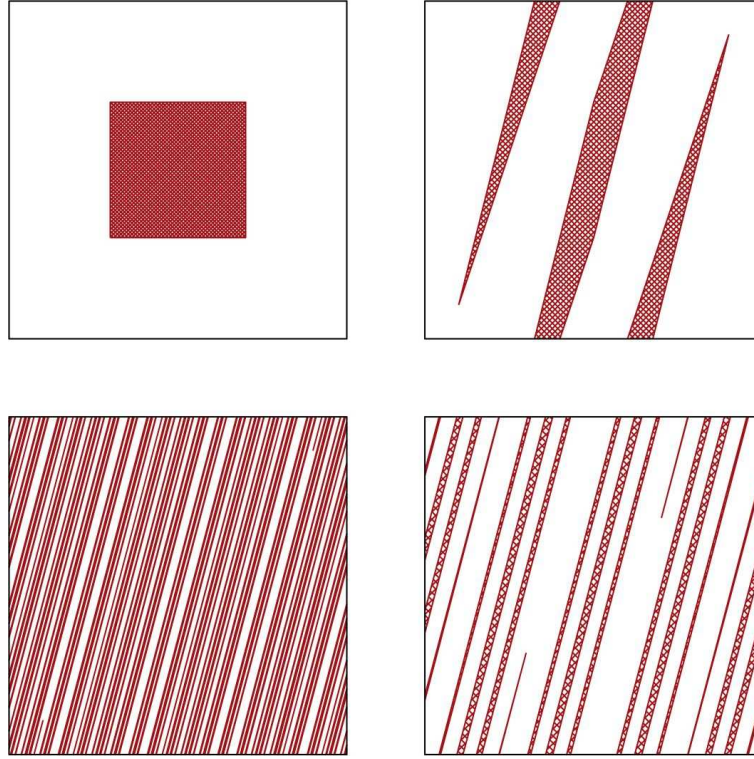


Figure 3: Zeroth, first, second, and third iterates of the generalized cat map with $p = 2$, acting on an initial square distribution (clockwise from upper left).



Figure 4: Evolution of a pixelated blobfish under the $p = 2$ generalized cat map.

thogonal to $|\Psi\rangle$, the reduced density matrix ρ_A does not correspond to a 'pure state' in that it is not a projector. It has two degenerate eigenvalues at $\lambda = \frac{1}{2}$. The quantity $S_A = -\text{Tr} \rho_A \ln \rho_A = \ln 2$ is the *quantum entanglement entropy* for the spin singlet.

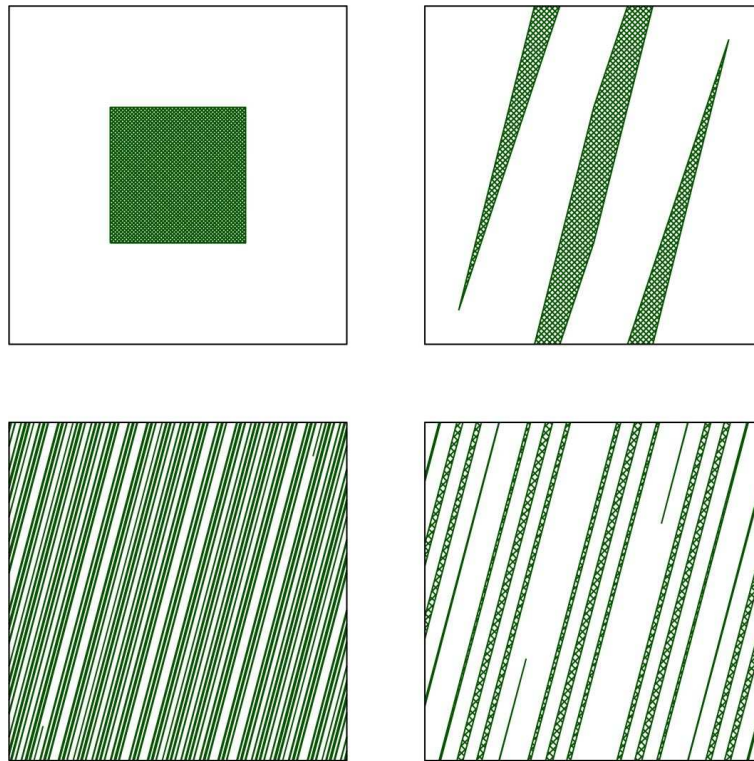


Figure 5: Zeroth, first, second, and third iterates of the generalized cat map with $p = 3$, acting on an initial square distribution (clockwise from upper left).

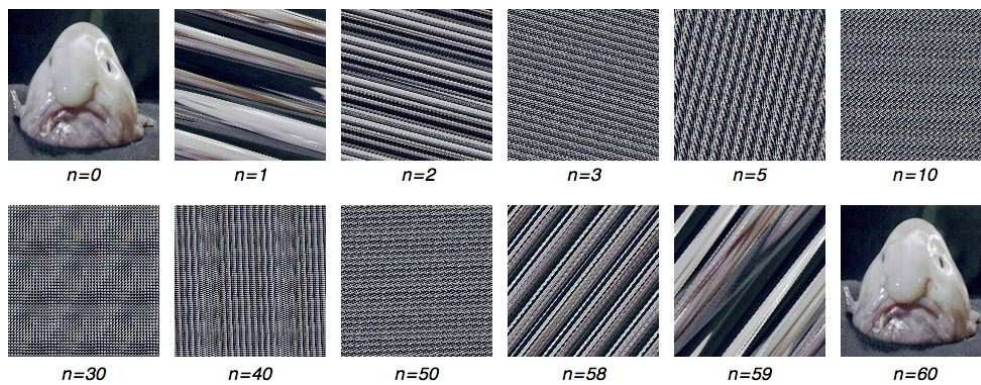


Figure 6: Evolution of a pixelated blobfish under the $p = 3$ generalized cat map.

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #3 SOLUTIONS

(1) Consider a generalization of the situation in §4.4 of the notes where now three reservoirs are in thermal contact, with any pair of systems able to exchange energy.

- (a) Assuming interface energies are negligible, what is the total density of states $D(E)$? Your answer should be expressed in terms of the densities of states functions $D_{1,2,3}$ for the three individual systems.
- (b) Find an expression for $P(E_1, E_2)$, which is the joint probability distribution for system 1 to have energy E_1 while system 2 has energy E_2 and the total energy of all three systems is $E_1 + E_2 + E_3 = E$.
- (c) Extremize $P(E_1, E_2)$ with respect to $E_{1,2}$. Show that this requires the temperatures for all three systems must be equal: $T_1 = T_2 = T_3$. Writing $E_j = E_j^* + \delta E_j$, where E_j^* is the extremal solution ($j = 1, 2$), expand $\ln P(E_1^* + \delta E_1, E_2^* + \delta E_2)$ to second order in the variations δE_j . Remember that

$$S = k_B \ln D \quad , \quad \left(\frac{\partial S}{\partial E} \right)_{V,N} = \frac{1}{T} \quad , \quad \left(\frac{\partial^2 S}{\partial E^2} \right)_{V,N} = -\frac{1}{T^2 C_V} .$$

- (d) Assuming a Gaussian form for $P(E_1, E_2)$ as derived in part (c), find the variance of the energy of system 1,

$$\text{Var}(E_1) = \langle (E_1 - E_1^*)^2 \rangle .$$

Solution :

- (a) The total density of states is a convolution:

$$D(E) = \int_{-\infty}^{\infty} dE_1 \int_{-\infty}^{\infty} dE_2 \int_{-\infty}^{\infty} dE_3 D_1(E_1) D_2(E_2) D_3(E_3) \delta(E - E_1 - E_2 - E_3) .$$

- (b) The joint probability density $P(E_1, E_2)$ is given by

$$P(E_1, E_2) = \frac{D_1(E_1) D_2(E_2) D_3(E - E_1 - E_2)}{D(E)} .$$

- (c) We set the derivatives $\partial \ln P / \partial E_{1,2} = 0$, which gives

$$\frac{\partial \ln P}{\partial E_1} = \frac{\partial \ln D_1}{\partial E_1} - \frac{\partial D_3}{\partial E_3} = 0 \quad , \quad \frac{\partial \ln P}{\partial E_2} = \frac{\partial \ln D_2}{\partial E_2} - \frac{\partial D_3}{\partial E_3} = 0 ,$$

where $E_3 = E - E_1 - E_2$ in the argument of $D_3(E_3)$. Thus, we have

$$\frac{\partial \ln D_1}{\partial E_1} = \frac{\partial \ln D_2}{\partial E_2} = \frac{\partial \ln D_3}{\partial E_3} \equiv \frac{1}{T}.$$

Expanding $\ln P(E_1^* + \delta E_1, E_2^* + \delta E_2)$ to second order in the variations δE_j , we find the first order terms cancel, leaving

$$\ln P(E_1^* + \delta E_1, E_2^* + \delta E_2) = \ln P(E_1^*, E_2^*) - \frac{(\delta E_1)^2}{2k_B T^2 C_1} - \frac{(\delta E_2)^2}{2k_B T^2 C_2} - \frac{(\delta E_1 + \delta E_2)^2}{2k_B T^2 C_3} + \dots,$$

where $\partial^2 \ln D_j / \partial E^2 = -1/2k_B T^2 C_j$, with C_j the heat capacity at constant volume and particle number. Thus,

$$P(E_1, E_2) = \frac{\sqrt{\det(\mathcal{C}^{-1})}}{2\pi k_B T^2} \exp\left(-\frac{1}{2k_B T^2} C_{ij}^{-1} \delta E_i \delta E_j\right),$$

where the matrix \mathcal{C}^{-1} is defined as

$$\mathcal{C}^{-1} = \begin{pmatrix} C_1^{-1} + C_3^{-1} & C_3^{-1} \\ C_3^{-1} & C_2^{-1} + C_3^{-1} \end{pmatrix}.$$

One finds

$$\det(\mathcal{C}^{-1}) = C_1^{-1} C_2^{-1} + C_1^{-1} C_3^{-1} + C_2^{-1} C_3^{-1}.$$

The prefactor in the above expression for $P(E_1, E_2)$ has been fixed by the normalization condition $\int dE_1 \int dE_2 P(E_1, E_2) = 1$.

(d) Integrating over E_2 , we obtain $P(E_1)$:

$$P(E_1) = \int_{-\infty}^{\infty} dE_2 P(E_1, E_2) = \frac{1}{\sqrt{2\pi k_B \tilde{C}_1 T^2}} e^{-(\delta E_1)^2 / 2k_B \tilde{C}_1 T^2},$$

where

$$\tilde{C}_1 = \frac{C_2^{-1} + C_3^{-1}}{C_1^{-1} C_2^{-1} + C_1^{-1} C_3^{-1} + C_2^{-1} C_3^{-1}}.$$

Thus,

$$\langle (\delta E_1)^2 \rangle = \int_{-\infty}^{\infty} dE_1 (\delta E_1)^2 = k_B \tilde{C}_1 T^2.$$

(2) Consider a two-dimensional gas of identical classical, noninteracting, massive relativistic particles with dispersion $\varepsilon(\mathbf{p}) = \sqrt{\mathbf{p}^2 c^2 + m^2 c^4}$.

(a) Compute the free energy $F(T, V, N)$.

(b) Find the entropy $S(T, V, N)$.

(c) Find an equation of state relating the fugacity $z = e^{\mu/k_B T}$ to the temperature T and the pressure p .

Solution :

(a) We have $Z = (\zeta A)^N / N!$ where A is the area and

$$\zeta(T) = \int \frac{d^2 p}{h^2} e^{-\beta \sqrt{p^2 c^2 + m^2 c^4}} = \frac{2\pi}{(\beta \hbar c)^2} (1 + \beta m c^2) e^{-\beta m c^2} .$$

To obtain this result it is convenient to change variables to $u = \beta \sqrt{p^2 c^2 + m^2 c^4}$, in which case $p dp = u du / \beta^2 c^2$, and the lower limit on u is $m c^2$. The free energy is then

$$F = -k_B T \ln Z = N k_B T \ln \left(\frac{2\pi \hbar^2 c^2 N}{(k_B T)^2 A} \right) - N k_B T \ln \left(1 + \frac{m c^2}{k_B T} \right) + N m c^2 .$$

where we are taking the thermodynamic limit with $N \rightarrow \infty$.

(b) We have

$$S = -\frac{\partial F}{\partial T} = -N k_B \ln \left(\frac{2\pi \hbar^2 c^2 N}{(k_B T)^2 A} \right) + N k_B \ln \left(1 + \frac{m c^2}{k_B T} \right) + N k_B \left(\frac{m c^2 + 2 k_B T}{m c^2 + k_B T} \right) .$$

(c) The grand partition function is

$$\Xi(T, V, \mu) = e^{-\beta \Omega} = e^{\beta p V} = \sum_{N=0}^{\infty} Z_N(T, V, N) e^{\beta \mu N} .$$

We then find $\Xi = \exp(\zeta A e^{\beta \mu})$, and

$$p = \frac{(k_B T)^3}{2\pi(\hbar c)^2} \left(1 + \frac{m c^2}{k_B T} \right) e^{(\mu - m c^2)/k_B T} .$$

Note that

$$n = \frac{\partial(\beta p)}{\partial \mu} = \frac{p}{k_B T} \implies p = n k_B T .$$

(3) A three-level system has energy levels $\varepsilon_0 = 0$, $\varepsilon_1 = \Delta$, and $\varepsilon_2 = 4\Delta$. Find the free energy $F(T)$, the entropy $S(T)$ and the heat capacity $C(T)$.

Solution :

We have

$$Z = \text{Tr} e^{-\beta H} = 1 + e^{-\beta \Delta} + e^{-4\beta \Delta} .$$

The free energy is

$$F = -k_B T \ln Z = -k_B T \ln(1 + e^{-\Delta/k_B T} + e^{-4\Delta/k_B T}) .$$

To find the entropy S , we differentiate with respect to temperature:

$$S = -\left. \frac{\partial F}{\partial T} \right|_{V,N} = k_B \ln(1 + e^{-\Delta/k_B T} + e^{-4\Delta/k_B T}) + \frac{\Delta}{T} \cdot \frac{e^{-\Delta/k_B T} + 4e^{-4\Delta/k_B T}}{1 + e^{-\Delta/k_B T} + e^{-4\Delta/k_B T}} .$$

Now differentiate with respect to T one last time to find

$$C_{V,N} = k_B \left(\frac{\Delta}{k_B T} \right)^2 \cdot \frac{e^{-\Delta/k_B T} + 16e^{-4\Delta/k_B T} + 9e^{-5\Delta/k_B T}}{(1 + e^{-\Delta/k_B T} + e^{-4\Delta/k_B T})^2} .$$

(4) Consider a many-body system with Hamiltonian $\hat{H} = \frac{1}{2}\hat{N}(\hat{N} - 1)U$, where \hat{N} is the particle number and $U > 0$ is an interaction energy. Assume the particles are identical and can be described using Maxwell-Boltzmann statistics, as we have discussed. Assuming $\mu = 0$, plot the entropy S and the average particle number N as functions of the scaled temperature $k_B T/U$. (You will need to think about how to impose a numerical cutoff in your calculations.)

Solution :

The grand partition function is

$$\Xi(T, \mu) = e^{-\beta\Omega} = e^{\beta pV} = \sum_{N=0}^{\infty} e^{-N(N-1)\beta U/2} ,$$

where we have taken $\mu = 0$ and we have assumed that each state of definite particle number $|N\rangle$, is nondegenerate. We then have the grand potential

$$\Omega(T, \mu) = -k_B T \ln \Xi = -k_B T \ln \left(\sum_{N=0}^{\infty} e^{-N(N-1)U/2k_B T} \right)$$

The entropy is

$$S = -\frac{\partial \Omega}{\partial T} = k_B \ln \left(\sum_{N=0}^{\infty} e^{-N(N-1)U/2k_B T} \right) + \frac{U}{2T} \cdot \frac{\sum_{N=0}^{\infty} N(N-1) e^{-N(N-1)U/2k_B T}}{\sum_{N=0}^{\infty} e^{-N(N-1)U/2k_B T}} .$$

This must be evaluated numerically. The results are shown in Fig. 1. Note that $\lim_{T \rightarrow 0} S(T) = k_B \ln 2$, which indicates a doubly degenerate ground state. This is because both $|N=0\rangle$ and $|N=1\rangle$ have energy $E_0 = E_1 = 0$.

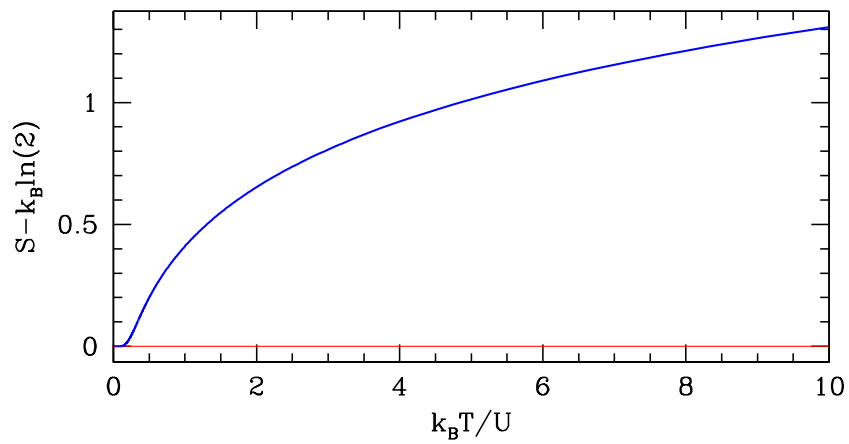


Figure 1: Entropy as a function of dimensionless temperature for problem #4. Note that $S(T = 0) = \ln 2$ because the states $|N = 0\rangle$ and $|N = 1\rangle$ are degenerate.

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #4 SOLUTIONS

(1) Consider a noninteracting classical gas with Hamiltonian

$$\mathcal{H} = \sum_{i=1}^N \varepsilon(\mathbf{p}_i),$$

where $\varepsilon(\mathbf{p})$ is the dispersion relation. Define

$$\xi(T) = h^{-d} \int d^d p e^{-\varepsilon(\mathbf{p})/k_B T}.$$

- (a) Find $F(T, V, N)$.
- (b) Find $G(T, p, N)$.
- (c) Find $\Omega(T, V, \mu)$.
- (d) Show that

$$\beta p \int_0^\infty dV e^{-\beta p V} Z(T, V, N) = e^{-G(T, p, N)/k_B T}.$$

Solution :

(a) We have $Z(T, V, N) = (V\xi)^N/N!$, so

$$F(T, V, N) = -k_B T \ln Z(T, V, N) = -Nk_B T \ln\left(\frac{V}{N}\right) - Nk_B T \ln \xi(T) - Nk_B T.$$

(b) G is obtained from F by Legendre transform: $G = F + pV$, i.e.

$$G(T, p, N) = -Nk_B T \ln\left(\frac{k_B T}{p}\right) - Nk_B T \ln \xi(T).$$

Note that we have used the ideal gas law $pV = Nk_B T$ here.

(c) Ω is obtained from F by Legendre transform: $\Omega = F - \mu N$. Another way to obtain Ω is to use the grand potential $\Xi = \exp(V\xi(T) e^{\mu/k_B T})$, whence

$$\Omega(T, V, \mu) = -Vk_B T \xi(T) e^{\mu/k_B T}.$$

(d) We have

$$Y(T, p, N) = \beta p \int_0^\infty dV e^{-\beta p V} Z(T, V, N) = \frac{\xi^N(T)}{N!} \beta p \int_0^\infty dV V^N e^{-\beta p V} = \left(\frac{k_B T \xi(T)}{p}\right)^N$$

Thus, $G(T, p, N) = -Nk_B T \ln(k_B T \xi/p)$. Note that if we normalize the volume integral differently and define

$$Y(T, p, N) = \int_0^\infty \frac{dV}{V_0} e^{-\beta p V} Z(T, V, N) = \left(\frac{k_B T}{p V_0} \right) \cdot \left(\frac{k_B T \xi(T)}{p} \right)^N,$$

we obtain $G(T, p, N) = -Nk_B T \ln(k_B T \xi/p) - k_B T \ln(k_B T/pV_0)$, which differs from the previous result only by an $\mathcal{O}(N^0)$ term, which is subextensive and hence negligible in the thermodynamic limit.

(2) A three-dimensional gas of magnetic particles in an external magnetic field H is described by the Hamiltonian

$$\mathcal{H} = \sum_i \left[\frac{\mathbf{p}_i^2}{2m} - \mu_0 H \sigma_i \right],$$

where $\sigma_i = \pm 1$ is the spin polarization of particle i and μ_0 is the magnetic moment per particle.

- Working in the ordinary canonical ensemble, derive an expression for the magnetization of system.
- Repeat the calculation for the grand canonical ensemble. Also, find an expression for the Landau free energy $\Omega(T, V, \mu)$.
- Calculate how much heat will be given off by the system when the magnetic field is reduced from H to zero at constant volume, constant temperature, and particle number.

Solution :

(a) The partition function trace is now an integral over all coordinates and momenta with measure $d\mu$ as before, plus a sum over all individual spin polarizations. Thus,

$$\begin{aligned} Z &= \text{Tr} e^{-\mathcal{H}/k_B T} = \frac{1}{N!} \prod_{i=1}^N \sum_{\sigma_i} \int \frac{d^3 x_i d^3 p_i}{h^3} e^{-\mathbf{p}_i^2/2mk_B T} e^{\mu_0 H \sigma_i/k_B T} \\ &= \frac{1}{N!} V^N \lambda_T^{-3N} \left[2 \cosh(\mu_0 H/k_B T) \right]^N, \end{aligned}$$

where $\lambda_T = (2\pi\hbar^2/mk_B T)^{1/2}$ is the thermal wavelength. The Helmholtz free energy is

$$\begin{aligned} F(T, V, H, N) &= -k_B T \ln Z(T, V, H, N) \\ &= -Nk_B T \ln \left(\frac{V}{N \lambda_T^3} \right) - Nk_B T \ln \cosh(\mu_0 H/k_B T) - Nk_B T (1 + \ln 2). \end{aligned}$$

The magnetization is then

$$M(T, V, H, N) = -\frac{\partial F}{\partial H} = N\mu_0 \tanh(\mu_0 H/k_B T) .$$

(b) The grand partition function is

$$\Xi(T, V, H, \mu) = \sum_{N=0}^{\infty} e^{\mu N/k_B T} Z(T, V, N) = \exp \left(V\lambda_T^{-3} \cdot 2 \cosh(\mu_0 H/k_B T) \cdot e^{\mu/k_B T} \right) .$$

Thus,

$$\Omega(T, V, H, \mu) = -k_B T \ln \Xi(T, V, \mu) = -V k_B T \lambda_T^{-3} \cdot 2 \cosh(\mu_0 H/k_B T) \cdot e^{\mu/k_B T} .$$

Then

$$M(T, V, H, \mu) = -\frac{\partial \Omega}{\partial H} = 2\mu_0 \cdot V\lambda_T^{-3} \cdot \sinh(\mu_0 H/k_B T) \cdot e^{\mu/k_B T} .$$

Note that

$$N(T, V, H, \mu) = -\frac{\partial \Omega}{\partial \mu} = V\lambda_T^{-3} \cdot \cosh(\mu_0 H/k_B T) \cdot e^{\mu/k_B T} ,$$

so $M = N\mu_0 \tanh(\mu_0 H/k_B T)$, which agrees with the result from part (a).

(c) Starting with our expression for $F(T, V, N)$ in part (a), we differentiate to find the entropy:

$$S(T, V, H, N) = -\frac{\partial F}{\partial T} = Nk_B \ln \cosh(\mu_0 H/k_B T) - \frac{N\mu_0 H}{T} \tanh(\mu_0 H/k_B T) + S(T, V, 0, N) ,$$

where $S(T, V, 0, N)$ is the entropy at $H = 0$, which we don't need to compute for this problem. The heat absorbed *by* the system is

$$\begin{aligned} Q &= \int dQ = TS(0) - TS(H) = Nk_B T \ln \cosh(\mu_0 H/k_B T) + N\mu_0 H \tanh(\mu_0 H/k_B T) \\ &= Nk_B T \left(x \tanh x - \ln \cosh x \right) , \end{aligned}$$

where $x = \mu_0 H/k_B T$. Defining $f(x) = x \tanh x - \ln \cosh x$, one has $f'(x) = x \operatorname{sech}^2 x$ which is positive for all $x > 0$. Since $f(x)$ is an even function with $f(0) = 0$, we conclude $f(x) > 0$ for $x \neq 0$. Thus, $Q > 0$, which means that the system absorbs heat under this process. *I.e.* the heat released by the system is $(-Q)$.

(3) A classical three-dimensional gas of noninteracting particles has the Hamiltonian

$$\mathcal{H} = \sum_{i=1}^N \left[A |\mathbf{p}_i|^s + B |\mathbf{q}_i|^t \right] ,$$

where s and t are nonnegative real numbers.

- (a) Find the free energy $F(T, V, N)$.
- (b) Find the average energy $E(T, V, N)$.
- (c) Find the grand potential $\Omega(T, V, \mu)$.

Remember the definition of the Gamma function, $\Gamma(z) = \int_{-\infty}^{\infty} du u^{z-1} e^{-u}$.

Solution :

(a) Working in the OCE, the partition function is $Z = \xi_p^N(T) \xi_q^N(T)/N!$, where

$$\xi_p(T) = \frac{1}{h^3} \int d^3p \exp(-Ap^s/k_B T)$$

$$\xi_q(T) = \int d^3q \exp(-Bq^t/k_B T) .$$

We focus first on the momentum integral, changing variables to $u = Ap^s/k_B T$. Then

$$u = \frac{Ap^s}{k_B T} \Rightarrow p = \left(\frac{k_B T u}{A}\right)^{1/s}, \quad p^2 dp = \left(\frac{k_B T}{A}\right)^{3/s} \cdot s^{-1} u^{(3/s)-1} du ,$$

and

$$\begin{aligned} \xi_p(T) &= \frac{1}{h^3} \int d^3p \exp(-Ap^s/k_B T) = \frac{4\pi}{h^3} \left(\frac{k_B T}{A}\right)^{3/s} \cdot \frac{1}{s} \int_{-\infty}^{\infty} du u^{(3/s)-1} e^{-u} \\ &= \frac{4\pi}{sh^3} \Gamma(3/s) \left(\frac{k_B T}{A}\right)^{3/s}, \end{aligned}$$

where we have used $z\Gamma(z) = \Gamma(z+1)$. *Mutatis mutandis*,

$$\xi_q(T) = \int d^3q \exp(-Bq^t/k_B T) = \frac{4\pi}{t} \Gamma(3/t) \left(\frac{k_B T}{B}\right)^{3/t} .$$

Thus, the free energy is

$$F(T, V, N) = -k_B T \ln Z = -Nk_B T \ln \left(\frac{\xi_p(T) \xi_q(T)}{N} \right) - Nk_B T .$$

(b) The average energy is

$$E = \frac{\partial}{\partial \beta} (\beta F) = \left(\frac{3}{s} + \frac{3}{t} \right) Nk_B T .$$

(c) The grand potential is $\Omega = -k_B T \ln \Xi$, and $\Xi = \exp\left(\xi_p(T) \xi_q(T) e^{\mu/k_B T}\right)$. Thus,

$$\Omega(T, V, N) = -k_B T \xi_p(T) \xi_q(T) e^{\mu/k_B T} .$$

Note that F and Ω are both independent of V , which means that the pressure p vanishes!

(4) A gas of nonrelativistic particles of mass m is held in a container at constant pressure p and temperature T . It is free to exchange energy with the outside world, but the particle number N remains fixed. Compute the variance in the system volume, $\text{Var}(V)$, and the ratio $(\Delta V)_{\text{rms}}/\langle V \rangle$. Use the Gibbs ensemble.

Solution : The Gibbs free energy is

$$G(T, p, N) = -N k_B T \ln \left(\frac{k_B T}{p \lambda_T^3} \right) ,$$

where $\lambda_T = (2\pi\hbar^2/mk_B T)^{1/2}$ is the thermal wavelength. Thus, with

$$Y = e^{-G/k_B T} = \int \frac{dV}{V_0} e^{-\beta p V} Z(T, V, N) ,$$

we have

$$\begin{aligned} \langle V \rangle &= -\frac{1}{\beta} \frac{1}{Y} \frac{\partial Y}{\partial p} = \frac{\partial G}{\partial p} = \frac{N k_B T}{p} \\ \text{Var}(V) &= \langle V^2 \rangle - \langle V \rangle^2 = \frac{1}{\beta^2} \left\{ \frac{1}{Y} \frac{\partial^2 Y}{\partial p^2} - \left(\frac{1}{Y} \frac{\partial Y}{\partial p} \right)^2 \right\} = -k_B T \frac{\partial^2 G}{\partial p^2} = N \left(\frac{k_B T}{p} \right)^2 . \end{aligned}$$

Thus, $(\Delta V)_{\text{RMS}} = \sqrt{\text{Var}(V)}/\langle V \rangle = N^{-1/2}$.

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #5 SOLUTIONS
PRACTICE MIDTERM EXAM

(1) A nonrelativistic gas of spin- $\frac{1}{2}$ particles of mass m at temperature T and pressure p is in equilibrium with a surface. There is no magnetic field in the bulk, but the surface itself is magnetic, so the energy of an adsorbed particle is $-\Delta - \mu_0 H \sigma$, where $\sigma = \pm 1$ is the spin polarization and H is the surface magnetic field. The surface has N_s adsorption sites.

- (a) Compute the Landau free energy of the gas $\Omega_{\text{gas}}(T, V, \mu)$. Remember that each particle has two spin polarization states.
- (b) Compute the Landau free energy of the surface $\Omega_{\text{surf}}(T, H, N_s)$. Remember that each adsorption site can be in one of three possible states: empty, occupied with $\sigma = +1$, and occupied with $\sigma = -1$.
- (c) Find an expression for the fraction $f(p, T, \Delta, H)$ of occupied adsorption sites.
- (d) Find the surface magnetization, $M = \mu_0(N_{\text{surf},\uparrow} - N_{\text{surf},\downarrow})$.

Solution :

(a) We have

$$\begin{aligned} \Xi_{\text{gas}}(T, V, \mu) &= \sum_{N=0}^{\infty} e^{N\mu/k_B T} Z(T, V, N) = \sum_{N=0}^{\infty} \frac{V^N}{N!} e^{N\mu/k_B T} 2^N \lambda_T^{-3N} \\ &= \exp\left(2V k_B T \lambda_T^{-3} e^{\mu/k_B T}\right), \end{aligned}$$

where $\lambda_T = \sqrt{2\pi\hbar^2/mk_B T}$ is the thermal wavelength. Thus,

$$\Omega_{\text{gas}} = -k_B T \ln \Xi_{\text{gas}} = -2V k_B T \lambda_T^{-3} e^{\mu/k_B T}.$$

(b) Each site on the surface is independent, with three possible energy states: $E = 0$ (vacant), $E = -\Delta - \mu_0 H$ (occupied with $\sigma = +1$), and $E = -\Delta + \mu_0 H$ (occupied with $\sigma = -1$). Thus,

$$\Xi_{\text{surf}}(T, H, N_s) = \left(1 + e^{(\mu+\Delta+\mu_0 H)/k_B T} + e^{(\mu+\Delta-\mu_0 H)/k_B T}\right)^{N_s}.$$

The surface free energy is

$$\Omega_{\text{surf}}(T, H, N_s) = -k_B T \ln \Xi_{\text{surf}} = -N_s k_B T \ln\left(1 + 2e^{(\mu+\Delta)/k_B T} \cosh(\mu_0 H/k_B T)\right).$$

(c) The fraction of occupied surface sites is $f = \langle N_{\text{surf}}/N_s \rangle$. Thus,

$$f = -\frac{1}{N_s} \frac{\partial \Omega_{\text{surf}}}{\partial \mu} = \frac{2 e^{(\mu+\Delta)/k_B T} \cosh(\mu_0 H/k_B T)}{1 + 2 e^{(\mu+\Delta)/k_B T} \cosh(\mu_0 H/k_B T)} = \frac{2}{2 + e^{-(\mu+\Delta)/k_B T} \text{sech}(\mu_0 H/k_B T)}.$$

To find $f(p, T, \Delta, H)$, we must eliminate μ in favor of p , the pressure in the gas. This is easy! From $\Omega_{\text{gas}} = -pV$, we have $p = 2k_B T \lambda_T^{-3} e^{\mu/k_B T}$, hence

$$e^{-\mu/k_B T} = \frac{2k_B T}{p \lambda_T^3}.$$

Thus,

$$f(p, T, \Delta, H) = \frac{p \lambda_T^3}{p \lambda_T^3 + k_B T e^{-\Delta/k_B T} \text{sech}(\mu_0 H/k_B T)}.$$

Note that $f \rightarrow 1$ when $\Delta \rightarrow \infty$, when $T \rightarrow 0$, when $p \rightarrow \infty$, or when $H \rightarrow \infty$.

(d) The surface magnetization is

$$\begin{aligned} M &= -\frac{\partial \Omega_{\text{surf}}}{\partial H} = N_s \mu_0 \cdot \frac{2 e^{(\mu+\Delta)/k_B T} \sinh(\mu_0 H/k_B T)}{1 + 2 e^{(\mu+\Delta)/k_B T} \cosh(\mu_0 H/k_B T)} \\ &= \frac{N_s \mu_0 p \lambda_T^3 \tanh(\mu_0 H/k_B T)}{p \lambda_T^3 + k_B T e^{-\Delta/k_B T} \text{sech}(\mu_0 H/k_B T)}. \end{aligned}$$

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #6 SOLUTIONS

(1) $\nu = 8$ moles of a diatomic ideal gas are subjected to a cyclic quasistatic process, the thermodynamic path for which is an ellipse in the (V, p) plane. The center of the ellipse lies at $(V_0, p_0) = (0.25 \text{ m}^3, 1.0 \text{ bar})$. The semimajor axes of the ellipse are $\Delta V = 0.10 \text{ m}^3$ and $\Delta p = 0.20 \text{ bar}$.

- (a) What is the temperature at $(V, p) = (V_0 + \Delta V, p_0)$?
- (b) Compute the net work per cycle done by the gas.
- (c) Compute the internal energy difference $E(V_0 - \Delta V, p_0) - E(V_0, p_0 - \Delta p)$.
- (d) Compute the heat Q absorbed by the gas along the upper half of the cycle.

Solution :

(a) The temperature is $T = pV/\nu R$. With $V = V_0 + \Delta V = 0.35 \text{ m}^3$ and $p = p_0 = 1.0 \text{ bar}$, we have

$$T = \frac{(10^5 \text{ Pa})(0.35 \text{ m}^3)}{(8 \text{ mol})(8.31 \text{ J/mol K})} = 530 \text{ K} .$$

(b) The area of an ellipse is π times the product of the semimajor axis lengths.

$$\oint p dV = \pi (\Delta p)(\Delta V) = \pi (0.20 \times 10^6 \text{ bar}) (0.10 \text{ m}^3) = 6.3 \text{ kJ} .$$

(c) For a diatomic ideal gas, $E = \frac{5}{2}pV$. Thus,

$$\Delta E = \frac{5}{2}(V_0 \Delta p - p_0 \Delta V) = \frac{5}{2}(-0.05 \times 10^5 \text{ J}) = -13 \text{ kJ} .$$

(d) We have $Q = \Delta E + W$, with

$$W = 2 p_0 \Delta V + \frac{\pi}{2}(\Delta p)(\Delta V) = 23 \text{ kJ} ,$$

which is the total area under the top half of the ellipse. The difference in energy is given by $\Delta E = \frac{5}{2} p_0 \cdot 2\Delta V = 5 p_0 \Delta V$, so

$$Q = \Delta E + W = 7 p_0 \Delta V + \frac{\pi}{2}(\Delta p)(\Delta V) = 73 \text{ kJ} .$$

(2) Determine which of the following differentials are exact and which are inexact.

- (a) $xy dx + xy dy$
- (b) $(x + y^{-1}) dx - xy^{-2} dy$
- (c) $xy^3 dx + 3x^2y^2 dy$
- (d) $(\ln y + \ln z) dx + xy^{-1} dy + xz^{-1} dz$

Solution :

Recall $dF = \sum_i A_i(\mathbf{x}) dx_i$ is exact if $\frac{\partial A_i}{\partial x_j} = \frac{\partial A_j}{\partial x_i}$ for all i and j . Thus,

(a) $dF = xy dx + xy dy$ is inexact, since $\partial A_x/\partial y = x$ but $\partial A_y/\partial x = y$. However, $dF = xy d(x + y)$, $(xy)^{-1}dF = d(x + y)$ is exact.

(b) $dF = (x + y^{-1}) dx - xy^{-2} dy = d(\frac{1}{2}x^2 + xy^{-1})$ is exact.

(c) $dF = xy^3 dx + 3x^2y^2 dy$ is inexact, since $\partial A_x/\partial y = 3xy^2$ but $\partial A_y/\partial x = 6xy^2$. However, $dF = x d(xy^3)$, so $x^{-1}dF = d(xy^3)$ is exact.

(d) $dF = (\ln y + \ln z) dx + xy^{-1} dy + xz^{-1} dz = d(x \ln y + x \ln z)$ is exact.

(3) Liquid mercury at atmospheric pressure and temperature $T = 0^\circ \text{C}$ has a molar volume of $14.72 \text{ cm}^3/\text{mol}$ and a specific heat at constant pressure of $c_p = 28.0 \text{ J/mol}\cdot\text{K}$. Its coefficient of expansion is $\alpha = \frac{1}{V}(\frac{\partial V}{\partial T})_p = 1.81 \times 10^{-4}/\text{K}$ and its isothermal compressibility is $\kappa_T = -\frac{1}{V}(\frac{\partial V}{\partial T})_T = 3.88 \times 10^{-12} \text{ cm}^2/\text{dyn}$. Find its specific heat at constant volume c_V and the ratio $\gamma = c_p/c_V$. [Reif problem 5.10]

Solution :

According to eqn. (2.307) in the notes,

$$c_p - c_V = \frac{vT\alpha_p^2}{\kappa_T} = \frac{(14.72 \times 10^{-6} \text{ m}^3/\text{mol})(273 \text{ K})(1.81 \times 10^{-4}/\text{K})^2}{3.88 \times 10^{-11} \text{ m s}^2/\text{kg}} = 3.39 \text{ J/K} .$$

Thus,

$$c_V = 24.6 \text{ J/K} \quad , \quad \gamma = \frac{c_p}{c_v} = \frac{28.0}{24.6} = 1.14 .$$

(4) ν moles of an ideal diatomic gas are driven along the cycle depicted in Fig. 1. Section AB is an adiabatic free expansion; section BC is an isotherm at temperature $T_A = T_B = T_C$; CD is an isobar, and DA is an isochore. The volume at B is given by $V_B = (1 - x)V_A + xV_C$, where $0 \leq x \leq 1$.

- (a) Find an expression for the total work W_{cycle} in terms of ν , T_A , V_A , V_C , and x .
- (b) Suppose $V_A = 1.0 \text{ L}$, $V_C = 5.0 \text{ L}$, $T_A = 500 \text{ K}$, and $\nu = 5$. What is the volume V_B such that $W_{\text{cycle}} = 0$?

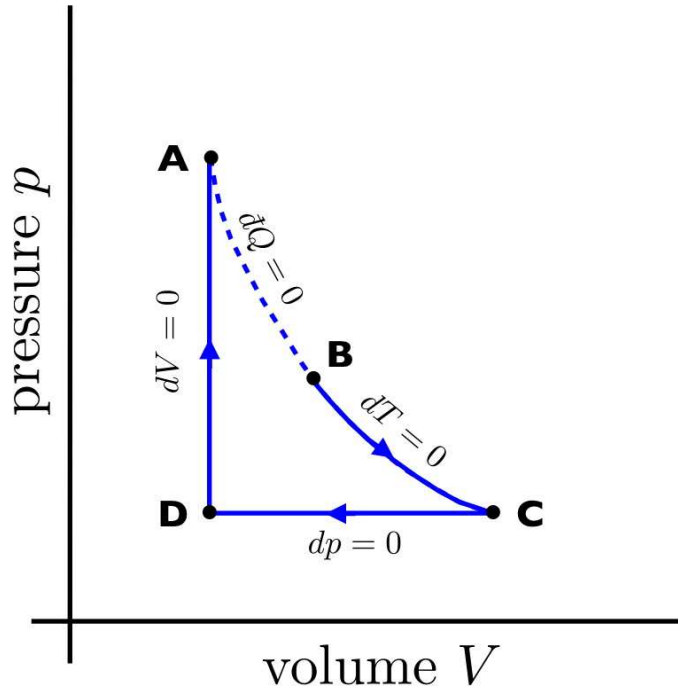


Figure 1: Thermodynamic cycle for problem 4, consisting of adiabatic free expansion (AB), isotherm (BC), isobar (CD), and isochore (DA).

Solution :

(a) We have $W_{AB} = W_{DA} = 0$, and

$$W_{BC} = \int_B^C p dV = \nu R T_A \int_B^C \frac{dV}{V} = \nu R T_A \ln\left(\frac{V_C}{V_B}\right)$$

$$W_{CD} = \int_C^D p dV = p_C (V_D - V_C) = -\nu R T_A \left(1 - \frac{V_A}{V_C}\right).$$

Thus,

$$W_{\text{CYC}} = \nu R T_A \left[\ln\left(\frac{V_C}{V_B}\right) - 1 + \frac{V_A}{V_C} \right].$$

(b) Setting $V_B = (1 - x)V_A + xV_C$, and defining $r \equiv V_A/V_C$, we have

$$W_{\text{CYC}} = \nu R T_A \left(-\ln(x + (1 - x)r) + 1 - r \right),$$

and setting $W_{\text{CYC}} = 0$ we obtain $x = x^*$, with

$$x^* = \frac{e^{r-1} - r}{1 - r}.$$

For $V_A = 1.0 \text{ L}$ and $V_C = 5.0 \text{ L}$, we have $r = \frac{1}{5}$ and $x^* = 0.31$, corresponding to $V_B = 2.2 \text{ L}$.

(5) A strange material found stuck to the bottom of a seat in Warren Lecture Hall 2001 obeys the thermodynamic relation $E(S, V, N) = aS^6/V^2N^3$, where a is a dimensionful constant.

- What are the MKS dimensions of a ?
- Find the equation of state relating p , V , N , and T .
- Find the coefficient of thermal expansion $\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_p$. Express your answer in terms of intensive quantities p , T , and $n = N/V$.
- Find the isothermal compressibility $\kappa = -\frac{1}{V} \left(\frac{\partial V}{\partial p} \right)_T$. Express your answer in terms of intensive quantities p , T , and $n = N/V$.

Solution :

(a) From $[E] = \text{J}$, $[S] = \text{J/K}$, and $[V] = \text{m}^3$, we obtain $[a] = \text{m}^6 \text{K}^5/\text{J}^5$.

(b) We have

$$T = \left(\frac{\partial E}{\partial S} \right)_{VN} = \frac{6aS^5}{V^2N^3}, \quad p = - \left(\frac{\partial E}{\partial V} \right)_{SN} = \frac{2aS^6}{V^3N^3}.$$

We can eliminate S by finding the ratio T^6/p^5 :

$$\frac{T^6}{p^5} = \frac{6^6}{2^5} \cdot \frac{aV^3}{N^3} = 1458 a n^{-3}.$$

This is an equation of state, which we can recast as

$$p(T, n) = \frac{T^{6/5} n^{3/5}}{(1458 a)^{1/5}}.$$

Contrast this with the ideal gas law, $p = nk_B T$. For parts (c) and (d) it is useful to take the logarithm, and obtain

$$6 \ln T = 5 \ln p + 3 \ln V - 3 \ln N + \ln(1458 a).$$

(c) The coefficient of volume expansion is

$$\alpha_p = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_{pN} = \left(\frac{\partial \ln V}{\partial T} \right)_{pN} = \frac{2}{T}.$$

(d) The isothermal compressibility is

$$\kappa_T = -\frac{1}{V} \left(\frac{\partial V}{\partial p} \right)_{TN} = -\left(\frac{\partial \ln V}{\partial p} \right)_{TN} = \frac{5}{3p}.$$

PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #7 SOLUTIONS

(1) Using the chain rule from multivariable calculus (see §2.16 of the lecture notes), solve the following:

- (a) Find $(\partial N/\partial T)_{S,p}$ in terms of T , N , S , and $C_{p,N}$.
- (b) Experimentalists can measure $C_{V,N}$ but for many problems it is theoretically easier to work in the grand canonical ensemble, whose natural variables are (T, V, μ) . Show that

$$C_{V,N} = \left(\frac{\partial E}{\partial T} \right)_{V,z} - \left(\frac{\partial E}{\partial z} \right)_{T,V} \left(\frac{\partial N}{\partial T} \right)_{V,z} / \left(\frac{\partial N}{\partial z} \right)_{T,V},$$

where $z = \exp(\mu/k_B T)$ is the fugacity.

Solution :

(a) We have

$$\left(\frac{\partial N}{\partial T} \right)_{S,p} = \frac{\partial(N, S, p)}{\partial(T, S, p)} = \frac{\partial(N, S, p)}{\partial(N, T, p)} \cdot \frac{\partial(N, T, p)}{\partial(T, S, p)} = -\frac{NC_{p,N}}{TS}.$$

(b) Using the chain rule,

$$\begin{aligned} C_{V,N} &= \frac{\partial(E, V, N)}{\partial(T, V, N)} = \frac{\partial(E, V, N)}{\partial(T, V, z)} \cdot \frac{\partial(T, V, z)}{\partial(T, V, N)} \\ &= \left[\left(\frac{\partial E}{\partial T} \right)_{V,z} \left(\frac{\partial N}{\partial z} \right)_{T,V} - \left(\frac{\partial E}{\partial z} \right)_{T,V} \left(\frac{\partial N}{\partial T} \right)_{V,z} \right] \cdot \left(\frac{\partial z}{\partial N} \right)_{T,V} \\ &= \left(\frac{\partial E}{\partial T} \right)_{V,z} - \left(\frac{\partial E}{\partial z} \right)_{T,V} \left(\frac{\partial N}{\partial T} \right)_{V,z} / \left(\frac{\partial N}{\partial z} \right)_{T,V}. \end{aligned}$$

(2) Consider the equation of state,

$$p = \frac{R^2 T^2}{a + vRT},$$

where $v = N_A V/N$ is the molar volume and a is a constant.

- (a) Find an expression for the molar energy $\varepsilon(T, v)$. Assume that in the limit $v \rightarrow \infty$, where the ideal gas law $pv = RT$ holds, that the gas is ideal with $\varepsilon(v \rightarrow \infty, T) = \frac{1}{2}fRT$.

(b) Find the molar specific heat $c_{V,N}$.

Solution :

(a) We fix N throughout the analysis. As shown in §2.10.2 of the lecture notes,

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

Defining the molar energy $\varepsilon = E/\nu = N_A E/N$ and the molar volume $v = V/\nu = N_A V/N$, we can write the above equation as

$$\left(\frac{\partial \varepsilon}{\partial v}\right)_T = T \left(\frac{\partial p}{\partial T}\right)_v - p = p \left[\left(\frac{\partial \ln p}{\partial \ln T}\right)_v - 1 \right].$$

Now from the equation of state, we have

$$\ln p = 2 \ln T - \ln(a + vRT) + 2 \ln R,$$

hence

$$\left(\frac{\partial \ln p}{\partial \ln T}\right)_v = 2 - \frac{vRT}{a + vRT}.$$

Plugging this into our formula for $\left(\frac{\partial \varepsilon}{\partial v}\right)_T$, we have

$$\left(\frac{\partial \varepsilon}{\partial v}\right)_T = \frac{ap}{a + vRT} = \frac{aR^2T^2}{(a + vRT)^2}.$$

Now we integrate with respect to v at fixed T , using the method of partial fractions. After some grinding, we arrive at

$$\varepsilon(T, v) = \omega(T) - \frac{aRT}{(a + vRT)}.$$

In the limit $v \rightarrow \infty$, the second term on the RHS tends to zero. This is the ideal gas limit, hence we must have $\omega(T) = \frac{1}{2}fRT$, where $f = 3$ for a monatomic gas, $f = 5$ for diatomic, etc. Thus,

$$\varepsilon(T, v) = \frac{1}{2}fRT - \frac{aRT}{a + vRT} = \frac{1}{2}fRT - \frac{a}{v} + \frac{a^2}{v(a + vRT)}.$$

(b) To find the molar specific heat, we compute

$$c_{V,N} = \left(\frac{\partial \varepsilon}{\partial T}\right)_v = \frac{1}{2}fR - \frac{a^2R}{(a + vRT)^2}.$$

(3) A van der Waals gas undergoes an adiabatic free expansion from initial volume V_i to final volume V_f . The equation of state is given in §2.10.3 of the lecture notes. The number of particles N is held constant.

- (a) If the initial temperature is T_i , what is the final temperature T_f ?
 (b) Find an expression for the change in entropy ΔS of the gas.

Solution :

(a) This part is done for you in §2.10.5 of the notes. One finds

$$\Delta T = T_f - T_i = \frac{2a}{fR} \left(\frac{1}{v_f} - \frac{1}{v_i} \right).$$

(b) Consider a two-legged thermodynamic path, consisting first of a straight leg from (T_i, V_i) to (T_i, V_f) , and second of a straight leg from (T_i, V_f) to (T_f, V_f) . We then have

$$\Delta S = \overbrace{\int_{V_i}^{V_f} dV \left(\frac{\partial S}{\partial V} \right)_{T_i, N}}^{\Delta S_1} + \overbrace{\int_{T_i}^{T_f} dT \left(\frac{\partial S}{\partial T} \right)_{V_f, N}}^{\Delta S_2}.$$

Along the first leg we use

$$\left(\frac{\partial S}{\partial V} \right)_{T, N} = \left(\frac{\partial p}{\partial T} \right)_{V, N} = \frac{R}{v - b}$$

and we then find

$$\Delta S_1 = R \ln \left(\frac{v_f - b}{v_i - b} \right).$$

Along the second leg, we have

$$\Delta S_2 = \int_{T_i}^{T_f} dT \left(\frac{\partial S}{\partial T} \right)_{V_f, N} = \int_{T_i}^{T_f} dT \frac{C_{V_f, N}}{T} = \frac{1}{2} f R \int_{T_i}^{T_f} \frac{dT}{T} = \frac{1}{2} f R \ln \left(\frac{T_f}{T_i} \right).$$

Thus,

$$\Delta S = R \ln \left(\frac{v_f - b}{v_i - b} \right) + \frac{1}{2} f R \ln \left[1 + \frac{2a}{fRT_i} \left(\frac{1}{v_f} - \frac{1}{v_i} \right) \right].$$

**PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #8 SOLUTIONS**

(1) For the Dieterici equation of state,

$$p(V - Nb) = Nk_B T e^{-Na/Vk_B T},$$

find the virial coefficients $B_2(T)$ and $B_3(T)$.

Solution :

We first write the equation of state as $p = p(n, T)$ where $n = N/V$:

$$p = \frac{nk_B T}{1 - bn} e^{-an/k_B T}.$$

Next, we expand in powers of the density n :

$$\begin{aligned} p &= nk_B T (1 + bn + b^2 n^2 + \dots) (1 - \beta a n + \frac{1}{2} \beta^2 a^2 n^2 + \dots) \\ &= nk_B T \left[1 + (b - \beta a) n + (b^2 - \beta a b + \frac{1}{2} \beta^2 a^2) n^2 + \dots \right] \\ &= nk_B T \left[1 + B_2 n + B_3 n^2 + \dots \right], \end{aligned}$$

where $\beta = 1/k_B T$. We can now read off the virial coefficients:

$$B_2(T) = b - \frac{a}{k_B T}, \quad B_3 = b^2 - \frac{ab}{k_B T} + \frac{a^2}{2k_B^2 T^2}.$$

(2) Consider a gas of particles with dispersion $\varepsilon(\mathbf{k}) = \varepsilon_0 |\mathbf{k}\ell|^{5/2}$, where ε_0 is an energy scale and ℓ is a length scale.

- (a) Find the density of states $g(\varepsilon)$ in $d = 2$ and $d = 3$ dimensions.
- (b) Find the virial coefficients $B_2(T)$ and $B_3(T)$ in $d = 2$ and $d = 3$ dimensions.
- (c) Find the heat capacity $C_V(T)$ in $d = 3$ dimensions for photon statistics.

Solution :

(a) For $\varepsilon(\mathbf{k}) = \varepsilon_0 |\mathbf{k}\ell|^\alpha$ we have

$$\begin{aligned} g(\varepsilon) &= \int \frac{d^d k}{(2\pi)^d} \delta(\varepsilon - \varepsilon(\mathbf{k})) = \frac{\Omega_d}{(2\pi)^d} \int_0^\infty dk k^{d-1} \frac{\delta(k - (\varepsilon/\varepsilon_0)^{1/\alpha}/\ell)}{\alpha \varepsilon_0 \ell^\alpha k^{\alpha-1}} \\ &= \frac{\Omega_d}{(2\pi)^d} \frac{1}{\alpha \varepsilon_0 \ell^d} \left(\frac{\varepsilon}{\varepsilon_0} \right)^{\frac{d}{\alpha}-1} \Theta(\varepsilon). \end{aligned}$$

Thus, for $\alpha = \frac{5}{2}$,

$$g_{d=2}(\varepsilon) = \frac{1}{5\pi\varepsilon_0\ell^2} \left(\frac{\varepsilon}{\varepsilon_0}\right)^{-1/5} \Theta(\varepsilon) \quad , \quad g_{d=3}(\varepsilon) = \frac{1}{5\pi\varepsilon_0\ell^3} \left(\frac{\varepsilon}{\varepsilon_0}\right)^{1/5} \Theta(\varepsilon) .$$

(b) We must compute the coefficients

$$\begin{aligned} C_j &= \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) e^{-j\varepsilon/k_B T} = \frac{\Omega_d}{(2\pi)^d} \frac{1}{\alpha\varepsilon_0\ell^d} \int_0^{\infty} d\varepsilon \left(\frac{\varepsilon}{\varepsilon_0}\right)^{\frac{d}{\alpha}-1} e^{-j\varepsilon/k_B T} \\ &= \frac{\Omega_d \Gamma(d/\alpha)}{(2\pi)^d} \frac{1}{\alpha\ell^d} \left(\frac{k_B T}{j\varepsilon_0}\right)^{d/\alpha} \equiv j^{-d/\alpha} \lambda_T^{-d} , \end{aligned}$$

where

$$\lambda_T \equiv \frac{2\pi\ell}{[\Omega_d \Gamma(\frac{d}{\alpha})/\alpha]^{1/d}} \left(\frac{\varepsilon_0}{k_B T}\right)^{1/\alpha} .$$

Then

$$\begin{aligned} B_2(T) &= \mp \frac{C_2}{2C_1^2} = \mp 2^{-(\frac{d}{\alpha}+1)} \lambda_T^d \\ B_3(T) &= \frac{C_2^2}{C_1^4} - \frac{2C_3}{C_1^3} = \left[4^{-\frac{d}{\alpha}} - \frac{2}{3} \cdot 3^{-\frac{d}{\alpha}}\right] \lambda_T^{2d} . \end{aligned}$$

We have $\alpha = \frac{5}{2}$, so $\frac{d}{\alpha} = \frac{4}{5}$ for $d = 2$ and $\frac{6}{5}$ for $d = 3$.

(c) For photon statistics, the energy is

$$E(T, V) = V \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \varepsilon \frac{1}{e^{\varepsilon/k_B T} - 1} = \frac{V\Omega_d \varepsilon_0}{(2\pi\ell)^d \alpha} \Gamma\left(\frac{d}{\alpha} + 1\right) \zeta\left(\frac{d}{\alpha} + 1\right) \left(\frac{k_B T}{\varepsilon_0}\right)^{\frac{d}{\alpha}+1}$$

Thus,

$$C_V = \frac{\partial E}{\partial T} = \frac{V\Omega_d k_B}{(2\pi\ell)^d \alpha} \Gamma\left(\frac{d}{\alpha} + 2\right) \zeta\left(\frac{d}{\alpha} + 1\right) \left(\frac{k_B T}{\varepsilon_0}\right)^{\frac{d}{\alpha}} .$$

(3) At atmospheric pressure, what would the temperature T have to be in order that the electromagnetic energy density should be identical to the energy density of a monatomic ideal gas?

Solution :

The pressure is $p = 1.0 \text{ atm} \simeq 10^5 \text{ Pa}$. We set

$$\frac{E}{V} = \frac{3}{2} p = \frac{2\pi^2}{30} \frac{(k_B T)^4}{(\hbar c)^3} ,$$

and solve for T :

$$T = \frac{1}{1.38 \times 10^{-23} \text{ J/K}} \cdot \left[\frac{45}{2\pi^2} \cdot (10^5 \text{ Pa}) \cdot \left(1970 \text{ eV } \text{\AA} \cdot 1.602 \times 10^{-19} \frac{\text{J}}{\text{eV}} \cdot 10^{-10} \frac{\text{m}}{\text{\AA}} \right)^3 \right]^{1/4}$$

$$= 1.19 \times 10^5 \text{ K} .$$

(4) Find the internal energy and heat capacity for a two-dimensional crystalline insulator, according to the Debye model.

Solution :

We have

$$\Omega(T, V) = N k_B T \int_0^\infty d\omega g(\omega) \ln \left[2 \sinh \left(\frac{\hbar\omega}{2k_B T} \right) \right] .$$

The internal energy is given by

$$E(T, V) = \frac{\partial(\beta\Omega)}{\partial\beta} = \frac{1}{2} N \int_0^\infty d\omega g(\omega) \hbar\omega \operatorname{ctnh} \left(\frac{\hbar\omega}{2k_B T} \right) .$$

In the three-dimensional Debye model, the phonon density of states per unit cell is

$$g(\omega) = \frac{9\omega^2}{\omega_D^3} \Theta(\omega_D - \omega) ,$$

where ω_D is the Debye frequency. Thus,

$$E(T) = \frac{9N\hbar}{2\omega_D^3} \int_0^{\omega_D} d\omega \omega^3 \operatorname{ctnh} \left(\frac{\hbar\omega}{2k_B T} \right)$$

$$= \frac{72N}{(\hbar\omega_D)^3} (k_B T)^4 \int_0^{\frac{\hbar\omega_D}{2k_B T}} ds s^3 \operatorname{ctnh}(s) .$$

In $d = 2$ dimensions, we must replace the phonon density of states with

$$g(\omega) = \frac{4\omega}{\omega_D^2} \Theta(\omega_D - \omega) .$$

This guarantees that the integrated phonon density of states per unit cell is 2, which is the number of acoustic phonon modes in two dimensions. We then have

$$\begin{aligned}
 E(T) &= \frac{2\hbar}{\omega_D^2} N \int_0^{\omega_D} d\omega \omega^2 \operatorname{ctnh} \left(\frac{\hbar\omega}{2k_B T} \right) \\
 &= \frac{16N}{(\hbar\omega_D)^2} (k_B T)^3 \int_0^{\frac{\hbar\omega_D}{2k_B T}} ds s^2 \operatorname{ctnh}(s) .
 \end{aligned}$$

The heat capacity is

$$\begin{aligned}
 C_V &= \frac{\partial E}{\partial T} = \frac{N\hbar^2}{k_B T^2 \omega_D^2} \int_0^{\omega_D} d\omega \omega^3 \operatorname{csch}^2 \left(\frac{\hbar\omega}{2k_B T} \right) \\
 &= 16Nk_B \left(\frac{k_B T}{\hbar\omega_D} \right)^2 \int_0^{\frac{\hbar\omega_D}{2k_B T}} ds s^2 \operatorname{csch}^2(s) .
 \end{aligned}$$

One can check that $\lim_{T \rightarrow \infty} C_V(T) = 2Nk_B$, which is the appropriate Dulong-Petit limit.

**PHYSICS 140A : STATISTICAL PHYSICS
HW ASSIGNMENT #9 SOLUTIONS**

- (1) For a system of noninteracting $S = 0$ bosons obeying the dispersion $\varepsilon(\mathbf{k}) = \hbar v|\mathbf{k}|$.
- (a) Find the density of states per unit volume $g(\varepsilon)$.
 - (b) Determine the critical temperature for Bose-Einstein condensation in three dimensions.
 - (c) Find the condensate fraction n_0/n for $T < T_c$.
 - (d) For this dispersion, is there a finite transition temperature in $d = 2$ dimensions? If not, explain why. If so, compute $T_c^{(d=2)}$.

Solution :

(a) The density of states in d dimensions is

$$g(\varepsilon) = \int \frac{d^d k}{(2\pi)^d} \delta(\varepsilon - \hbar v k) = \frac{\Omega_d}{(2\pi)^d} \frac{\varepsilon^{d-1}}{(\hbar v)^d}.$$

(b) The condition for $T = T_c$ is to write $n = n(T_c, \mu = 0)$:

$$n = \int_0^\infty d\varepsilon \frac{g(\varepsilon)}{e^{\varepsilon/k_B T_c} - 1} = \frac{1}{2\pi^2 (\hbar v)^3} \int_0^\infty d\varepsilon \frac{\varepsilon^2}{e^{\varepsilon/k_B T_c} - 1} = \frac{\zeta(3)}{\pi^2} \left(\frac{k_B T_c}{\hbar v} \right)^3.$$

Thus,

$$k_B T_c = \left(\frac{\pi^2}{\zeta(3)} \right)^{1/3} \hbar v n^{1/3}.$$

(c) For $T < T_c$, we have

$$n = n_0 + \frac{\zeta(3)}{\pi^2} \left(\frac{k_B T}{\hbar v} \right)^3.$$

Thus,

$$\frac{n_0}{n} = 1 - \left(\frac{T}{T_c(n)} \right)^3.$$

(d) In $d = 2$ we have

$$n = \frac{1}{2\pi (\hbar v)^2} \int_0^\infty d\varepsilon \frac{\varepsilon}{e^{\varepsilon/k_B T_c} - 1} = \frac{\zeta(2)}{2\pi} \left(\frac{k_B T_c}{\hbar v} \right)^2$$

and hence

$$k_B T_c^{(d=2)} = \hbar v \sqrt{\frac{2\pi n}{\zeta(2)}}.$$

(2) Using the argument we used in class and in §5.4.2 of the notes, predict the surface temperatures of the remaining planets in our solar system. In each case, compare your answers with the most reliable source you can find. In cases where there are discrepancies, try to come up with a convincing excuse.

Solution :

Relevant planetary data are available from

<http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html>

and from Wikipedia. According to the derivation in the notes, we have

$$T = \left(\frac{R_\odot}{2a}\right)^{1/2} T_\odot,$$

where $R_\odot = 6.96 \times 10^5$ km and $T_\odot = 5780$ K. From this equation and the reported values for a for each planet, we obtain the following table:

	Mercury	Venus	Earth	Mars	Jupiter	Saturn	Uranus	Neptune	Pluto
a (10^8 km)	0.576	1.08	1.50	2.28	7.78	14.3	28.7	45.0	59.1
$T_{\text{surf}}^{\text{obs}}$ (K)	340*	735 [†]	288 [‡]	210	112	84	53	55	44
$T_{\text{surf}}^{\text{pred}}$ (K)	448	327	278	226	122	89.1	63.6	50.8	44.3

Table 1: Planetary data from GSU web site and from Wikipedia. Observed temperatures are averages. * mean equatorial temperature. [†] mean temperature below cloud cover.

Note that we have included Pluto, because since my childhood Pluto has always been the ninth planet to me. We see that our simple formula works out quite well except for Mercury and Venus. Mercury, being so close to the sun, has enormous temperature fluctuations as a function of location. Venus has a whopping greenhouse effect.

(3) Read carefully the new and improved §5.5.4 of the lecture notes (“Melting and the Lindemann criterion”). Using the data in Table 5.1, and looking up the atomic mass and lattice constant of tantalum (Ta), find the temperature T_L where the Lindemann criterion predicts Ta should melt.

Solution :

One finds the mass of tantalum is $M = 181 \text{ amu}$, and the lattice constant is $a = 3.30 \text{ \AA}$. Thus,

$$\Theta^* = \frac{109 \text{ K}}{M[\text{amu}](a[\text{\AA}])^2} = 55.3 \text{ mK} .$$

From the table in the lecture notes, the Debye temperature is $\Theta_D = 246 \text{ K}$ and the melting point is $T_{\text{melt}} = 2996 \text{ K}$. The Lindemann temperature is

$$T_L = \left(\frac{\eta^2 \Theta_D}{\Theta^*} - 1 \right) \frac{\Theta_D}{4} = 2674 \text{ K} ,$$

where $\eta = 0.10$. Close enough for government work.

(4) For ideal Fermi gases in $d = 1, 2,$ and 3 dimensions, compute at $T = 0$ the average fermion velocity.

Solution :

At $T = 0$ the average velocity is

$$\langle v \rangle = \int_0^{k_F} dk k^{d-1} \frac{\hbar k}{m} \Bigg/ \int_0^{k_F} dk k^{d-1} = \frac{d}{d+1} \cdot \frac{\hbar k_F}{m} .$$

The number density is

$$n = \frac{\mathbf{g} \Omega_d}{(2\pi)^d} \int_0^{k_F} dk k^{d-1} = \frac{\mathbf{g} \Omega_d k_F^d}{(2\pi)^d d} \quad \Rightarrow \quad k_F = 2\pi \left(\frac{d}{\mathbf{g} \Omega_d} \right)^{1/d} n^{1/d} .$$

Putting these together we can obtain the average velocity in terms of the density n and physical constants. (OK! OK! I mean average speed!)

(5) Consider a three-dimensional Fermi gas of $S = \frac{1}{2}$ particles obeying the dispersion relation $\varepsilon(\mathbf{k}) = A |\mathbf{k}|^4$.

- Compute the density of states $g(\varepsilon)$.
- Compute the molar heat capacity.
- Compute the lowest order nontrivial temperature dependence for $\mu(T)$ at low temperatures. *I.e.* compute the $\mathcal{O}(T^2)$ term in $\mu(T)$.

Solution :

(a) The density of states in $d = 3$ ($g = 2S + 1 = 2$) is given by

$$g(\varepsilon) = \frac{1}{\pi^2} \int_0^\infty dk k^2 \delta(\varepsilon - \varepsilon(k)) = \frac{1}{\pi^2} k^2(\varepsilon) \left. \frac{dk}{d\varepsilon} \right|_{k=(\varepsilon/A)^{1/4}} = \frac{\varepsilon^{-1/4}}{4\pi^2 A^{3/4}}.$$

(b) The molar heat capacity is

$$c_V = \frac{\pi^2}{3n} R g(\varepsilon_F) k_B T = \frac{\pi^2 R}{4} \cdot \frac{k_B T}{\varepsilon_F},$$

where $\varepsilon_F = \hbar^2 k_F^2 / 2m$ can be expressed in terms of the density using $k_F = (3\pi^2 n)^{1/3}$, which is valid for any isotropic dispersion in $d = 3$. In deriving this formula we had to express the density n , which enters in the denominator in the above expression, in terms of ε_F . But this is easy:

$$n = \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon) = \frac{1}{3\pi^2} \left(\frac{\varepsilon_F}{A} \right)^{3/4}.$$

(c) We have (Lecture Notes, §5.7.5)

$$\delta\mu = -\frac{\pi^2}{6} (k_B T)^2 \frac{g'(\varepsilon_F)}{g(\varepsilon_F)} = \frac{\pi^2}{24} \cdot \frac{(k_B T)^2}{\varepsilon_F}.$$

Thus,

$$\mu(n, T) = \varepsilon_F(n) + \frac{\pi^2}{24} \cdot \frac{(k_B T)^2}{\varepsilon_F(n)} + \mathcal{O}(T^4),$$

where $\varepsilon_F(n) = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}$.

**PHYSICS 140A : STATISTICAL PHYSICS
MIDTERM EXAM SOLUTIONS**

Consider a classical gas of indistinguishable particles in three dimensions with Hamiltonian

$$\hat{H} = \sum_{i=1}^N \left\{ A |\mathbf{p}_i|^3 - \mu_0 H S_i \right\},$$

where A is a constant, and where $S_i \in \{-1, 0, +1\}$ (*i.e.* there are three possible spin polarization states).

(a) Compute the free energy $F_{\text{gas}}(T, H, V, N)$.

(b) Compute the magnetization density $m_{\text{gas}} = M_{\text{gas}}/V$ as a function of temperature, pressure, and magnetic field.

The gas is placed in thermal contact with a surface containing N_s adsorption sites, each with adsorption energy $-\Delta$. The surface is metallic and shields the adsorbed particles from the magnetic field, so the field at the surface may be approximated by $H = 0$.

(c) Find the Landau free energy for the surface, $\Omega_{\text{surf}}(T, N_s, \mu)$.

(d) Find the fraction $f_0(T, \mu)$ of empty adsorption sites.

(e) Find the gas pressure $p^*(T, H)$ at which $f_0 = \frac{1}{2}$.

Solution :

(a) The single particle partition function is

$$\zeta(T, V, H) = V \int \frac{d^3p}{h^3} e^{-Ap^3/k_B T} \sum_{S=-1}^1 e^{\mu_0 H S/k_B T} = \frac{4\pi V k_B T}{3A h^3} \cdot \left(1 + 2 \cosh(\mu_0 H/k_B T) \right).$$

The N -particle partition function is $Z_{\text{gas}}(T, H, V, N) = \zeta^N/N!$, hence

$$F_{\text{gas}} = -N k_B T \left[\ln \left(\frac{4\pi V k_B T}{3N A h^3} \right) + 1 \right] - N k_B T \ln \left(1 + 2 \cosh(\mu_0 H/k_B T) \right)$$

(b) The magnetization density is

$$m_{\text{gas}}(T, p, H) = -\frac{1}{V} \frac{\partial F}{\partial H} = \frac{p \mu_0}{k_B T} \cdot \frac{2 \sinh(\mu_0 H/k_B T)}{1 + 2 \cosh(\mu_0 H/k_B T)}$$

We have used the ideal gas law, $pV = N k_B T$ here.

(c) There are four possible states for an adsorption site: empty, or occupied by a particle with one of three possible spin polarizations. Thus, $\Xi_{\text{surf}}(T, N_s, \mu) = \xi^{N_s}$, with

$$\xi(T, \mu) = 1 + 3 e^{(\mu+\Delta)/k_B T}.$$

Thus,

$$\Omega_{\text{surf}}(T, N_s, \mu) = -N_s k_B T \ln \left(1 + 3 e^{(\mu+\Delta)/k_B T} \right)$$

(d) The fraction of empty adsorption sites is $1/\xi$, *i.e.*

$$f_0(T, \mu) = \frac{1}{1 + 3 e^{(\mu+\Delta)/k_B T}}$$

(e) Setting $f_0 = \frac{1}{2}$, we obtain the equation $3 e^{(\mu+\Delta)/k_B T} = 1$, or

$$e^{\mu/k_B T} = \frac{1}{3} e^{-\Delta/k_B T} .$$

We now need the fugacity $z = e^{\mu/k_B T}$ in terms of p , T , and H . To this end, we compute the Landau free energy of the gas,

$$\Omega_{\text{gas}} = -pV = -k_B T \zeta e^{\mu/k_B T} .$$

Thus,

$$p^*(T, H) = \frac{k_B T \zeta}{V} e^{\mu/k_B T} = \frac{4\pi(k_B T)^2}{9Ah^3} \cdot \left(1 + 2 \cosh(\mu_0 H/k_B T) \right) e^{-\Delta/k_B T}$$

**PHYSICS 140A : STATISTICAL PHYSICS
FINAL EXAMINATION
(do all four problems)**

(1) The entropy for a peculiar thermodynamic system has the form

$$S(E, V, N) = Nk_B \left\{ \left(\frac{E}{N\varepsilon_0} \right)^{1/3} + \left(\frac{V}{Nv_0} \right)^{1/2} \right\},$$

where ε_0 and v_0 are constants with dimensions of energy and volume, respectively.

- (a) Find the equation of state $p = p(T, V, N)$.
[5 points]
- (b) Find the work done along an isotherm in the (V, p) plane between points A and B in terms of the temperature T , the number of particles N , and the pressures p_A and p_B .
[10 points]
- (c) Find $\mu(T, p)$.
[10 points]

Solution :

(a) (a) We have

$$p = T \left(\frac{\partial S}{\partial V} \right)_{E, N} = \frac{k_B T}{2v_0} \left(\frac{V}{Nv_0} \right)^{-1/2}.$$

(b) We use the result of part (a) to obtain

$$W_{AB} = \int_A^B p dV = Nk_B T \left(\frac{V}{Nv_0} \right)^{1/2} \Big|_A^B = \frac{N(k_B T)^2}{2v_0} \left(\frac{1}{p_B} - \frac{1}{p_A} \right).$$

(c) We have

$$\mu = T \left(\frac{\partial S}{\partial N} \right)_{E, V} = \frac{2}{3} k_B T \left(\frac{E}{N\varepsilon_0} \right)^{1/3} + \frac{1}{2} k_B T \left(\frac{V}{Nv_0} \right)^{1/2}.$$

The temperature is given by

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_{V, N} = \frac{k_B}{3\varepsilon_0} \left(\frac{E}{N\varepsilon_0} \right)^{-2/3}.$$

Thus, using

$$\frac{E}{N\varepsilon_0} = \left(\frac{k_B T}{3\varepsilon_0} \right)^{3/2}, \quad \frac{V}{Nv_0} = \left(\frac{k_B T}{2p v_0} \right)^2,$$

we obtain

$$\mu(T, p) = \frac{2(k_B T)^{3/2}}{3\sqrt{3}\varepsilon_0^{1/2}} + \frac{(k_B T)^2}{4pv_0}.$$

(2) Consider a set of N noninteracting crystalline defects characterized by a dipole moment $\mathbf{p} = p_0 \hat{\mathbf{n}}$, where $\hat{\mathbf{n}}$ can point in any of six directions: $\pm\hat{\mathbf{x}}$, $\pm\hat{\mathbf{y}}$, and $\pm\hat{\mathbf{z}}$. In the absence of an external field, the energies for these configurations are $\varepsilon(\pm\hat{\mathbf{x}}) = \varepsilon(\pm\hat{\mathbf{y}}) = \varepsilon_0$ and $\varepsilon(\pm\hat{\mathbf{z}}) = 0$.

- (a) Find the free energy $F(T, N)$.
[10 points]
- (b) Now let there be an external electric field $\mathbf{E} = E \hat{\mathbf{z}}$. The energy in the presence of the field is augmented by $\Delta\varepsilon = -\mathbf{p} \cdot \mathbf{E}$. Compute the total dipole moment $\mathbf{P} = \sum_i \langle \mathbf{p}_i \rangle$.
[5 points]
- (c) Compute the electric susceptibility $\chi_E^{zz} = \frac{1}{V} \frac{\partial P_z}{\partial E_z}$ at $\mathbf{E} = 0$.
[5 points]
- (d) Find an expression for the entropy $S(T, N, E)$ when $\varepsilon_0 = 0$.
[5 points]

Solution :

(a) We have $Z = \xi^N$ where the single particle partition function is

$$\xi = \text{Tr} e^{-\beta h} = 4e^{-\beta\varepsilon_0} + 2.$$

Thus,

$$F(T, N) = -k_B T \ln Z = -Nk_B T \ln \left(2 + 4e^{-\varepsilon_0/k_B T} \right).$$

(b) Including effects of the electric field, we have

$$F(T, N) = -k_B T \ln Z = -Nk_B T \ln \left(2 \cosh \left(\frac{p_0 E}{k_B T} \right) + 4e^{-\varepsilon_0/k_B T} \right).$$

The electric polarization is clearly aligned along $\hat{\mathbf{z}}$, *i.e.* $\mathbf{P} = P(T, N, E) \hat{\mathbf{z}}$, with

$$P = - \left(\frac{\partial F}{\partial E} \right)_{T, N} = \frac{Np_0 \sinh(p_0 E/k_B T)}{2e^{-\varepsilon_0/k_B T} + \cosh(p_0 E/k_B T)}.$$

(c) We expand P to linear order in E and differentiate, yielding

$$\chi_E^{zz} = \frac{N}{V} \cdot \frac{1}{2e^{-\varepsilon_0/k_B T} + 1} \cdot \frac{p_0^2}{k_B T}.$$

(d) Setting $\varepsilon_0 = 0$, we have

$$F(T, N) = -Nk_B T \ln\left(4 + 2 \cosh(p_0 E/k_B T)\right).$$

The entropy is then

$$S = -\left(\frac{\partial F}{\partial T}\right)_N = Nk_B \left[\ln\left(4 + 2 \cosh(p_0 E/k_B T)\right) - \frac{(p_0 E/k_B T) \sinh(p_0 E/k_B T)}{2 + \cosh(p_0 E/k_B T)} \right].$$

(3) A bosonic gas is known to have a power law density of states $g(\varepsilon) = A\varepsilon^\sigma$ per unit volume, where σ is a real number.

(a) Experimentalists measure T_c as a function of the number density n and make a log-log plot of their results. They find a beautiful straight line with slope $\frac{3}{7}$. That is, $T_c(n) \propto n^{3/7}$. Assuming the phase transition they observe is an ideal Bose-Einstein condensation, find the value of σ .

[5 points]

(b) For $T < T_c$, find the heat capacity C_V .

[5 points]

(c) For $T > T_c$, find an expression for $p(T, z)$, where $z = e^{\beta\mu}$ is the fugacity. Recall the definition of the polylogarithm (or generalized Riemann zeta function)¹,

$$\text{Li}_q(z) \equiv \frac{1}{\Gamma(q)} \int_0^\infty dt \frac{t^{q-1}}{z^{-1}e^t - 1} = \sum_{n=1}^\infty \frac{z^n}{n^q},$$

where $\Gamma(q) = \int_0^\infty dt t^{q-1} e^{-t}$ is the Gamma function.

[5 points]

(d) If these particles were fermions rather than bosons, find (i) the Fermi energy $\varepsilon_F(n)$ and (ii) the pressure $p(n)$ as functions of the density n at $T = 0$.

[10 points]

Solution :

(a) At $T = T_c$, we have $\mu = 0$ and $n_0 = 0$, hence

$$n = \int_{-\infty}^\infty d\varepsilon \frac{g(\varepsilon)}{e^{\varepsilon/k_B T_c} - 1} = \Gamma(1 + \sigma) \zeta(1 + \sigma) A (k_B T_c)^{1+\sigma}.$$

¹In the notes and in class we used the notation $\zeta_q(z)$ for the polylogarithm, but for those of you who have yet to master the scribal complexities of the Greek ζ , you can use the notation $\text{Li}_q(z)$ instead.

Thus, $T_c \propto n^{\frac{1}{1+\sigma}} = n^{3/7}$ which means $\sigma = \frac{4}{3}$.

(b) For $T < T_c$ we have $\mu = 0$, but the condensate carries no energy. Thus,

$$\begin{aligned} E &= V \int_{-\infty}^{\infty} d\varepsilon \frac{\varepsilon g(\varepsilon)}{e^{\varepsilon/k_B T} - 1} = \Gamma(2 + \sigma) \zeta(2 + \sigma) A (k_B T)^{2+\sigma} \\ &= \Gamma\left(\frac{10}{3}\right) \zeta\left(\frac{10}{3}\right) A (k_B T)^{10/3} . \end{aligned}$$

Thus,

$$C_V = \Gamma\left(\frac{13}{3}\right) \zeta\left(\frac{10}{3}\right) A (k_B T)^{7/3} ,$$

where we have used $z \Gamma(z) = \Gamma(z + 1)$.

(c) The pressure is $p = -\Omega/V$, which is

$$\begin{aligned} p(T, z) &= -k_B T \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \ln(1 - z e^{-\varepsilon/k_B T}) = -A k_B T \int_0^{\infty} d\varepsilon \varepsilon^\sigma \ln(1 - z e^{-\varepsilon/k_B T}) \\ &= \frac{A}{1 + \sigma} \int_0^{\infty} d\varepsilon \frac{\varepsilon^{1+\sigma}}{z^{-1} e^{\varepsilon/k_B T} - 1} = \Gamma(1 + \sigma) A (k_B T)^{2+\sigma} \text{Li}_{2+\sigma}(z) \\ &= \Gamma\left(\frac{7}{3}\right) A (k_B T)^{10/3} \text{Li}_{10/3}(z) . \end{aligned}$$

(d) The Fermi energy is obtained from

$$n = \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon) = \frac{A \varepsilon_F^{1+\sigma}}{1 + \sigma} \quad \Rightarrow \quad \varepsilon_F(n) = \left(\frac{(1 + \sigma) n}{A} \right)^{\frac{1}{1+\sigma}} = \left(\frac{7n}{3A} \right)^{3/7} .$$

We obtain the pressure from $p = -\left(\frac{\partial E}{\partial V}\right)_N$. The energy is

$$E = V \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon) \varepsilon = V \cdot \frac{A \varepsilon_F^{2+\sigma}}{2 + \sigma} \propto V^{-\frac{1}{1+\sigma}} .$$

Thus, $p = \frac{1}{1+\sigma} \cdot \frac{E}{V}$, i.e.

$$p(n) = \frac{A \varepsilon_F^{2+\sigma}}{(1 + \sigma)(2 + \sigma)} = \frac{3}{10} \left(\frac{7}{3}\right)^{3/7} A^{-3/7} n^{10/7} .$$

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

(a) Consider a three-dimensional gas of N classical particles of mass m in a uniform gravitational field g . Assume $z \geq 0$ and $\mathbf{g} = -g\hat{z}$. Find the heat capacity C_V .
[7 points]

(b) Consider a system with a single phase space coordinate ϕ which lives on a circle. Now consider three dynamical systems on this phase space:

$$(i) \dot{\phi} = 0 \quad , \quad (ii) \dot{\phi} = 1 \quad , \quad (iii) \dot{\phi} = 2 - \cos \phi .$$

For each of these systems, tell whether it is recurrent, ergodic, both, or neither, and explain your reasoning.

[6 points]

(c) Explain Boltzmann's H -theorem.

[6 points]

(d) ν moles of gaseous Argon at an initial temperature T_A and volume $V_A = 1.0$ L undergo an adiabatic free expansion to an intermediate state of volume $V_B = 2.0$ L. After coming to equilibrium, this process is followed by a reversible adiabatic expansion to a final state of volume $V_C = 3.0$ L. Let S_A denote the initial entropy of the gas. Find the temperatures $T_{B,C}$ and the entropies $S_{B,C}$. Then repeat the calculation assuming the first expansion (from A to B) is a reversible adiabatic expansion and the second (from B to C) an adiabatic free expansion.

[6 points]

Solution :

(a) The partition function is

$$Z = \frac{A^N}{N!} \left(\lambda_T^{-3} \int_0^\infty dz e^{-mgz/k_B T} \right)^N = \frac{1}{N!} \left(\frac{k_B T A}{mg \lambda_T^3} \right)^N ,$$

where A is the cross-sectional area. Thus,

$$F = -Nk_B T \ln \left(\frac{k_B T A}{Nmg \lambda_T^3} \right) - Nk_B T .$$

We then have

$$C_V = -T \frac{\partial^2 F}{\partial T^2} = \frac{5}{2} Nk_B .$$

(b) Recurrence means a system will come arbitrarily close to revisiting any allowed point in phase space. Ergodicity means time averages may be replaced by phase space averages. With these definitions, we see that

- (i) $\dot{\phi} = 0$: recurrent but not ergodic
- (ii) $\dot{\phi} = 1$: both recurrent and ergodic
- (iii) $\dot{\phi} = 2 - \cos \phi$: recurrent but not ergodic .

If by recurrent we mean "in every neighborhood \mathcal{N} of a point ϕ_0 there exists a point which returns to \mathcal{N} after a finite number of iterations of the τ -advance mapping g_τ , then $\dot{\phi} = 0$ surely is recurrent. because all points remain fixed under these dynamics. With $\dot{\phi} = 1$, we have $\phi(t) = t$, which winds around the phase space with uniform angular frequency. This is both recurrent as well as ergodic. For $\dot{\phi} = 2 - \cos \phi$, we have $\dot{\phi} > 0$ so the motion is constantly winding around the phase space, *i.e.* it doesn't get stuck at a fixed point. So it is recurrent, but not ergodic, because the phase space velocity is relatively slow in the vicinity of $\phi = 0$ and relatively fast in the vicinity of $\phi = \pi$, and time averages will weigh more heavily the neighborhood of $\phi = 0$.

(c) If a probability distribution P_i evolves according to a master equation,

$$\dot{P}_i = \sum_j (W_{ji}P_j - W_{ij}P_i),$$

then one can construct a quantity $H(t)$ which is a function of the distribution and which satisfies $\dot{H} \leq 0$. Explicitly, one has

$$H(t) = \sum_i P_i(t) \ln(P_i(t)/P_i^{\text{eq}}),$$

where P_i^{eq} is the equilibrium distribution, which is a fixed point of the master equation. Any such probability distribution therefore evolves *irreversibly*.

(d) Argon is a monatomic ideal gas, thus $\gamma = c_p/c_v = \frac{5}{3}$. The adiabatic equation of state is $d(TV^{\gamma-1}) = 0$. The entropy of a monatomic ideal gas is $S = \frac{3}{2}Nk_B \ln(E/N) + Nk_B \ln(V/N) + Na$ where a is a constant. During an adiabatic free expansion, $\Delta E = Q = W = 0$. We can now construct the following table:

	T_B	T_C	$S_B - S_A$	$S_C - S_A$
AB free / BC reversible	T_A	$(3/2)^{-2/3} T_A$	$\nu R \ln 2$	$\nu R \ln 2$
AB reversible / BC free	$2^{-2/3} T_A$	$2^{-2/3} T_A$	0	$\nu R \ln(3/2)$

(5) Match the Jonathan Coulton song lines in the left column with their following lines in the right column.

[30 quatloos extra credit]

- | | |
|---|--|
| (a) That was a joke – haha – fat chance | (1) I can see the day unfold in front of me |
| (b) Saw a vision in his head | (2) I'm glad to see you take constructive criticism well |
| (c) I try to medicate my concentration haze | (3) And this mountain is covered with wolves |
| (d) I've been patient, I've been gracious | (4) A bulbous pointy form |
| (e) I guess we'll table this for now | (5) Hearing the whirr of the servos inside |
| (f) She'll eye me suspiciously | (6) Anyway this cake is great |

Solution :

(a) 6 (b) 4 (c) 1 (d) 3 (e) 2 (f) 5

**PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #1 SOLUTIONS**

(1) Consider a spin-1 Ising chain with Hamiltonian

$$\hat{H} = -J \sum_n S_n S_{n+1},$$

where each S_n takes possible values $\{-1, 0, 1\}$.

(a) Find the transfer matrix for the this model.

(b) Find an expression for the free energy $F(T, J, N)$ for an N -site chain and for an N -site ring.

(c) Suppose a magnetic field term $\hat{H}' = -\mu_0 H \sum_n S_n$ is included. Find the transfer matrix.

Solution :

(a) The transfer matrix is

$$R_{SS'} = e^{\beta J S S'} = \begin{pmatrix} e^{\beta J} & 1 & e^{-\beta J} \\ 1 & 1 & 1 \\ e^{-\beta J} & 1 & e^{\beta J} \end{pmatrix}.$$

(b) The partition function is

$$Z_{\text{ring}} = \text{Tr}(R^N) \quad , \quad Z_{\text{chain}} = \sum_{S, S'} [R^{N-1}]_{SS'}.$$

We can derive the eigenvalues and eigenvectors of R almost by inspection. Clearly one eigenvector is

$$\psi_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \quad , \quad \lambda_0 = 2 \sinh \beta J.$$

The remaining two eigenvectors are orthogonal to $\psi^{(0)}$ and may be written as

$$\psi_{\pm} = \frac{1}{\sqrt{2 + \alpha^2}} \begin{pmatrix} 1 \\ \alpha \\ 1 \end{pmatrix} ,$$

where there are two possible solutions for α which we call α_{\pm} . Applying R to ψ_{\pm} , we have

$$\begin{aligned} 2 \cosh \beta J + \alpha &= \lambda \\ 2 + \alpha &= \lambda \alpha \end{aligned}$$

Using the second equation to solve for λ , we have $\lambda = 1 + 2\alpha^{-1}$. Plugging this into the first equation, we obtain

$$\alpha_{\pm} = \frac{1}{2} - \cosh \beta J \pm \sqrt{\left(\frac{1}{2} - \cosh \beta J\right)^2 + 2}$$

and

$$\lambda_{\pm} = \frac{1}{2} + \cosh \beta J \pm \sqrt{\frac{9}{4} - \cosh \beta J + \cosh^2 \beta J}$$

The roots α_{\pm} satisfy $\alpha_+ \alpha_- = -2$, which guarantees that $\langle \psi_+ | \psi_- \rangle = 0$. Note that

$$\langle S | \psi_0 \rangle \langle \psi_0 | S' \rangle = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

$$\langle S | \psi_{\pm} \rangle \langle \psi_{\pm} | S' \rangle = \frac{1}{2 + \alpha_{\pm}^2} \begin{pmatrix} 1 & \alpha_{\pm} & 1 \\ \alpha_{\pm} & \alpha_{\pm}^2 & \alpha_{\pm} \\ 1 & \alpha_{\pm} & 1 \end{pmatrix}$$

and, for any J ,

$$[R^J]_{SS'} = \lambda_+^J \cdot \langle S | \psi_+ \rangle \langle \psi_+ | S' \rangle + \lambda_0^J \cdot \langle S | \psi_0 \rangle \langle \psi_0 | S' \rangle + \lambda_-^J \cdot \langle S | \psi_- \rangle \langle \psi_- | S' \rangle.$$

Thus,

$$Z_{\text{ring}} = \lambda_+^N + \lambda_0^N + \lambda_-^N$$

$$Z_{\text{chain}} = \lambda_+^{N-1} \cdot \frac{(\alpha_+ + 2)^2}{\alpha_+^2 + 2} + \lambda_-^{N-1} \cdot \frac{(\alpha_- + 2)^2}{\alpha_-^2 + 2}$$

$$= \frac{(2\lambda_+ - 3)^2 \cdot \lambda_+^{N-1}}{2(\lambda_+ - 2)^2 + 1} + \frac{(2\lambda_- - 3)^2 \cdot \lambda_-^{N-1}}{2(\lambda_- - 2)^2 + 1}.$$

(c) With a magnetic field, we have

$$R_{SS'} = e^{\beta J S S'} e^{\beta \mu_0 H (S+S')/2} = \begin{pmatrix} e^{\beta(J+\mu_0 H)} & e^{\beta \mu_0 H/2} & e^{-\beta J} \\ e^{\beta \mu_0 H/2} & 1 & e^{-\beta \mu_0 H/2} \\ e^{-\beta J} & e^{-\beta \mu_0 H/2} & e^{\beta(J-\mu_0 H)} \end{pmatrix}.$$

(2) Use the high temperature expansion to derive the spin-spin correlation functions for a spin- $\frac{1}{2}$ ($\sigma_n = \pm 1$) Ising chain and Ising ring. Compare with the results in chapter 6 of the lecture notes.

Solution :

The spin-spin correlation function $C_{kl} = \langle \sigma_k \sigma_l \rangle$ is expressed as a ratio Y_{kl}/Z as in eqn. 6.51 of the Lecture Notes (LN). For the chain, the only diagram which contributes to Z is $\Gamma = \{\emptyset\}$, i.e. the trivial empty lattice. This is because there is no way to form closed loops on a chain. Thus $Z_{\text{ring}} = 2^N (\cosh \beta J)^{N-1}$ since the number of links is $N_L = N - 1$ (see LN eqn. 6.45). For the chain, in addition to the empty lattice, there is one closed loop that can be formed which includes every link of the chain. Thus $Z_{\text{chain}} = 2^N (\cosh \beta J)^N (1 + x^N)$, where $x = \tanh \beta J$. As for the numerator $Y_{kl'}$ on the chain there is only one possible string,

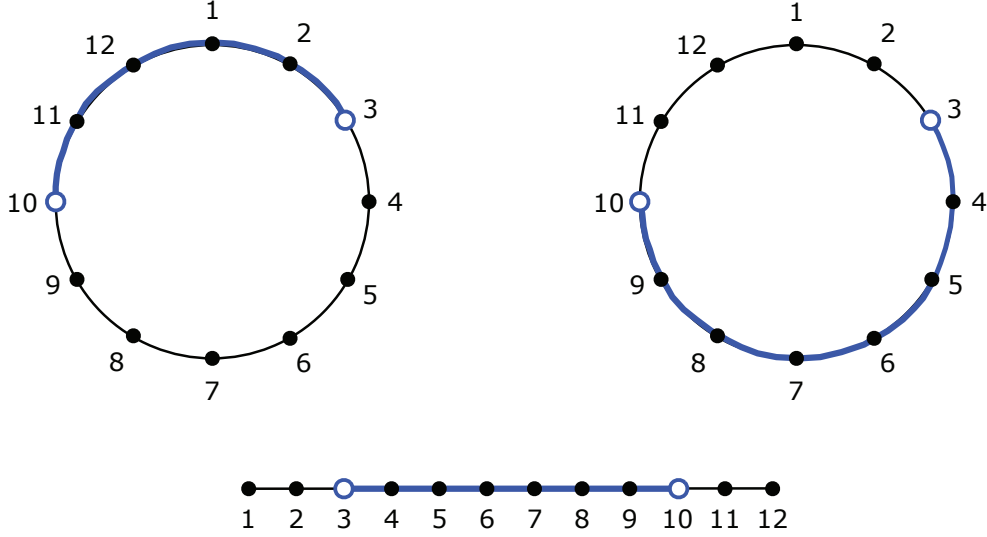


Figure 1: Diagrams for the numerator of the high temperature expansion of the spin-spin correlation function on an Ising ring and chain.

shown in fig. 1, which extends between sites k and l . Thus $Y_{kl}^{\text{chain}} = 2^N (\cosh \beta J)^{N-1} x^{|k-l|}$. On the ring there are two possible strings, since the ring is multiply connected. Thus $Y_{kl}^{\text{ring}} = 2^N (\cosh \beta J)^N (x^{|k-l|} + x^{N-|k-l|})$. Therefore,

$$C_{kl}^{\text{chain}} = x^{|k-l|} \quad , \quad C_{kl}^{\text{ring}} = \frac{x^{|k-l|} + x^{N-|k-l|}}{1 + x^N} .$$

(3) Consider an N -site Ising ring, with N even. Let $K = J/k_B T$ be the dimensionless ferromagnetic coupling ($K > 0$), and $\mathcal{H}(K, N) = H/k_B T = -K \sum_{n=1}^N \sigma_n \sigma_{n+1}$ the dimensionless Hamiltonian. The partition function is $Z(K, N) = \text{Tr} e^{-\mathcal{H}(K, N)}$. By 'tracing out' over the even sites, show that

$$Z(K, N) = e^{-N'c} Z(K', N') ,$$

where $N' = N/2$, $c = c(K)$ and $K' = K'(K)$. Thus, the partition function of an N site ring with dimensionless coupling K is related to the partition function for the same model on an $N' = N/2$ site ring, at some renormalized coupling K' , up to a constant factor. The essential step in the proof is showing that

$$\sum_{\sigma_{2k}=\pm} e^{K\sigma_{2k}(\sigma_{2k-1}+\sigma_{2k+1})} = e^{-c} e^{K'\sigma_{2k-1}\sigma_{2k+1}}$$

for some c and K' .

Solution :

We have

$$\sum_{\sigma_{2k}=\pm} e^{K\sigma_{2k}(\sigma_{2k-1}+\sigma_{2k+1})} = 2 \cosh (K\sigma_{2k-1} + K\sigma_{2k+1}) \equiv e^{-c} e^{K'\sigma_{2k-1}\sigma_{2k+1}}$$

Consider the cases $(\sigma_{2k-1}, \sigma_{2k+1}) = (1, 1)$ and $(1, -1)$, respectively. These yield two equations,

$$\begin{aligned} 2 \cosh 2K &= e^{-c} e^{K'} \\ 2 &= e^{-c} e^{-K'} . \end{aligned}$$

From these we derive

$$c(K) = -\ln 2 - \frac{1}{2} \ln \cosh K$$

and

$$K'(K) = \frac{1}{2} \ln \cosh 2K .$$

This last equation is a realization of the *renormalization group*. By thinning the degrees of freedom, we derive an effective coupling K' valid at a new length scale. In our case, it is easy to see that $K' < K$ so the coupling gets weaker and weaker at longer length scales. This is consistent with the fact that the one-dimensional Ising model is disordered at all finite temperatures.

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #2 SOLUTIONS

(1) For each of the cluster diagrams in Fig. 1, find the symmetry factor s_γ and write an expression for the cluster integral b_γ .

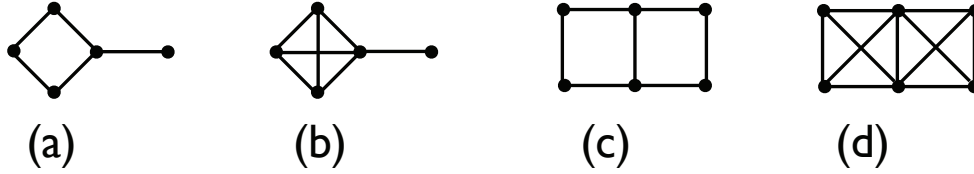


Figure 1: Cluster diagrams for problem 1.

Solution : Choose labels as in Fig. 2, and set $x_{n_\gamma} \equiv 0$ to cancel out the volume factor in the definition of b_γ .

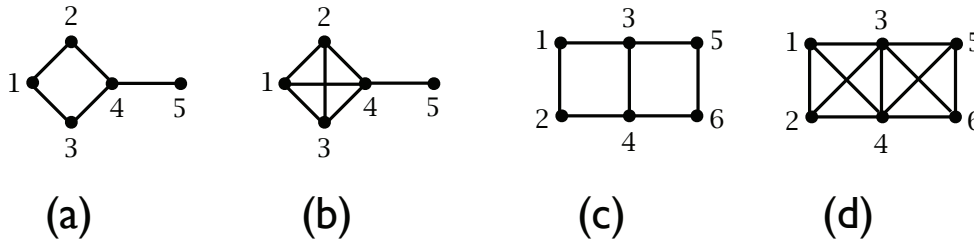


Figure 2: Labeled cluster diagrams.

(a) The symmetry factor is $s_\gamma = 2$, so

$$b_\gamma = \frac{1}{2} \int d^d x_1 \int d^d x_2 \int d^d x_3 \int d^d x_4 f(r_{12}) f(r_{13}) f(r_{24}) f(r_{34}) f(r_4).$$

(b) Sites 1, 2, and 3 may be permuted in any way, so the symmetry factor is $s_\gamma = 6$. We then have

$$b_\gamma = \frac{1}{6} \int d^d x_1 \int d^d x_2 \int d^d x_3 \int d^d x_4 f(r_{12}) f(r_{13}) f(r_{24}) f(r_{34}) f(r_{14}) f(r_{23}) f(r_4).$$

(c) The diagram is symmetric under reflections in two axes, hence $s_\gamma = 4$. We then have

$$b_\gamma = \frac{1}{4} \int d^d x_1 \int d^d x_2 \int d^d x_3 \int d^d x_4 \int d^d x_5 f(r_{12}) f(r_{13}) f(r_{24}) f(r_{34}) f(r_{35}) f(r_4) f(r_5).$$

(d) The diagram is symmetric with respect to the permutations (12), (34), (56), and (15)(26). Thus, $s_\gamma = 2^4 = 16$. We then have

$$b_\gamma = \frac{1}{16} \int d^d x_1 \int d^d x_2 \int d^d x_3 \int d^d x_4 \int d^d x_5 f(r_{12}) f(r_{13}) f(r_{14}) f(r_{23}) f(r_{24}) f(r_{34}) f(r_{35}) f(r_{45}) f(r_3) f(r_4) f(r_5).$$

(2) Compute the partition function for the one-dimensional Tonks gas of hard rods of length a on a ring of circumference L . This is slightly tricky, so here are some hints. Once again, assume a particular ordering so that $x_1 < x_2 < \dots < x_N$. Due to translational invariance, we can define the positions of particles $\{2, \dots, N\}$ relative to that of particle 1, which we initially place at $x_1 = 0$. Then periodicity means that $x_N \leq L - a$, and in general one then has

$$x_{j-1} + a \leq x_j \leq L - (N - j + 1)a .$$

Now integrate over $\{x_2, \dots, x_N\}$ subject to these constraints. Finally, one does the x_1 integral, which is over the entire ring, but which must be corrected to eliminate overcounting from cyclic permutations. How many cyclic permutations are there?

Solution :

There are N cyclic permutations, hence

$$Z(T, L, N) = \lambda_T^{-N} \frac{L}{N} \int_a^{Y_2} dx_2 \int_{x_2+a}^{Y_3} dx_3 \cdots \int_{x_{N-1}+a}^{Y_N} dx_N = \frac{L(L - Na)^{N-1} \lambda_T^{-N}}{N!} .$$

(3) Consider a three-dimensional gas of point particles interacting according to the potential

$$u(r) = \begin{cases} +\Delta_0 & \text{if } r \leq a \\ -\Delta_1 & \text{if } a < r \leq b \\ 0 & \text{if } b < r , \end{cases}$$

where $\Delta_{0,1}$ are both positive. Compute the second virial coefficient $B_2(T)$ and find a relation which determines the inversion temperature in a throttling process.

Solution :

The Mayer function is

$$f(r) = \begin{cases} e^{-\Delta_0/k_B T} - 1 & \text{if } r \leq 0 \\ e^{\Delta_1/k_B T} - 1 & \text{if } a < r \leq b \\ 0 & \text{if } b < r . \end{cases}$$

The second virial coefficient is

$$\begin{aligned} B_2(T) &= -\frac{1}{2} \int d^3r f(r) \\ &= \frac{2\pi a^3}{3} \cdot \left[(1 - e^{-\Delta_0/k_B T}) + (s^3 - 1) (1 - e^{\Delta_1/k_B T}) \right] , \end{aligned}$$

where $s = b/a$. The inversion temperature is a solution of the equation $B_2(T) = TB_2'(T)$, which gives

$$s^3 - 1 = \frac{1 + \left(\frac{\Delta_0}{k_B T} - 1\right) e^{-\Delta_0/k_B T}}{1 + \left(\frac{\Delta_1}{k_B T} + 1\right) e^{\Delta_1/k_B T}}.$$

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #3 SOLUTIONS

(1) How would you define the pair distribution function $g_{ab}(r)$ for a molecular liquid? You might wish to define \mathbf{x}_{Ii}^a as the position of the i^{th} atom of species a in molecule I and then define an appropriate thermodynamic average, assuming all the molecules are identical. With this in mind, Interpret physically the pair distribution functions for liquid water from Fig. 6.13 of the lecture notes. The density n_a is the number density of species a .

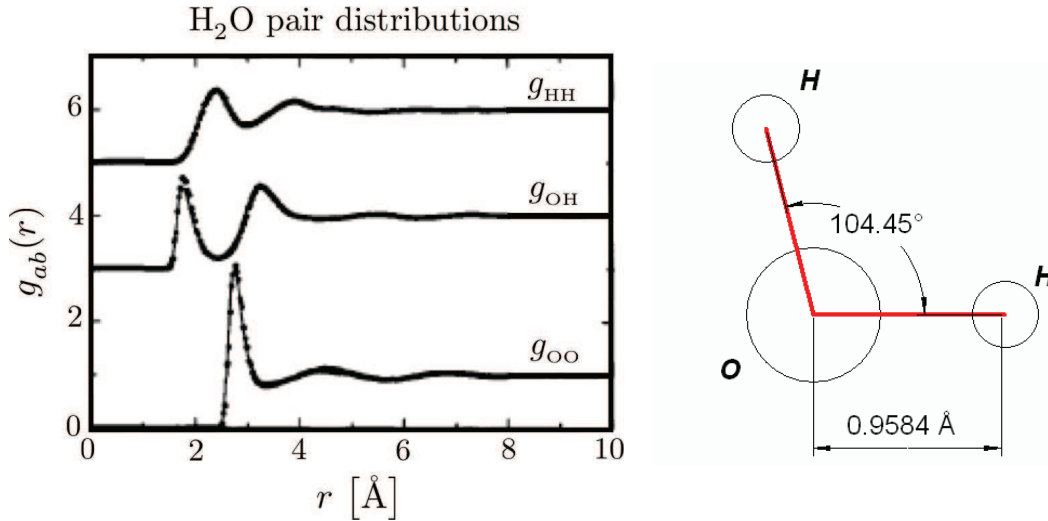


Figure 1: Left: Monte Carlo results for pair distribution functions of liquid water. From A. K. Soper, *Chem. Phys.* **202**, 295 (1996). Right: geometry of the water molecule.

Solution:

The figure is reproduced above in Fig. 1. The generalized pair distribution function for molecular systems is defined as

$$g_{ab}(r, r') = \frac{1}{n_a n_b} \left\langle \sum_{I \neq J}^M \sum_{i=1}^{\nu_a} \sum_{j=1}^{\nu_b} \delta(r - \mathbf{x}_{Ii}^a) \delta(r' - \mathbf{x}_{Jj}^b) \right\rangle,$$

where \mathbf{x}_{Ii}^a is the position of the i^{th} atom of species a in molecule I . Here ν_a is the number of atoms of species a in each molecule. We assume all the molecules are equivalent.

With this in mind, we turn to Fig. 1. Let's first consider g_{OH} . There are two clear peaks in the distribution located at $r_1 \approx 1.8 \text{ \AA}$ and $r_2 \approx 3.3 \text{ \AA}$. According to Fig. 2, the O-H separation within a single molecule is $a \approx 0.96 \text{ \AA}$, so the peak at r_1 is not due to intramolecular correlation (*i.e.* on the same molecule). Indeed, intramolecular correlations are excluded in the above definition of g_{ab} . The peak at r_1 is due to the correlation of a given oxygen atom with a hydrogen atom on the closest other water molecule. That this peak occurs at a smaller separation than the first peaks in g_{HH} and g_{OO} makes sense from the point of view of electrostatics: O is negatively charged and H is positively charged. What about the peak

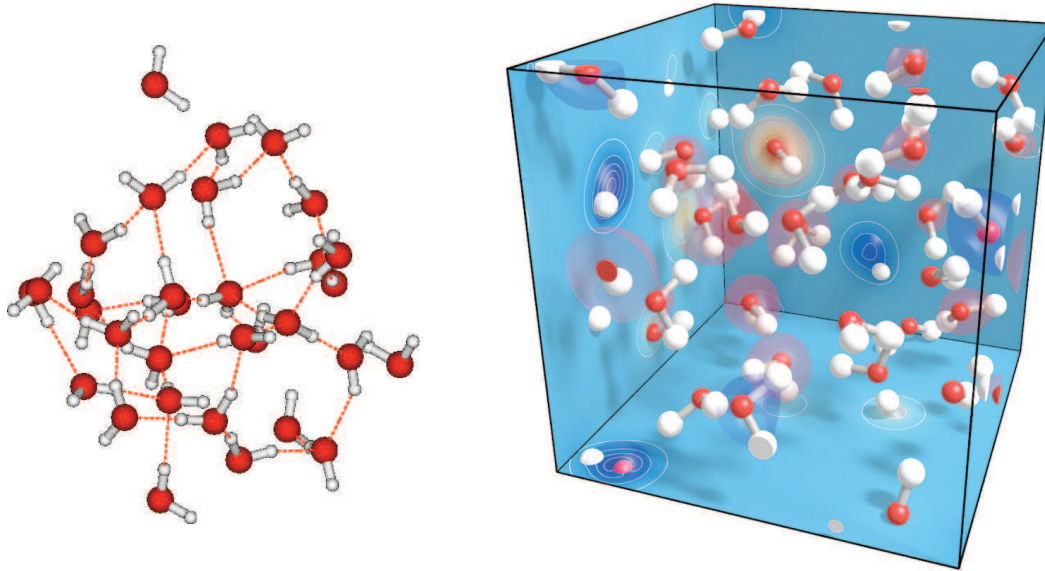


Figure 2: Two views of the local structure in liquid water. Left: molecular dynamics simulations (Univ. Oulu NMR group). Right: Quantum Monte Carlo simulations by D. Ceperley and J. Gergely (see <http://www.nccs.gov/2009/06/01/supercomputing-tests-the-waters>). Note the periodic boundary conditions.

at r_2 ? For a crude estimate, draw a triangle with side lengths $r_1 + a$ and a and an angle $\phi = 105.45^\circ$ between them. The remaining side length c is then computed from the law of cosines. For $r_1 = 1.8 \text{ \AA}$ and $a = 0.96 \text{ \AA}$, one finds $c = 3.2 \text{ \AA}$, which is very close to the observed value of r_2 . Thus, the second peak in g_{OH} is probably due to the second hydrogen atom on the closest other water molecule.

Next, consider g_{HH} . The first two peaks occur at $r_3 \approx 2.4 \text{ \AA}$ and $r_4 \approx 3.9 \text{ \AA}$. The difference of 1.5 \AA is very close to the separation between two hydrogen atoms within a given water molecule: $2a \sin(\frac{1}{2}\phi) = 1.515 \text{ \AA}$.

Finally, consider g_{OO} . There is a pronounced peak at a separation $r_5 \approx 2.8 \text{ \AA}$. Relatively speaking, there is less of a trough before the next peak, which itself is much smaller, than observed in either of the g_{OH} and g_{HH} distributions. This is because in the latter cases the presence of one hydrogen is strongly correlated with the presence of another on the same molecule.

(2) Consider a liquid where the interaction potential is $u(r) = \Delta_0 (a/r)^k$, where Δ_0 and a are energy and length scales, respectively. Assume that the pair distribution function is given by $g(r) \approx e^{-u(r)/k_{\text{B}}T}$. Compute the equation of state. For what values of k do your expressions converge?

Solution:

According to the virial equation of state in eqn. 6.157 of the Lecture Notes,

$$p = nk_{\text{B}}T - \frac{2}{3}\pi n^2 \int_0^{\infty} dr r^3 g(r) u'(r) .$$

Substituting for $u(r)$ and $g(r)$ as in the statement of the problem, we change variables to

$$s \equiv \frac{u(r)}{k_{\text{B}}T} \Rightarrow ds = \frac{u'(r)}{k_{\text{B}}T} dr ,$$

so

$$r = a \left(\frac{\Delta_0}{k_{\text{B}}T} \right)^{1/k} s^{-1/k}$$

and

$$r^3 g(r) u'(r) dr = k_{\text{B}}T a^3 \left(\frac{\Delta_0}{k_{\text{B}}T} \right)^{3/k} s^{-3/k} e^{-s} ds .$$

We then have

$$\begin{aligned} p &= nk_{\text{B}}T + \frac{2}{3}\pi n^3 a^3 k_{\text{B}}T \left(\frac{\Delta_0}{k_{\text{B}}T} \right)^{3/k} \int_0^{\infty} ds s^{-3/k} e^{-s} \\ &= nk_{\text{B}}T \left\{ 1 + \frac{2}{3}\pi \Gamma\left(1 - \frac{3}{k}\right) na^3 \left(\frac{\Delta_0}{k_{\text{B}}T} \right)^{3/k} \right\} . \end{aligned}$$

Note that a minus sign appears because we must switch the upper and lower limits on the s integral. This expression converges provided $k < 0$ or $k > 3$.

(3) Consider a charge Q impurity located at the origin of a two-dimensional metallic plane. You may model the plane initially as a noninteracting Fermi gas in the presence of a neutralizing background. The Poisson equation is

$$\nabla^2 \phi = 4\pi e [n(\boldsymbol{\rho}) - n_0] \delta(z) - 4\pi Q \delta(\boldsymbol{\rho}) \delta(z) ,$$

where $\boldsymbol{r} = (\boldsymbol{\rho}, z)$ is decomposed into a two-dimensional vector $\boldsymbol{\rho}$ and the scalar z , and where n_0 is the number density of electrons at $|\boldsymbol{\rho}| = \infty$.

- (a) Using the Thomas-Fermi approach, find the two-dimensional electron number density $n(\boldsymbol{\rho})$ in terms of the local potential $\phi(\boldsymbol{\rho}, 0)$.
- (b) By Fourier transformation, show that

$$\hat{\phi}(\boldsymbol{k}, q) = \frac{4\pi Q}{\boldsymbol{k}^2 + q^2} - \frac{4\pi n_0 e^2}{\epsilon_{\text{F}}} \frac{\hat{\chi}(\boldsymbol{k})}{\boldsymbol{k}^2 + q^2} ,$$

where \boldsymbol{k} is a two-dimensional wavevector, and

$$\hat{\chi}(\boldsymbol{k}) = \int_{-\infty}^{\infty} \frac{dq}{2\pi} \hat{\phi}(\boldsymbol{k}, q) .$$

- (c) Solve for $\hat{\chi}(\mathbf{k})$ and then for $\hat{\phi}(\mathbf{k}, q)$.
- (d) Derive an expression for the potential $\phi(\boldsymbol{\rho}, z)$.
- (e) Derive an expression for the local charge density $\varrho(\boldsymbol{\rho}) = en_0 - en(\boldsymbol{\rho})$. Show that $\varrho(\boldsymbol{\rho}) = \frac{Q}{2\pi\lambda^2} f(\rho/\lambda)$, where λ is a screening length and $f(s)$ is some function, and expression for which you should derive. Sketch $f(s)$.

Solution:

(a) In two dimensions we have

$$n = 2 \int \frac{d^2k}{(2\pi)^2} \Theta(k_F - k) = \frac{k_F^2}{2\pi} = \frac{m\varepsilon_F}{\pi\hbar^2},$$

where we have used $\varepsilon_F = \hbar^2 k_F^2 / 2m$. In the presence of a potential, the energy levels are shifted and it is the electrochemical potential $\varepsilon_F^\infty = \varepsilon_F - e\phi$ which is constant throughout the system. Thus, the local electron density is

$$n(\boldsymbol{\rho}) = \frac{m}{\pi\hbar^2} \left[\varepsilon_F^\infty + e\phi(\boldsymbol{\rho}, 0) \right] = n_0 + \frac{me}{\pi\hbar^2} \phi(\boldsymbol{\rho}, 0).$$

Here, $\phi(\mathbf{r}) = \phi(\boldsymbol{\rho}, z)$ is the electrostatic potential in three-dimensional space. When we restrict to the $z = 0$ plane we write $\phi(\boldsymbol{\rho}, 0)$.

(b) We now have

$$\nabla^2 \phi = \frac{4}{a_B} \phi(\boldsymbol{\rho}, 0) \delta(z) - 4\pi Q \delta(\boldsymbol{\rho}) \delta(z),$$

where $a_B = \hbar^2 / me^2$ is the Bohr radius. Now we take the Fourier transform by multiplying the above equation by $e^{i\mathbf{k}\cdot\boldsymbol{\rho}} e^{iqz}$ and then integrating over all $\boldsymbol{\rho}$ and z . This gives

$$-(\mathbf{k}^2 + q^2) \hat{\phi}(\mathbf{k}, q) = \frac{4}{a_B} \overbrace{\int_{-\infty}^{\infty} \frac{dq}{2\pi} \hat{\phi}(\mathbf{k}, q)}^{\hat{\chi}(\mathbf{k})} - 4\pi Q,$$

hence

$$\hat{\phi}(\mathbf{k}, q) = \frac{4\pi Q}{\mathbf{k}^2 + q^2} - \frac{4}{a_B} \frac{\hat{\chi}(\mathbf{k})}{\mathbf{k}^2 + q^2}.$$

(c) To solve for $\hat{\chi}(\mathbf{k})$ we integrate the above equation over q and use the fact that

$$\int_{-\infty}^{\infty} \frac{dq}{2\pi} \frac{e^{iqz}}{\mathbf{k}^2 + q^2} = \frac{e^{-|kz|}}{2|\mathbf{k}|}.$$

Thus,

$$\hat{\chi}(\mathbf{k}) = \frac{2\pi Q}{|\mathbf{k}|} - \frac{2}{|\mathbf{k}a_B|} \hat{\chi}(\mathbf{k})$$

Thus,

$$\hat{\chi}(\mathbf{k}) = \frac{2\pi Q}{|\mathbf{k}| + \lambda^{-1}},$$

where $\lambda = \frac{1}{2}a_B$. Plugging this back into our equation for $\hat{\phi}(\mathbf{k}, q)$, we obtain

$$\hat{\phi}(\mathbf{k}, q) = \frac{4\pi Q \cdot |\mathbf{k}\lambda|}{(\mathbf{k}^2 + q^2)(1 + |\mathbf{k}\lambda|)}.$$

(d) Now we Fourier transform back to real space:

$$\begin{aligned} \phi(\boldsymbol{\rho}, z) &= \int \frac{d^2k}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{dq}{2\pi} \hat{\phi}(\mathbf{k}, q) e^{i\mathbf{k}\cdot\boldsymbol{\rho}} e^{iqz} \\ &= \int \frac{d^2k}{(2\pi)^2} \frac{e^{-|kz|}}{2|\mathbf{k}|} \cdot \frac{4\pi Q |\mathbf{k}\lambda|}{1 + |\mathbf{k}\lambda|} \cdot e^{i\mathbf{k}\cdot\boldsymbol{\rho}} \\ &= \frac{Q}{\lambda} F(\rho/\lambda, |z|/\lambda), \end{aligned}$$

where

$$F(\sigma, \zeta) = \int_0^{\infty} du \frac{u}{1+u} J_0(\sigma u) e^{-\zeta u},$$

where $J_0(s)$ is the Bessel function of order zero.

(e) We have

$$\varrho(\boldsymbol{\rho}) = e[n_0 - n(\boldsymbol{\rho})] = -\frac{Q}{2\pi\lambda^2} F(\rho/\lambda, 0).$$

Note

$$\begin{aligned} F(\rho/\lambda, 0) &= \int_0^{\infty} du \frac{u J_0(u\rho/\lambda)}{1+u} = \frac{\lambda}{\rho} - \int_0^{\infty} du \frac{J_0(u\rho/\lambda)}{1+u} \\ &= \frac{\lambda}{\rho} + \frac{1}{2}\pi Y_0(\rho/\lambda) - \frac{1}{2}\pi \mathbf{H}_0(\rho/\lambda), \end{aligned}$$

where $Y_0(s)$ is a Bessel function of the second kind and $\mathbf{H}_0(s)$ is the Struve function. Asymptotically¹ we obtain

$$\varrho(\boldsymbol{\rho}) = \frac{Q}{2\pi\lambda^2} \left\{ \sum_{n=1}^{p-1} (-1)^n \Gamma^2\left(\frac{1}{2} + n\right) \left(\frac{2\lambda}{\rho}\right)^{(2n+1)} + \mathcal{O}(2\lambda/\rho)^{2p+1} \right\}.$$

Note that $\varrho(\boldsymbol{\rho}) \propto \rho^{-3}$ at large distances. In the above formula, p is arbitrary. Since $\Gamma(z + \frac{1}{2}) \sim z \ln z - z$, the optimal value of p to minimize the remainder in the sum is $p \approx \rho/2\lambda$. See Fig. 3 for a sketch.

¹See Gradshteyn and Ryzhik §8.554, then use $\Gamma(z)\Gamma(1-z) = \pi \csc(\pi z)$.

```
Integrate[BesselJ[0, u a] / (1 + u), {u, 0, Infinity}, Assumptions -> Re[a] > 0 && Abs[Im[a]] == 0]
```

$$\frac{1}{2} \pi (-\text{BesselY}[0, a] + \text{StruveH}[0, a])$$

```
F[x_] := 1/x + 1/2 pi (BesselY[0, x] - StruveH[0, x])
```

```
Plot[F[x], {x, 0, 10}, AxesLabel -> {sigma, F[sigma, 0]}, PlotStyle -> Thick]
```

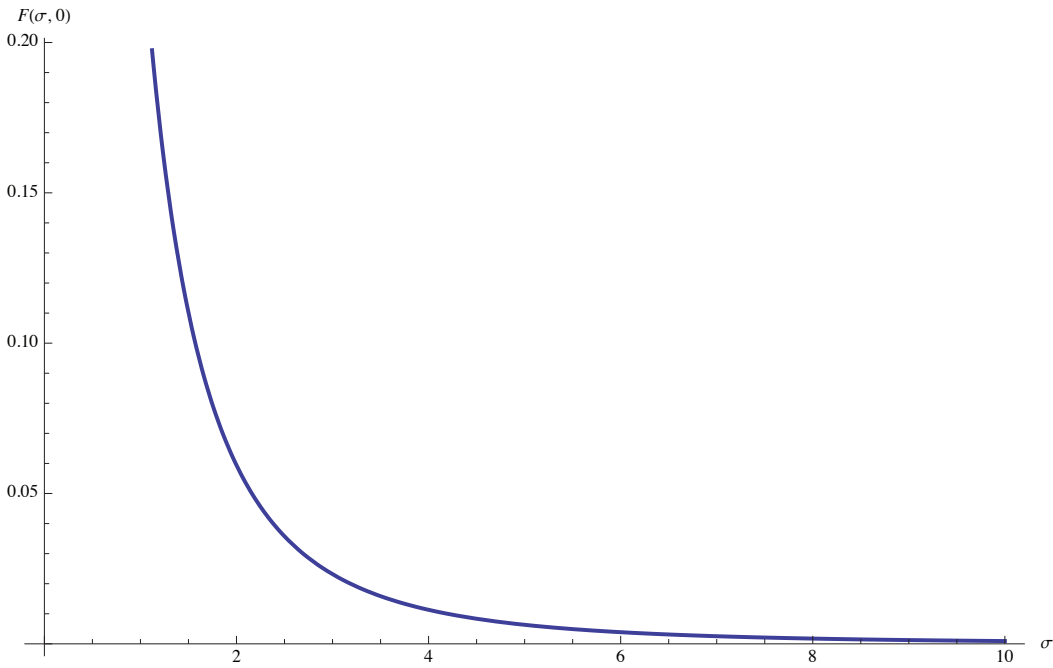


Figure 3: Plot of the screening charge density in units of $-Q/2\pi\lambda^2$ for problem (3).

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #4 SOLUTIONS

(1) The Dieterici equation of state is

$$p(v - b) = RT \exp\left(-\frac{a}{vRT}\right).$$

- (a) Find the critical point (p_c, v_c, T_c) for this equation of state
- (b) Writing $\bar{p} = p/p_c$, $\bar{v} = v/v_c$, and $\bar{T} = T/T_c$, rewrite the equation of state in the form $\bar{p} = \bar{p}(\bar{v}, \bar{T})$.
- (c) *For the brave only!* Writing $\bar{p} = 1 + \pi$, $\bar{T} = 1 + t$, and $\bar{v} = 1 + \epsilon$, find $\epsilon_{\text{liq}}(t)$ and $\epsilon_{\text{gas}}(t)$ for $0 < (-t) \ll 1$, working to lowest nontrivial order in $(-t)$.

Solution :

(a) We have

$$p = \frac{RT}{v - b} e^{-a/vRT},$$

hence

$$\left(\frac{\partial p}{\partial v}\right)_T = p \cdot \left\{ -\frac{1}{v - b} + \frac{a}{v^2 RT} \right\}.$$

Setting the LHS of the above equation to zero, we then have

$$\frac{v^2}{v - b} = \frac{a}{RT} \quad \Rightarrow \quad f(u) \equiv \frac{u^2}{u - 1} = \frac{a}{bRT},$$

where $u = v/b$ is dimensionless. Setting $f'(u^*) = 0$ yields $u^* = 2$, hence $f(u)$ on the interval $u \in (1, \infty)$ has a unique global minimum at $u = 2$, where $f(2) = 4$. Thus,

$$v_c = 2b, \quad T_c = \frac{a}{4bR}, \quad p_c = \frac{a}{4b^2} e^{-2}.$$

(b) In terms of the dimensionless variables \bar{p} , \bar{v} , and \bar{T} , the equation of state takes the form

$$\bar{p} = \frac{\bar{T}}{2\bar{v} - 1} \exp\left(2 - \frac{2}{\bar{v}\bar{T}}\right).$$

When written in terms of the dimensionless deviations π , ϵ , and t , this becomes

$$\pi = \left(\frac{1 + t}{1 + 2\epsilon}\right) \exp\left(\frac{2(\epsilon + t + \epsilon t)}{1 + \epsilon + t + \epsilon t}\right) - 1.$$

Expanding via Taylor's theorem, one finds

$$\pi(\epsilon, t) = 3t - 2t\epsilon + 2t^2 - \frac{2}{3}\epsilon^3 + 2\epsilon^2 t - 4\epsilon t^2 - \frac{2}{3}t^3 + \dots$$

Thus,

$$\pi_{\epsilon t} \equiv \frac{\partial^2 \pi}{\partial \epsilon \partial t} = -2 \quad , \quad \pi_{\epsilon \epsilon \epsilon} \equiv \frac{\partial^3 \pi}{\partial \epsilon^3} = -4 \quad ,$$

and according to the results in §7.2.2 of the Lecture Notes, we have

$$\epsilon_{L,G} = \mp \left(\frac{6 \pi_{\epsilon t}}{\pi_{\epsilon \epsilon \epsilon}} \right)^{1/2} = \mp (-3t)^{1/2} \quad .$$

(2) Consider a ferromagnetic spin-1 triangular lattice Ising model . The Hamiltonian is

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

where $S_i^z \in \{-1, 0, +1\}$ on each site i , H is a uniform magnetic field, and where the first sum is over all links of the lattice.

- (a) Derive the mean field Hamiltonian \hat{H}_{MF} for this model.
- (b) Derive the free energy per site F/N within the mean field approach.
- (c) Derive the self consistent equation for the local moment $m = \langle S_i^z \rangle$.
- (d) Find the critical temperature $T_c(H = 0)$.
- (e) Assuming $|H| \ll k_B |T - T_c| \ll J$, expand the dimensionless free energy $f = F/6NJ$ in terms of $\theta = T/T_c$, $h = H/k_B T_c$, and m . Minimizing with respect to m , find an expression for the dimensionless magnetic susceptibility $\chi = \partial m / \partial h$ close to the critical point.

Solution :

(a) Writing $S_i^z = m + \delta S_i^z$, where $m = \langle S_i^z \rangle$ and expanding \hat{H} to linear order in the fluctuations δS_i^z , we find

$$\hat{H}_{\text{MF}} = \frac{1}{2} N z J m^2 - (H + z J m) \sum_i S_i^z \quad ,$$

where $z = 6$ for the triangular lattice.

(b) The free energy per site is

$$\begin{aligned} F/N &= \frac{1}{2} z J m^2 - k_B T \ln \text{Tr} e^{(H+zJm)S^z} \\ &= \frac{1}{2} z J m^2 - k_B T \ln \left\{ 1 + 2 \cosh \left(\frac{H + z J m}{k_B T} \right) \right\} . \end{aligned}$$

(c) The mean field equation is $\partial F/\partial m = 0$, which is equivalent to $m = \langle S_i^z \rangle$. We obtain

$$m = \frac{2 \sinh\left(\frac{H+zJm}{k_B T}\right)}{1 + 2 \cosh\left(\frac{H+zJm}{k_B T}\right)}.$$

(d) To find T_c , we set $H = 0$ in the mean field equation:

$$\begin{aligned} m &= \frac{2 \sinh(\beta z J m)}{1 + 2 \cosh(\beta z J m)} \\ &= \frac{2}{3} \beta z J m + \mathcal{O}(m^3). \end{aligned}$$

The critical temperature is obtained by setting the slope on the RHS of the above equation to unity. Thus,

$$T_c = \frac{2zJ}{3k_B}.$$

So for the triangular lattice, where $z = 6$, one has $T_c = 4J/k_B$.

(e) Scaling T and H as indicated, the mean field equation becomes

$$m = \frac{2 \sinh((m+h)/\theta)}{1 + 2 \cosh((m+h)/\theta)} = \frac{m+h}{\theta/\theta_c} + \dots,$$

where $\theta_c = \frac{2}{3}$, and where we assume $\theta > \theta_c$. Solving for $m(h)$, we have

$$m = \frac{h}{1 - \frac{\theta_c}{\theta}} = \frac{\theta_c h}{\theta - \theta_c} + \mathcal{O}((\theta - \theta_c)^2).$$

Thus, $\chi = \theta_c/(\theta - \theta_c)$, which reflects the usual mean field susceptibility exponent $\gamma = 1$.

(3) Consider the antiferromagnetic *quantum* Heisenberg model on a bipartite lattice:

$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

where $J > 0$ and the sum is over the links of the lattice.

- (a) Break up the lattice into a *dimer covering* (a dimer is a pair of nearest neighbor sites)¹. Denote one sublattice as A and the other as B. You are to develop a mean field theory of interacting dimers in the presence of a self-consistent *staggered field*

$$\langle \mathbf{S}_A \rangle = -\langle \mathbf{S}_B \rangle \equiv m \hat{\mathbf{z}}.$$

¹There are exponentially many such dimer coverings, *i.e.* the number grows as $e^{\alpha N}$ where N is the number of lattice sites. Think about tiling a chessboard with dominoes. The mathematical analysis of this problem was performed by H. N. V. Temperley and M. E. Fisher, *Phil. Mag.* **6**, 1061 (1961).

The mean field Hamiltonian then breaks up into a sum over dimer Hamiltonians

$$\begin{aligned}\mathcal{H}_{\text{dimer}} &= J\mathbf{S}_A \cdot \mathbf{S}_B + (z-1)J\langle \mathbf{S}_B \rangle \cdot \mathbf{S}_A + (z-1)J\langle \mathbf{S}_A \rangle \cdot \mathbf{S}_B \\ &= J\mathbf{S}_A \cdot \mathbf{S}_B - H_s(S_A^z - S_B^z)\end{aligned}$$

where the effective staggered field is $H_s = (z-1)Jm$, and z is the lattice coordination number. Find the eigenvalues of the dimer Hamiltonian when $S = \frac{1}{2}$.

- (b) Define $x = 2h/J$. What is the self-consistent equation for x when $T = 0$? Under what conditions is there a nontrivial solution? What then is the self-consistent staggered magnetization?

Hint: Write your mean field Hamiltonian as a 4×4 matrix using the basis states $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$. It should be block diagonal in such a way which allows an easy calculation of the eigenvalues.

Solution :

(a) The mean field Hamiltonian,

$$\mathcal{H} = J\mathbf{S}_A \cdot \mathbf{S}_B - H_s(S_A^z - S_B^z),$$

is written in matrix form (for $S = \frac{1}{2}$) as

$$\mathcal{H} = \begin{pmatrix} \overbrace{\begin{matrix} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle \\ \frac{1}{4}J & 0 \\ 0 & -\frac{1}{4}J - H_s \end{matrix}} & \begin{matrix} |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \\ 0 & 0 \\ \frac{1}{2}J & 0 \\ \frac{1}{4}J + H_s & 0 \end{matrix} \\ \begin{matrix} |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \\ \frac{1}{4}J + H_s & 0 \\ 0 & 0 \\ 0 & \frac{1}{4}J \end{matrix} & \end{pmatrix}.$$

Clearly the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are eigenstates of \mathcal{H} with eigenvalues $\frac{1}{4}J$. The other two eigenvalues are easily found to be

$$\lambda_{\pm} = -\frac{1}{4}J \pm \sqrt{H_s^2 + \frac{1}{4}J^2},$$

(b) The ground state eigenvector is then

$$|\Psi_0\rangle = \alpha|\uparrow\downarrow\rangle + \beta|\downarrow\uparrow\rangle,$$

with

$$\frac{\beta}{\alpha} = x - \sqrt{1+x^2},$$

with $x = 2H_s/J$. The staggered moment is then

$$m = \langle S_A^z \rangle = \frac{1}{2} \frac{|\alpha|^2 - |\beta|^2}{|\alpha|^2 + |\beta|^2} = \frac{x}{2\sqrt{1+x^2}}.$$

Since $m = \frac{1}{2}x/(z-1)$, we have $\sqrt{1+x^2} = (z-1)$, or

$$m = \frac{\sqrt{z(z-2)}}{2(z-1)}$$

for the staggered magnetization. For $z = 4$ (square lattice) we find $m = \frac{\sqrt{2}}{3} \simeq 0.471$, which is 94% of the full moment $S = \frac{1}{2}$. Spin wave theory gives $m \simeq S - 0.19 \simeq 0.31$, which is only 62% of the full moment for $S = \frac{1}{2}$.

Equivalently, we can compute the total energy per dipole,

$$\mathcal{E} = (z-1)Jm^2 + \lambda_-$$

where the first term is the mean field energy of the $(z-1)$ links per site treated in the mean field approximation. Minimizing with respect to m ,

$$\frac{\partial \mathcal{E}}{\partial m} = 2(z-1)Jm - \frac{(z-1)^2 J^2 m}{\sqrt{(z-1)^2 J^2 m^2 + \frac{1}{4}J^2}}. \quad (1)$$

Solving for m , we recover the result $m = \sqrt{z(z-2)}/2(z-1)$.

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #5 SOLUTIONS

(1) Consider the $S = 1$ Ising Hamiltonian

$$\hat{H} = -J \sum_{\langle ij \rangle} S_i^z S_j^z - H \sum_i S_i^z + \Delta \sum_i (S_i^z)^2,$$

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

- (a) Making the mean field approximation in the first term, but treating the other terms exactly, find the corresponding mean field Hamiltonian \hat{H}_{MF} .
- (b) Defining $\theta = k_B T / zJ$, $h = H / zJ$, and $\delta = \Delta / zJ$, find the free energy $f = F / NzJ$ as a function of θ , δ , h , and m .
- (c) Write the mean field equation for this model.

Solution :

(a) The mean field Hamiltonian is

$$\hat{H}_{\text{MF}} = \frac{1}{2} NzJm^2 - (H + zJm) \sum_i S_i^z + \Delta \sum_i (S_i^z)^2.$$

The mean field free energy is then

$$F_{\text{MF}} = \frac{1}{2} NzJm^2 - Nk_B T \ln \left[1 + 2 e^{-\Delta/k_B T} \cosh \left(\frac{H + zJm}{k_B T} \right) \right].$$

(b) The scaled free energy is

$$f = \frac{1}{2} m^2 - \theta \ln \left[1 + 2 e^{-\delta/\theta} \cosh \left(\frac{m + h}{\theta} \right) \right].$$

(c) The mean field equation is

$$\frac{\partial f}{\partial m} = m - \frac{\sinh \left(\frac{m+h}{\theta} \right)}{\frac{1}{2} \exp(\delta/\theta) + \cosh \left(\frac{m+h}{\theta} \right)} = 0.$$

(2) Consider a spin- S Ising model. The Hamiltonian is $\hat{H} = -J \sum_{\langle ij \rangle} S_i^z S_j^z$, where the individual spin polarizations take values $S_i^z \in \{-S, \dots, +S\}$. Find an expression for the mean field value of T_c . *Hint: Expand the free energy for small $m = \langle S_i^z \rangle$, and find what value of T makes the coefficient of the quadratic term vanish.*

Solution :

The mean field Hamiltonian is $\hat{H}_{\text{MF}} = -zJm \sum_i S_i^z$, hence the mean field free energy is

$$F_{\text{MF}} = \frac{1}{2}NzJm^2 - Nk_{\text{B}}T \ln \sum_{j=-S}^S e^{jzJm/k_{\text{B}}T} .$$

Note that

$$\sum_{j=-S}^S e^{ju} = e^{Su} \sum_{j=0}^{2S} e^{-ju} = e^{Su} \left(\frac{1 - e^{-(2S+1)u}}{1 - e^{-u}} \right) = \frac{\sinh((S + \frac{1}{2})u)}{\sinh(\frac{1}{2}u)} .$$

Thus,

$$f = \frac{1}{2}m^2 - \theta \ln \sinh((2S + 1)m/2\theta) + \theta \ln \sinh(m/2\theta) .$$

The mean field equation is

$$\frac{\partial f}{\partial m} = m - (S + \frac{1}{2}) \text{ctnh}[(S + \frac{1}{2})m/\theta] + \frac{1}{2} \text{ctnh}(m/2\theta) .$$

Now use the Laurent expansion for $\text{ctnh}(u) = \frac{1}{u} + \frac{u}{3} - \frac{u^3}{45} + \dots$ to obtain

$$m = \frac{1}{3}S(S + 1) \frac{m}{\theta} + \mathcal{O}(m^3) ,$$

from which we identify $\theta_c = \frac{1}{3}S(S + 1)$, or $T_c^{\text{MF}} = S(S + 1)zJ/3k_{\text{B}}$.

(3) Consider the O(2) model,

$$\hat{H} = -\frac{1}{2} \sum_{i,j} J_{ij} \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j - \mathbf{H} \cdot \sum_i \hat{\mathbf{n}}_i ,$$

where $\hat{\mathbf{n}}_i = \cos \phi_i \hat{\mathbf{x}} + \sin \phi_i \hat{\mathbf{y}}$. Consider the case of infinite range interactions, where $J_{ij} = J/N$ for all i, j , where N is the total number of sites.

(a) Show that

$$\exp \left[\frac{\beta J}{2N} \sum_{i,j} \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j \right] = \frac{N\beta J}{2\pi} \int d^2m e^{-N\beta Jm^2/2} e^{\beta Jm \cdot \sum_i \hat{\mathbf{n}}_i} .$$

(b) Using the definition of the modified Bessel function $I_0(z)$,

$$I_0(z) = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{z \cos \phi} ,$$

show that

$$Z = \text{Tr} e^{-\beta \hat{H}} = \int d^2m e^{-NA(\mathbf{m}, \mathbf{h})/\theta} ,$$

where $\theta = k_{\text{B}}T/J$ and $\mathbf{h} = \mathbf{H}/J$. Find an expression for $A(\mathbf{m}, \mathbf{h})$.

- (c) Find the equation which extremizes $A(\mathbf{m}, \mathbf{h})$ as a function of \mathbf{m} .
- (d) Look up the properties of $I_0(z)$ and write down the first few terms in the Taylor expansion of $A(\mathbf{m}, \mathbf{h})$ for small m and h . Solve for θ_c .

Solution :

(a) We have

$$\frac{\hat{H}}{k_B T} = -\frac{J}{2Nk_B T} \left(\sum_i \hat{\mathbf{n}}_i \right)^2 - \frac{\mathbf{H}}{k_B T} \cdot \sum_i \hat{\mathbf{n}}_i.$$

Therefore

$$\begin{aligned} e^{-\hat{H}/k_B T} &= \exp \left[\frac{1}{2N\theta} \left(\sum_i \hat{\mathbf{n}}_i \right)^2 + \frac{\mathbf{h}}{\theta} \cdot \sum_i \hat{\mathbf{n}}_i \right] \\ &= \frac{N}{2\pi\theta} \int d^2 m \exp \left[-\frac{Nm^2}{2\theta} + \left(\frac{\mathbf{m} + \mathbf{h}}{\theta} \right) \cdot \sum_i \hat{\mathbf{n}}_i \right]. \end{aligned}$$

(b) Integrating the previous expression, we have

$$\begin{aligned} Z &= \text{Tr} e^{-\hat{H}/k_B T} = \prod_i \int \frac{d\hat{\mathbf{n}}_i}{2\pi} e^{-\hat{H}\{\hat{\mathbf{n}}_i\}/k_B T} \\ &= \frac{N}{2\pi\theta} \int d^2 m e^{-Nm^2/2\theta} \left[I_0(|\mathbf{m} + \mathbf{h}|/\theta) \right]^N. \end{aligned}$$

Thus, we identify

$$A(\mathbf{m}, \mathbf{h}) = \frac{1}{2} m^2 - \theta \ln I_0(|\mathbf{m} + \mathbf{h}|/\theta) - \frac{\theta}{N} \ln(N/2\pi\theta).$$

(c) Extremizing with respect to the vector \mathbf{m} , we have

$$\frac{\partial A}{\partial \mathbf{m}} = \mathbf{m} - \frac{\mathbf{m} + \mathbf{h}}{|\mathbf{m} + \mathbf{h}|} \cdot \frac{I_1(|\mathbf{m} + \mathbf{h}|/\theta)}{I_0(|\mathbf{m} + \mathbf{h}|/\theta)} = 0,$$

where $I_1(z) = I_0'(z)$. Clearly any solution requires that \mathbf{m} and \mathbf{h} be colinear, hence

$$m = \frac{I_1((m+h)/\theta)}{I_0((m+h)/\theta)}.$$

(d) To find θ_c , we first set $h = 0$. We then must solve

$$m = \frac{I_1(m/\theta)}{I_0(m/\theta)}.$$

The modified Bessel function $I_\nu(z)$ has the expansion

$$I_\nu(z) = \left(\frac{1}{2}z\right)^\nu \sum_{k=0}^{\infty} \frac{\left(\frac{1}{4}z^2\right)^k}{k! \Gamma(k + \nu + 1)} .$$

Thus,

$$I_0(z) = 1 + \frac{1}{4}z^2 + \dots$$

$$I_1(z) = \frac{1}{2}z + \frac{1}{16}z^3 + \dots ,$$

and therefore $I_1(z)/I_0(z) = \frac{1}{2}z - \frac{1}{16}z^3 + \mathcal{O}(z^5)$, and we read off $\theta_c = \frac{1}{2}$.

PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #6 SOLUTIONS

(1) Consider a q -state Potts model on the body-centered cubic (BCC) lattice. The Hamiltonian is given by

$$\hat{H} = -J \sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j},$$

where $\sigma_i \in \{1, \dots, q\}$ on each site.

- (a) Following the mean field treatment in §7.5.3 of the Lecture Notes, write $x = \langle \delta_{\sigma_i, 1} \rangle = q^{-1} + s$, and expand the free energy in powers of s up through terms of order s^4 . Neglecting all higher order terms in the free energy, find the critical temperature θ_c , where $\theta = k_B T / zJ$ as usual. Indicate whether the transition is first order or second order (this will depend on q).
- (b) For second order transitions, the truncated Landau expansion is sufficient, since we care only about the sign of the quadratic term in the free energy. First order transitions involve a discontinuity in the order parameter, so any truncation of the free energy as a power series in the order parameter involves an approximation. Find a way to numerically determine $\theta_c(q)$ based on the full mean field (*i.e.* variational density matrix) free energy. Compare your results with what you found in part (a), and sketch both sets of results for several values of q .

Solution :

(a) The expansion of the free energy $f(s, \theta)$ is given in eqn. 7.129 of the notes (set $h = 0$). We have

$$f = f_0 + \frac{1}{2}a s^2 - \frac{1}{3}y s^3 + \frac{1}{4}b s^4 + \mathcal{O}(s^5),$$

with

$$a = \frac{q(q\theta - 1)}{q - 1}, \quad y = \frac{(q - 2)q^3\theta}{2(q - 1)^2}, \quad b = \frac{1}{3}q^3\theta \left[1 + (q - 1)^{-3} \right].$$

For $q = 2$ we have $y = 0$, and there is a second order phase transition when $a = 0$, *i.e.* $\theta = q^{-1}$. For $q > 2$, there is a cubic term in the Landau expansion, and this portends a first order transition. Restricting to the quartic free energy above, a first order at $a > 0$ transition preempts what would have been a second order transition at $a = 0$. The transition occurs for $y^2 = \frac{9}{2}ab$. Solving for θ , we obtain

$$\theta_c^L = \frac{6(q^2 - 3q + 3)}{(5q^2 - 14q + 14)q}.$$

The value of the order parameter s just below the first order transition temperature is

$$s(\theta_c^-) = \sqrt{2a/b},$$

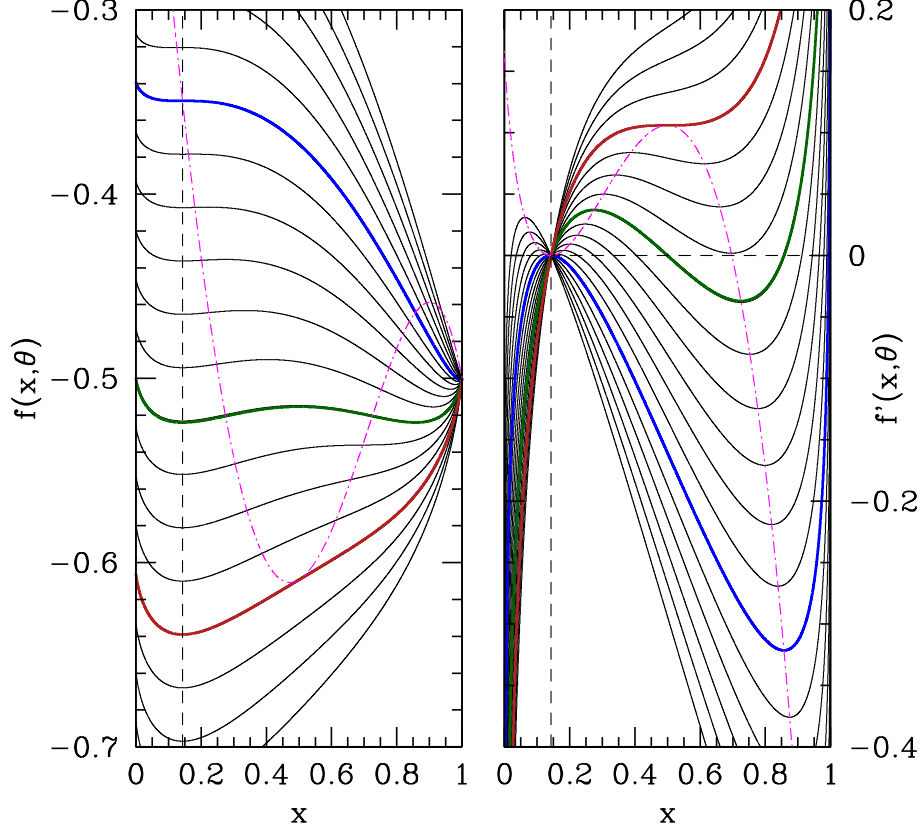


Figure 1: Variational free energy of the $q = 7$ Potts model *versus* variational parameter x . Left: free energy $f(x, \theta)$. Right: derivative $f'(x, \theta)$ with respect to the x . The dot-dash magenta curve in both cases is the locus of points for which the second derivative $f''(x, \theta)$ with respect to x vanishes. Three characteristic temperatures are marked $\theta = q^{-1}$ (blue), where the coefficient of the quadratic term in the Landau expansion changes sign; $\theta = \theta_0$ (red), where there is a saddle-node bifurcation and above which the free energy has only one minimum at $x = q^{-1}$ (symmetric phase); and $\theta = \theta_c$ (green), where the first order transition occurs.

where a and b are evaluated at $\theta = \theta_c$

(b) The full variational free energy, neglecting constants, is

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

Therefore

$$\begin{aligned} \frac{\partial f}{\partial x} &= -x + \frac{1-x}{q-1} + \theta \ln x - \theta \ln \left(\frac{1-x}{q-1} \right) \\ \frac{\partial^2 f}{\partial x^2} &= -\frac{q}{q-1} + \frac{\theta}{x(1-x)}. \end{aligned}$$

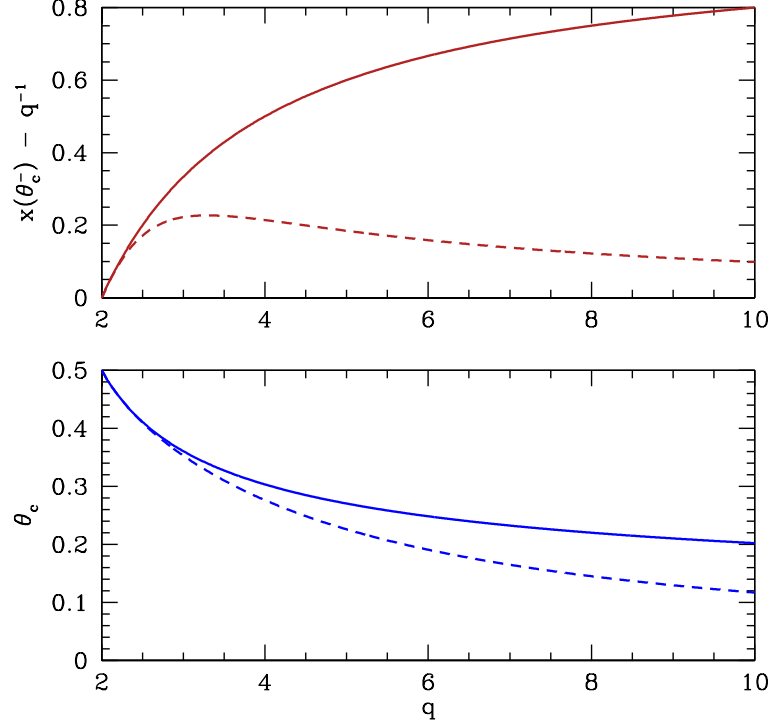


Figure 2: Comparisons of order parameter jump at θ_c (top) and critical temperature θ_c (bottom) for untruncated (solid lines) and truncated (dashed lines) expansions of the mean field free energy. Note the agreement as $q \rightarrow 2$, where the jump is small and a truncated expansion is then valid.

Solving for $\frac{\partial^2 f}{\partial x^2} = 0$, we obtain

$$x_{\pm} = \frac{1}{2} \pm \frac{1}{2} \sqrt{1 - \frac{\theta}{\theta_0}},$$

where $\theta_0 = q/4(q-1)$. For temperatures below θ_0 , the function $f(x, \theta)$ has three extrema: two local minima and one local maximum. The points x_{\pm} lie between either minimum and the maximum. The situation is depicted in fig. 1 for the case $q = 7$. To locate the first order transition, we must find the temperature θ_c for which the two minima are degenerate. This can be done numerically, but there is an analytic solution:

$$\theta_c^{\text{MF}} = \frac{q-2}{2(q-1)\ln(q-1)}, \quad s(\theta_c^-) = \frac{q-2}{q}.$$

A comparison of these results with those from part (a) is shown in fig. 2.

(2) Find v_c , T_c , and p_c for the equation of state,

$$p = \frac{RT}{v-b} - \frac{\alpha}{v^3}.$$

Solution :

We find $p'(v)$:

$$\frac{\partial p}{\partial v} = -\frac{RT}{(v-b)^2} + \frac{3\alpha}{v^4}.$$

Setting this to zero yields the equation

$$f(u) \equiv \frac{u^4}{(u-1)^2} = \frac{3\alpha}{RTb^2},$$

where $u \equiv v/b$ is dimensionless. The function $f(u)$ on the interval $[1, \infty]$ has a minimum at $u = 2$, where $f_{\min} = f(2) = 16$. This determines the critical temperature, by setting the RHS of the above equation to f_{\min} . Then evaluate $p_c = p(v_c, T_c)$. One finds

$$v_c = 2b \quad , \quad T_c = \frac{3\alpha}{16Rb^2} \quad , \quad p_c = \frac{\alpha}{16b^3}.$$

(3) Consider the $O(3)$ model,

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

where each $\hat{\mathbf{n}}_i$ is a three-dimensional unit vector.

(a) Writing

$$\hat{\mathbf{n}}_i = \mathbf{m} + \delta\hat{\mathbf{n}}_i,$$

with $\mathbf{m} = \langle \hat{\mathbf{n}}_i \rangle$ and $\delta\hat{\mathbf{n}}_i = \hat{\mathbf{n}}_i - \mathbf{m}$, derive the mean field Hamiltonian.

(b) Compute the mean field free energy $f(m, \theta, \mathbf{h})$, where $\theta = k_B T / zJ$ and $\mathbf{h} = \mathbf{H} / zJ$, with $f = F / NzJ$. Here z is the lattice coordination number and N the total number of lattice sites, as usual. You may assume that $\mathbf{m} \parallel \mathbf{h}$. Note that the trace over the local degree of freedom at each site i is given by

$$\text{Tr}_i \longleftrightarrow \int \frac{d\hat{\mathbf{n}}_i}{4\pi},$$

where the integral is over all solid angle.

(c) Find the critical point (θ_c, h_c) .

(d) Find the behavior of the magnetic susceptibility $\chi = \partial m / \partial h$ as a function of temperature θ just above θ_c .

Solution :

(a) Making the mean field *Ansatz*, one obtains the effective field $\mathbf{H}_{\text{eff}} = \mathbf{H} + zJ\mathbf{m}$, and the mean field Hamiltonian

$$\hat{H}_{\text{MF}} = \frac{1}{2}NzJm^2 - (\mathbf{H} + zJ\mathbf{m}) \cdot \sum_i \hat{\mathbf{n}}_i.$$

(b) We assume that $\mathbf{m} \parallel \mathbf{h}$, in which case

$$\begin{aligned} f(m, \theta, h) &= \frac{1}{2}m^2 - \theta \int \frac{d\hat{\mathbf{n}}}{4\pi} e^{(m+h)\hat{\mathbf{z}} \cdot \hat{\mathbf{n}}/\theta} \\ &= \frac{1}{2}m^2 - \theta \ln \left(\frac{\sinh((m+h)/\theta)}{(m+h)/\theta} \right). \end{aligned}$$

Here we have without loss of generality taken \mathbf{h} to lie in the $\hat{\mathbf{z}}$ direction.

(c) We expand $f(m, \theta, h)$ for small m and θ , obtaining

$$\begin{aligned} f(m, \theta, h) &= \frac{1}{2}m^2 - \frac{(m+h)^2}{3\theta} + \frac{(m+h)^4}{180\theta^3} + \dots \\ &= \frac{1}{2} \left(1 - \frac{2}{3\theta} \right) m^2 - \frac{2hm}{3\theta} + \frac{m^4}{180\theta^4} + \dots \end{aligned}$$

We now read off $h_c = 0$ and $\theta_c = \frac{2}{3}$.

(d) Setting $\partial f / \partial m = 0$, we obtain

$$\left(1 - \frac{\theta_c}{\theta} \right) m = \frac{\theta_c}{\theta} hm + \mathcal{O}(m^3).$$

We therefore have

$$m(h, \theta > \theta_c) = \frac{\theta_c h}{\theta - \theta_c} + \mathcal{O}(h^3) \quad , \quad \chi(\theta > \theta_c) = \frac{\partial m}{\partial h} \Big|_{h=0} = \frac{\theta_c}{\theta - \theta_c}.$$

**PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #7 SOLUTIONS**

(1) The Hamiltonian for the three state (\mathbb{Z}_3) clock model is written

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

where each local unit vector $\hat{\mathbf{n}}_i$ can take one of three possible values:

$$\hat{\mathbf{n}} = \hat{\mathbf{x}} \quad , \quad \hat{\mathbf{n}} = -\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}} \quad , \quad \hat{\mathbf{n}} = -\frac{1}{2}\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}\hat{\mathbf{y}} .$$

- (a) Consider the \mathbb{Z}_3 clock model on a lattice of coordination number z . Make the mean field assumption $\langle \hat{\mathbf{n}}_i \rangle = m\hat{\mathbf{x}}$. Expanding the Hamiltonian to linear order in the fluctuations, derive the mean field Hamiltonian for this model \hat{H}_{MF} .
- (b) Rescaling $\theta = k_{\text{B}}T/zJ$ and $f = F/NzJ$, where N is the number of sites, find $f(m, \theta)$.
- (c) Find the mean field equation.
- (d) Is the transition second order or first order?
- (e) Show that this model is equivalent to the three state Potts model. Is the \mathbb{Z}_4 clock model equivalent to the four state Potts model? Why or why not?

Solution :

(a) The mean field Hamiltonian is

$$\hat{H}_{\text{MF}} = \frac{1}{2}NzJm^2 - zJm\hat{\mathbf{x}} \cdot \sum_i \hat{\mathbf{n}}_i .$$

(b) We have

$$\begin{aligned} f(m, \theta) &= \frac{1}{2}m^2 - \theta \ln \text{Tr}_{\hat{\mathbf{n}}} e^{m\hat{\mathbf{x}} \cdot \hat{\mathbf{n}}/\theta} \\ &= \frac{1}{2}m^2 - \theta \ln \left(\frac{1}{3}e^{m/\theta} + \frac{2}{3}e^{-m/2\theta} \right) \\ &= \frac{1}{2} \left(1 - \frac{1}{2\theta} \right) m^2 - \frac{m^3}{24\theta^2} + \frac{m^4}{64\theta^3} + \mathcal{O}(m^5) . \end{aligned}$$

Here we have defined $\text{Tr}_{\hat{\mathbf{n}}} = \frac{1}{3} \sum_{\hat{\mathbf{n}}} \hat{\mathbf{n}}$ as the normalized trace. The last line is somewhat tedious to obtain, but is not necessary for this problem.

(c) The mean field equation is

$$0 = \frac{\partial f}{\partial m} = m - \frac{e^{m/\theta} - e^{-m/2\theta}}{e^{m/\theta} + 2e^{-m/2\theta}} .$$

$\varepsilon_{\sigma\sigma'}^{\text{clock}}$	0°	120°	240°
0°	$-J$	$\frac{1}{2}J$	$\frac{1}{2}J$
120°	$\frac{1}{2}J$	$-J$	$\frac{1}{2}J$
240°	$\frac{1}{2}J$	$\frac{1}{2}J$	$-J$

Table 1: \mathbb{Z}_3 clock model energy matrix.

$\varepsilon_{\sigma\sigma'}^{\text{Potts}}$	A	B	C
A	$-\tilde{J}$	0	0
B	0	$-\tilde{J}$	0
C	0	0	$-\tilde{J}$

Table 2: $q = 3$ Potts model energy matrix.

Expanding the RHS to lowest order in m and setting the slope to 1, we find $\theta_c = \frac{1}{2}$.

(d) Since $f(m, \theta) \neq f(-m, \theta)$, the Landau expansion of the free energy (other than constants) should include terms of all orders starting with $\mathcal{O}(m^2)$. This means that there will in general be a cubic term, hence we expect a first order transition.

(e) Let $\varepsilon(\hat{n}, \hat{n}') = -J\hat{n} \cdot \hat{n}'$ be the energy for a given link. The unit vectors \hat{n} and \hat{n}' can each point in any of three directions, which we can label as 0° , 120° , and 240° . The matrix of possible bond energies is shown in Tab. 1.

Now consider the $q = 3$ Potts model, where the local states are labeled $|A\rangle$, $|B\rangle$, and $|C\rangle$. The Hamiltonian is

$$\hat{H} = -\tilde{J} \sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j}.$$

The interaction energy matrix for the Potts model is given in Tab. 2.

We can in each case label the three states by a local variable $\sigma \in \{1, 2, 3\}$, corresponding, respectively, to 0° , 120° , and 240° for the clock model and to A, B, and C for the Potts model. We then observe

$$\varepsilon_{\sigma\sigma'}^{\text{clock}}(J) = \varepsilon_{\sigma\sigma'}^{\text{Potts}}\left(\frac{3}{2}J\right) + \frac{1}{2}J.$$

Thus, the free energies satisfy

$$F^{\text{clock}}(J) = \frac{1}{4}NzJ + F^{\text{Potts}}\left(\frac{3}{2}J\right),$$

and the models are equivalent. However, the \mathbb{Z}_q clock model and q -state Potts model are *not* equivalent for $q > 3$. Can you see why? *Hint: construct the corresponding energy matrices for $q = 4$.*

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

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

Here $\Psi(\mathbf{r})$ 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 $\langle \Psi(\mathbf{r}) \rangle$. Note that the free energy is a functional of the two independent fields $\Psi(\mathbf{r})$ and $\Psi^*(\mathbf{r})$, where Ψ^* is the complex conjugate of Ψ . Alternatively, one can consider F a functional of the real and imaginary parts of Ψ .

- (a) Show that one can rescale the field Ψ and the coordinates \mathbf{r} 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 \mathbf{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 \mathbf{r} and \mathbf{x} .

- (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 $\psi(\mathbf{x})$.
- (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 .
- (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 :

(a) 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 $\tilde{\mathbf{x}} = \xi\mathbf{x}$ 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) 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) 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) 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

$$F(a, R) = \frac{1}{4} \pi \varepsilon_0 \left\{ 1 - \frac{a^4}{(R^2 + a^2)^2} + 2 \ln \left(\frac{R^2}{a^2} + 1 \right) + \frac{R^2 a^2}{R^2 + a^2} \right\}.$$

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

$$V(r) = \frac{1}{2}\pi\varepsilon_0 \ln\left(\frac{r^2}{a^2} + 1\right).$$

This tends to $V(r) = \pi\varepsilon_0 \ln(d/a)$ 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 #8 SOLUTIONS

(1) Consider a monatomic ideal gas in the presence of a temperature gradient ∇T . Answer the following questions within the framework of the relaxation time approximation to the Boltzmann equation.

- (a) Compute the particle current j and show that it vanishes.
 (b) Compute the 'energy squared' current,

$$j_{\varepsilon^2} = \int d^3p \varepsilon^2 \mathbf{v} f(\mathbf{r}, \mathbf{p}, t) .$$

- (c) Suppose the gas is diatomic, so $c_p = \frac{7}{2}k_B$. Show explicitly that the particle current j is zero. *Hint: To do this, you will have to understand the derivation of eqn. 8.85 in the Lecture Notes and how this changes when the gas is diatomic. You may assume $Q_{\alpha\beta} = \mathbf{F} = 0$.*

Solution :

(a) Under steady state conditions, the solution to the Boltzmann equation is $f = f^0 + \delta f$, where f^0 is the equilibrium distribution and

$$\delta f = -\frac{\tau f^0}{k_B T} \cdot \frac{\varepsilon - c_p T}{T} \mathbf{v} \cdot \nabla T .$$

For the monatomic ideal gas, $c_p = \frac{5}{2}k_B$. The particle current is

$$\begin{aligned} j^\alpha &= \int d^3p v^\alpha \delta f \\ &= -\frac{\tau}{k_B T^2} \int d^3p f^0(\mathbf{p}) v^\alpha v^\beta (\varepsilon - \frac{5}{2}k_B T) \frac{\partial T}{\partial x^\beta} \\ &= -\frac{2n\tau}{3mk_B T^2} \frac{\partial T}{\partial x^\alpha} \langle \varepsilon (\varepsilon - \frac{5}{2}k_B T) \rangle , \end{aligned}$$

where the average over momentum/velocity is converted into an average over the energy distribution,

$$\tilde{P}(\varepsilon) = 4\pi v^2 \frac{dv}{d\varepsilon} P_M(v) = \frac{2}{\sqrt{\pi}} (k_B T)^{-3/2} \varepsilon^{1/2} \phi(\varepsilon) e^{-\varepsilon/k_B T} .$$

As discussed in the Lecture Notes, the average of a homogeneous function of ε under this distribution is given by

$$\langle \varepsilon^\alpha \rangle = \frac{2}{\sqrt{\pi}} \Gamma(\alpha + \frac{3}{2}) (k_B T)^\alpha .$$

Thus,

$$\langle \varepsilon (\varepsilon - \frac{5}{2}k_B T) \rangle = \frac{2}{\sqrt{\pi}} (k_B T)^2 \left\{ \Gamma(\frac{7}{2}) - \frac{5}{2} \Gamma(\frac{5}{2}) \right\} = 0 .$$

(b) Now we must compute

$$\begin{aligned} j_{\varepsilon^2}^\alpha &= \int d^3p v^\alpha \varepsilon^2 \delta f \\ &= -\frac{2n\tau}{3mk_B T^2} \frac{\partial T}{\partial x^\alpha} \langle \varepsilon^3 (\varepsilon - \frac{5}{2}k_B T) \rangle . \end{aligned}$$

We then have

$$\langle \varepsilon^3 (\varepsilon - \frac{5}{2}k_B T) \rangle = \frac{2}{\sqrt{\pi}} (k_B T)^4 \left\{ \Gamma(\frac{11}{2}) - \frac{5}{2} \Gamma(\frac{9}{2}) \right\} = \frac{105}{2} (k_B T)^4$$

and so

$$\mathbf{j}_{\varepsilon^2} = -\frac{35n\tau k_B}{m} (k_B T)^2 \nabla T .$$

(c) For diatomic gases in the presence of a temperature gradient, the solution to the linearized Boltzmann equation in the relaxation time approximation is

$$\delta f = -\frac{\tau f^0}{k_B T} \cdot \frac{\varepsilon(\Gamma) - c_p T}{T} \mathbf{v} \cdot \nabla T ,$$

where

$$\varepsilon(\Gamma) = \varepsilon_{\text{tr}} + \varepsilon_{\text{rot}} = \frac{1}{2} m \mathbf{v}^2 + \frac{L_1^2 + L_2^2}{2I} ,$$

where $L_{1,2}$ are components of the angular momentum about the instantaneous body-fixed axes, with $I \equiv I_1 = I_2 \gg I_3$. We assume the rotations about axes 1 and 2 are effectively classical, so equipartition gives $\langle \varepsilon_{\text{rot}} \rangle = 2 \times \frac{1}{2} k_B = k_B$. We still have $\langle \varepsilon_{\text{tr}} \rangle = \frac{3}{2} k_B$. Now in the derivation of the factor $\varepsilon(\varepsilon - c_p T)$ above, the first factor of ε came from the $v^\alpha v^\beta$ term, so this is translational kinetic energy. Therefore, with $c_p = \frac{7}{2} k_B$ now, we must compute

$$\langle \varepsilon_{\text{tr}} (\varepsilon_{\text{tr}} + \varepsilon_{\text{rot}} - \frac{7}{2} k_B T) \rangle = \langle \varepsilon_{\text{tr}} (\varepsilon_{\text{tr}} - \frac{5}{2} k_B T) \rangle = 0 .$$

So again the particle current vanishes.

Note added :

It is interesting to note that there is no particle current flowing in response to a temperature gradient when τ is energy-independent. This is a consequence of the fact that the pressure gradient ∇p vanishes. Newton's Second Law for the fluid says that $nm\dot{\mathbf{V}} + \nabla p = 0$, to lowest relevant order. With $\nabla p \neq 0$, the fluid will accelerate. In a pipe, for example, eventually a steady state is reached where the flow is determined by the fluid viscosity, which is one of the terms we just dropped. (This is called *Poiseuille flow*.) When p is constant, the local equilibrium distribution is

$$f^0(\mathbf{r}, \mathbf{p}) = \frac{p/k_B T}{(2\pi m k_B T)^{3/2}} e^{-\mathbf{p}^2/2mk_B T} ,$$

where $T = T(\mathbf{r})$. We then have

$$f(\mathbf{r}, \mathbf{p}) = f^0(\mathbf{r} - \mathbf{v}\tau, \mathbf{p}),$$

which says that no new collisions happen for a time τ after a given particle thermalizes. *I.e.* we evolve the streaming terms for a time τ . Expanding, we have

$$\begin{aligned} f &= f^0 - \frac{\tau \mathbf{p}}{m} \cdot \frac{\partial f^0}{\partial \mathbf{r}} + \dots \\ &= \left\{ 1 - \frac{\tau}{2k_B T^2} \left(\varepsilon(\mathbf{p}) - \frac{5}{2} k_B T \right) \frac{\mathbf{p}}{m} \cdot \nabla T + \dots \right\} f^0(\mathbf{r}, \mathbf{p}), \end{aligned}$$

which leads to $\mathbf{j} = 0$, assuming the relaxation time τ is energy-independent.

When the flow takes place in a restricted geometry, a dimensionless figure of merit known as the *Knudsen number*, $\text{Kn} = \ell/L$, where ℓ is the mean free path and L is the characteristic linear dimension associated with the geometry. For $\text{Kn} \ll 1$, our Boltzmann transport calculations of quantities like κ , η , and ζ hold, and we may apply the Navier-Stokes equations¹. In the opposite limit $\text{Kn} \gg 1$, the boundary conditions on the distribution are crucial. Consider, for example, the case $\ell = \infty$. Suppose we have ideal gas flow in a cylinder whose symmetry axis is \hat{x} . Particles with $v_x > 0$ enter from the left, and particles with $v_x < 0$ enter from the right. Their respective velocity distributions are

$$P_j(\mathbf{v}) = n_j \left(\frac{m}{2\pi k_B T_j} \right)^{3/2} e^{-mv^2/2k_B T_j},$$

where $j = \text{L}$ or R . The average current is then

$$\begin{aligned} j_x &= \int d^3v \left\{ n_L v_x P_L(\mathbf{v}) \Theta(v_x) + n_R v_x P_R(\mathbf{v}) \Theta(-v_x) \right\} \\ &= n_L \sqrt{\frac{2k_B T_L}{m}} - n_R \sqrt{\frac{2k_B T_R}{m}}. \end{aligned}$$

(2) Suppose the relaxation time is energy-dependent, with $\tau(\varepsilon) = \tau_0 e^{-\varepsilon/\varepsilon_0}$. Compute the particle current \mathbf{j} and energy current \mathbf{j}_ε flowing in response to a temperature gradient ∇T .

Solution :

Now we must compute

$$\begin{aligned} \begin{Bmatrix} j^\alpha \\ j_\varepsilon^\alpha \end{Bmatrix} &= \int d^3p \begin{Bmatrix} v^\alpha \\ \varepsilon v^\alpha \end{Bmatrix} \delta f \\ &= -\frac{2n}{3mk_B T^2} \frac{\partial T}{\partial x^\alpha} \langle \tau(\varepsilon) \begin{Bmatrix} \varepsilon \\ \varepsilon^2 \end{Bmatrix} \left(\varepsilon - \frac{5}{2} k_B T \right) \rangle, \end{aligned}$$

¹These equations may need to be supplemented by certain conditions which apply in the vicinity of solid boundaries.

where $\tau(\varepsilon) = \tau_0 e^{-\varepsilon/\varepsilon_0}$. We find

$$\begin{aligned}\langle e^{-\varepsilon/\varepsilon_0} \varepsilon^\alpha \rangle &= \frac{2}{\sqrt{\pi}} (k_B T)^{-3/2} \int_0^\infty d\varepsilon \varepsilon^{\alpha+1/2} e^{-\varepsilon/k_B T} e^{-\varepsilon/\varepsilon_0} \\ &= \frac{2}{\sqrt{\pi}} \Gamma\left(\alpha + \frac{3}{2}\right) (k_B T)^\alpha \left(\frac{\varepsilon_0}{\varepsilon_0 + k_B T}\right)^{\alpha+3/2}.\end{aligned}$$

Therefore,

$$\begin{aligned}\langle e^{-\varepsilon/\varepsilon_0} \varepsilon \rangle &= \frac{3}{2} k_B T \left(\frac{\varepsilon_0}{\varepsilon_0 + k_B T}\right)^{5/2} \\ \langle e^{-\varepsilon/\varepsilon_0} \varepsilon^2 \rangle &= \frac{15}{4} (k_B T)^2 \left(\frac{\varepsilon_0}{\varepsilon_0 + k_B T}\right)^{7/2} \\ \langle e^{-\varepsilon/\varepsilon_0} \varepsilon^3 \rangle &= \frac{105}{8} (k_B T)^3 \left(\frac{\varepsilon_0}{\varepsilon_0 + k_B T}\right)^{9/2}\end{aligned}$$

and

$$\begin{aligned}\mathbf{j} &= \frac{5n\tau_0 k_B^2 T}{2m} \frac{\varepsilon_0^{5/2}}{(\varepsilon_0 + k_B T)^{7/2}} \nabla T \\ \mathbf{j}_\varepsilon &= -\frac{5n\tau_0 k_B^2 T}{4m} \left(\frac{\varepsilon_0}{\varepsilon_0 + k_B T}\right)^{7/2} \left(\frac{2\varepsilon_0 - 5k_B T}{\varepsilon_0 + k_B T}\right) \nabla T.\end{aligned}$$

The previous results are obtained by setting $\varepsilon_0 = \infty$ and $\tau_0 = 1/\sqrt{2} n \bar{v} \sigma$. Note the strange result that κ becomes negative for $k_B T > \frac{2}{5} \varepsilon_0$.

(3) Use the linearized Boltzmann equation to compute the bulk viscosity ζ of an ideal gas.

- (a) Consider first the case of a monatomic ideal gas. Show that $\zeta = 0$ within this approximation. Will your result change if the scattering time is energy-dependent?
- (b) Compute ζ for a diatomic ideal gas.

Solution :

According to eqn. 8.111 in the Lecture Notes, the solution to the linearized Boltzmann equation in the relaxation time approximation is

$$\delta f = -\frac{\tau f^0}{k_B T} \left\{ m v^\alpha v^\beta \frac{\partial V_\alpha}{\partial x^\beta} - (\varepsilon_{\text{tr}} + \varepsilon_{\text{rot}}) \frac{k_B}{c_V} \nabla \cdot \mathbf{V} \right\}.$$

We also have

$$\text{Tr } \Pi = nm \langle v^2 \rangle = 2n \langle \varepsilon_{\text{tr}} \rangle = 3p - 3\zeta \nabla \cdot \mathbf{V}.$$

We then compute $\text{Tr } \Pi$:

$$\begin{aligned}\text{Tr } \Pi &= 2n \langle \varepsilon_{\text{tr}} \rangle = 3p - 3\zeta \nabla \cdot \mathbf{V} \\ &= 2n \int d\Gamma (f^0 + \delta f) \varepsilon_{\text{tr}}\end{aligned}$$

The f^0 term yields a contribution $3nk_{\text{B}}T = 3p$ in all cases, which agrees with the first term on the RHS of the equation for $\text{Tr } \Pi$. Therefore

$$\zeta \nabla \cdot \mathbf{V} = -\frac{2}{3}n \int d\Gamma \delta f \varepsilon_{\text{tr}}.$$

(a) For the monatomic gas, $\Gamma = \{p_x, p_y, p_z\}$. We then have

$$\begin{aligned}\zeta \nabla \cdot \mathbf{V} &= \frac{2n\tau}{3k_{\text{B}}T} \int d^3p f^0(\mathbf{p}) \varepsilon \left\{ m v^\alpha v^\beta \frac{\partial V_\alpha}{\partial x^\beta} - \frac{\varepsilon}{c_V/k_{\text{B}}} \nabla \cdot \mathbf{V} \right\} \\ &= \frac{2n\tau}{3k_{\text{B}}T} \left\langle \left(\frac{2}{3} - \frac{k_{\text{B}}}{c_V} \right) \varepsilon \right\rangle \nabla \cdot \mathbf{V} = 0.\end{aligned}$$

Here we have replaced $m v^\alpha v^\beta \rightarrow \frac{1}{3}m v^2 = \frac{2}{3}\varepsilon_{\text{tr}}$ under the integral. If the scattering time is energy dependent, then we put $\tau(\varepsilon)$ inside the energy integral when computing the average, but this does not affect the final result: $\zeta = 0$.

(b) Now we must include the rotational kinetic energy in the expression for δf , and we have $c_V = \frac{5}{2}k_{\text{B}}$. Thus,

$$\begin{aligned}\zeta \nabla \cdot \mathbf{V} &= \frac{2n\tau}{3k_{\text{B}}T} \int d\Gamma f^0(\Gamma) \varepsilon_{\text{tr}} \left\{ m v^\alpha v^\beta \frac{\partial V_\alpha}{\partial x^\beta} - (\varepsilon_{\text{tr}} + \varepsilon_{\text{rot}}) \frac{k_{\text{B}}}{c_V} \nabla \cdot \mathbf{V} \right\} \\ &= \frac{2n\tau}{3k_{\text{B}}T} \left\langle \frac{2}{3}\varepsilon_{\text{tr}}^2 - \frac{k_{\text{B}}}{c_V} (\varepsilon_{\text{tr}} + \varepsilon_{\text{rot}}) \varepsilon_{\text{tr}} \right\rangle \nabla \cdot \mathbf{V},\end{aligned}$$

and therefore

$$\zeta = \frac{2n\tau}{3k_{\text{B}}T} \left\langle \frac{4}{15} \varepsilon_{\text{tr}}^2 - \frac{2}{5} k_{\text{B}} T \varepsilon_{\text{tr}} \right\rangle = \frac{4}{15} n \tau k_{\text{B}} T.$$

PHYSICS 140B : STATISTICAL PHYSICS
WINTER 2012 MIDTERM EXAM SOLUTIONS

(1) Consider the Planck equation of state,

$$p = -\frac{RT}{b} \ln\left(1 - \frac{b}{v}\right) - \frac{a}{v^2},$$

where a and b are constants, and $R = N_A k_B$ is the gas constant.

(a) What are the dimensions of a and b ?

Clearly $[a] = E \cdot V$ and $[b] = V$, where E and V stand for energy and volume, respectively.

(b) Recall the virial expansion of the equation of state,

$$p = nk_B T \left(1 + B_2 n + B_3 n^2 + \dots\right),$$

where $n = N_A/v$ is the number density. Find *all* the virial coefficients for the Planck equation. You should treat $B_{j=2}$ differently from $B_{j>2}$. Recall also that for $|\varepsilon| < 1$,

$$\ln(1 + \varepsilon) = \varepsilon - \frac{1}{2}\varepsilon^2 + \frac{1}{3}\varepsilon^3 - \dots = \sum_{k=1}^{\infty} (-1)^{k-1} \frac{\varepsilon^k}{k}.$$

Expanding the log, we have

$$\begin{aligned} p &= \frac{RT}{v} + \left(\frac{1}{2}bRT - a\right)v^{-2} + \sum_{k=3}^{\infty} \frac{b^{k-1}RT}{k} v^{-k} \\ &= nk_B T \left\{ 1 + \frac{1}{N_A} \left(\frac{b}{2} - \frac{a}{N_A k_B T}\right) n + \sum_{k=3}^{\infty} \frac{1}{k} \left(\frac{bn}{N_A}\right)^{k-1} \right\}, \end{aligned}$$

using $R = N_A k_B$. From this we read off

$$B_2 = \frac{1}{N_A} \left(\frac{b}{2} - \frac{a}{N_A k_B T}\right), \quad B_{k>2} = \frac{1}{k} \left(\frac{b}{N_A}\right)^{k-1}.$$

(c) Find the values v_c , T_c , and p_c at the critical point.

The critical point is one where $p(v)$ has an inflection point. Differentiating, we have

$$\begin{aligned} \frac{\partial p}{\partial v} &= -\frac{RT}{b} \cdot \frac{b}{v^2} \cdot \frac{1}{1 - \frac{b}{v}} + \frac{2a}{v^3} \\ &= -\frac{RT}{v(v-b)} + \frac{2a}{v^3}. \end{aligned}$$

Setting $\partial p/\partial v = 0$, we have

$$f(u) = \frac{u^2}{u-1} = \frac{2a}{bRT},$$

where $u = v/b$ is dimensionless. On the interval $u \in [1, \infty]$, the function $f(u)$ has a unique minimum, and setting $f'(u) = 0$ gives $u = 2$. The minimum value for f is then $f(2) = 4$. Thus, $v_c = 2$. Evaluating the above equation at the minimum of the LHS determines T_c , and plugging in we get $p_c = p(v_c, T_c)$. We find

$$v_c = 2b \quad , \quad T_c = \frac{2}{2bR} \quad , \quad p_c = (2 \ln 2 - 1) \cdot \frac{a}{4b^2}.$$

(2) The Hamiltonian for the four state (\mathbb{Z}_4) clock model is written

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

where each local unit vector $\hat{\mathbf{n}}_i$ can take one of four possible values: $\hat{\mathbf{n}}_i \in \{\hat{\mathbf{x}}, \hat{\mathbf{y}}, -\hat{\mathbf{x}}, -\hat{\mathbf{y}}\}$.

- (a) Consider the \mathbb{Z}_4 clock model on a lattice of coordination number z . Make the mean field assumption $\langle \hat{\mathbf{n}}_i \rangle = m\hat{\mathbf{x}}$. Expanding the Hamiltonian to linear order in the fluctuations, derive the mean field Hamiltonian for this model \hat{H}_{MF} .

The mean field Hamiltonian is

$$\hat{H}_{\text{MF}} = \frac{1}{2}NzJm^2 - zJm\hat{\mathbf{x}} \cdot \sum_i \hat{\mathbf{n}}_i.$$

- (b) Rescaling $\theta = k_B T/zJ$ and $f = F/NzJ$, where N is the number of sites, find $f(m, \theta)$. We have

$$\begin{aligned} f(m, \theta) &= \frac{1}{2}m^2 - \theta \ln \text{Tr}_{\hat{\mathbf{n}}} e^{m\hat{\mathbf{x}} \cdot \hat{\mathbf{n}}/\theta} \\ &= \frac{1}{2}m^2 - \theta \ln \left(\frac{1}{2} + \frac{1}{2} \cosh(m/\theta) \right) \\ &= \frac{1}{2} \left(1 - \frac{1}{2\theta} \right) m^2 + \frac{m^4}{96\theta^3} + \mathcal{O}(m^5). \end{aligned}$$

Here we have defined $\text{Tr}_{\hat{\mathbf{n}}} = \frac{1}{4} \sum_{\hat{\mathbf{n}}}$ as the normalized trace.

- (c) Find the mean field equation and the critical value θ_c . The mean field equation is

$$0 = \frac{\partial f}{\partial m} = m - \frac{\sinh(m/\theta)}{1 + \cosh(m/\theta)}.$$

Expanding the RHS to lowest order in m and setting the slope to 1, we find $\theta_c = \frac{1}{2}$.

- (d) Is the transition second order or first order? There is no cubic term in the Landau expansion, and the coefficient of the quartic term is positive. Second order.

PHYSICS 140B : STATISTICAL PHYSICS
WINTER 2012 ALTERNATE MIDTERM EXAM SOLUTIONS

(1) Consider the equation of state,

$$p = \frac{RT}{\sqrt{v^2 - b^2}} - \frac{a}{v^2}.$$

(a) Find v_c , T_c , and p_c at the critical point.

Look for the inflection point in p as a function of v . Differentiating,

$$\frac{\partial p}{\partial v} = -\frac{RTv}{(v^2 - b^2)^{3/2}} + \frac{2a}{v^3}.$$

With $u \equiv v/b$ dimensionless, we have

$$f(u) = \frac{u^4}{(u^2 - 1)^{3/2}} = \frac{2a}{bRT}.$$

On the interval $u \in [1, \infty]$, the function $f(u)$ has a unique minimum, since

$$f'(u) = \frac{u^3(u^2 - 4)}{(u^2 - 1)^{5/2}},$$

and hence $f'(u) = 0$ has a unique solution $u = 2$, where $f(2) = 16/3\sqrt{3}$. Thus,

$$v_c = 2b \quad , \quad T_c = \frac{3\sqrt{3}}{8} \frac{a}{b} \quad , \quad p_c = \frac{a}{8b^2}.$$

(b) Writing $\bar{p} = p/p_c$, $\bar{v} = v/v_c$, and $\bar{T} = T/T_c$, write the dimensionless equation of state, $\bar{p} = \bar{p}(\bar{v}, \bar{T})$.

Scaling out v_c , T_c , and p_c , one finds

$$\bar{p} = \frac{3\sqrt{3}\bar{T}}{\sqrt{4\bar{v}^2 - 1}} - \frac{2}{\bar{v}^2}.$$

Note that $\bar{p}(\bar{v} = 1, \bar{T} = 1) = 1$.

(2) The Hamiltonian for the three state (\mathbb{Z}_3) clock model is written

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

where each local unit vector \hat{n}_i can take one of three possible values:

$$\hat{n} = \hat{x} \quad , \quad \hat{n} = -\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y} \quad , \quad \hat{n} = -\frac{1}{2}\hat{x} - \frac{\sqrt{3}}{2}\hat{y}.$$

- (a) Consider the \mathbb{Z}_3 clock model on a lattice of coordination number z . Make the mean field assumption $\langle \hat{n}_i \rangle = m \hat{x}$. Expanding the Hamiltonian to linear order in the fluctuations, derive the mean field Hamiltonian for this model \hat{H}_{MF} .

The mean field Hamiltonian is

$$\hat{H}_{\text{MF}} = \frac{1}{2} N z J m^2 - z J m \hat{x} \cdot \sum_i \hat{n}_i .$$

- (b) Rescaling $\theta = k_{\text{B}} T / z J$ and $f = F / N z J$, where N is the number of sites, find $f(m, \theta)$. We have

$$\begin{aligned} f(m, \theta) &= \frac{1}{2} m^2 - \theta \ln \text{Tr}_{\hat{n}} e^{m \hat{x} \cdot \hat{n} / \theta} \\ &= \frac{1}{2} m^2 - \theta \ln \left(\frac{1}{3} e^{m/\theta} + \frac{2}{3} e^{-m/2\theta} \right) \\ &= \frac{1}{2} \left(1 - \frac{1}{2\theta} \right) m^2 - \frac{m^3}{24\theta^2} + \frac{m^4}{64\theta^3} + \mathcal{O}(m^5) . \end{aligned}$$

Here we have defined $\text{Tr}_{\hat{n}} = \frac{1}{3} \sum_{\hat{n}}$ as the normalized trace. The last line is somewhat tedious to obtain, but is not necessary for this problem.

- (c) Find the mean field equation. The mean field equation is

$$0 = \frac{\partial f}{\partial m} = m - \frac{e^{m/\theta} - e^{-m/2\theta}}{e^{m/\theta} + 2 e^{-m/2\theta}} .$$

Expanding the RHS to lowest order in m and setting the slope to 1, we find $\theta_c = \frac{1}{2}$.

- (d) Is the transition second order or first order?

Since $f(m, \theta) \neq f(-m, \theta)$, the Landau expansion of the free energy (other than constants) should include terms of all orders starting with $\mathcal{O}(m^2)$. This means that there will in general be a cubic term, hence we expect a first order transition.

**PHYSICS 140B : STATISTICAL PHYSICS
WINTER 2012 FINAL EXAM SOLUTIONS**

(1) Consider an Ising model on a square lattice with Hamiltonian

$$\hat{H} = -J \sum_{i \in A} \sum'_{j \in B} S_i \sigma_j ,$$

where the sum is over all nearest-neighbor pairs, such that i is on the A sublattice and j is on the B sublattice (this is the meaning of the prime on the j sum), as depicted in Fig. 1. The A sublattice spins take values $S_i \in \{-1, 0, +1\}$, while the B sublattice spins take values $\sigma_j \in \{-1, +1\}$.

- (a) Make the mean field assumptions $\langle S_i \rangle = m_A$ for $i \in A$ and $\langle \sigma_j \rangle = m_B$ for $j \in B$. Find the mean field free energy $F(T, N, m_A, m_B)$. Adimensionalize as usual, writing $\theta \equiv k_B T / zJ$ (with $z = 4$ for the square lattice) and $f = F / zJN$. Then write $f(\theta, m_A, m_B)$. [10 points]

Writing $S_i = m_A + \delta S_i$ and $\sigma_j = m_B + \delta \sigma_j$ and dropping the terms proportional to $\delta S_i \delta \sigma_j$, which are quadratic in fluctuations, one obtains the mean field Hamiltonian

$$\hat{H}_{\text{MF}} = \frac{1}{2} N z J m_A m_B - z J m_B \sum_{i \in A} S_i - z J m_A \sum_{j \in B} \sigma_j ,$$

with $z = 4$ for the square lattice. Thus, the internal field on each A site is $H_{\text{int,A}} = zJm_B$, and the internal field on each B site is $H_{\text{int,B}} = zJm_A$. The mean field free energy, $F_{\text{MF}} = -k_B T \ln Z_{\text{MF}}$, is then

$$F_{\text{MF}} = \frac{1}{2} N z J m_A m_B - \frac{1}{2} N k_B T \ln \left[1 + 2 \cosh(zJm_B / k_B T) \right] - \frac{1}{2} N k_B T \ln \left[2 \cosh(zJm_A / k_B T) \right] .$$

Adimensionalizing,

$$f(\theta, m_A, m_B) = \frac{1}{2} m_A m_B - \frac{1}{2} \theta \ln \left[1 + 2 \cosh(m_B / \theta) \right] - \frac{1}{2} \theta \ln \left[2 \cosh(m_A / \theta) \right] .$$

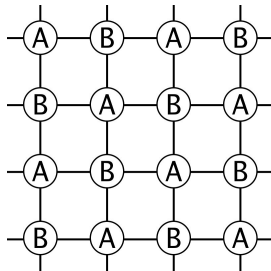


Figure 1: The square lattice and its A and B sublattices.

(b) Write down the two mean field equations (one for m_A and one for m_B). [10 points]

The mean field equations are obtained from $\partial f/\partial m_A = 0$ and $\partial f/\partial m_B = 0$. Thus,

$$m_A = \frac{2 \sinh(m_B/\theta)}{1 + 2 \cosh(m_B/\theta)}$$

$$m_B = \tanh(m_A/\theta).$$

(c) Expand the free energy $f(\theta, m_A, m_B)$ up to fourth order in the order parameters m_A and m_B . You may find the following useful:

$$\ln(2 \cosh x) = \ln 2 + \frac{x^2}{2} - \frac{x^4}{12} + \mathcal{O}(x^6) \quad , \quad \ln(1 + 2 \cosh x) = \ln 3 + \frac{x^2}{3} - \frac{x^4}{36} + \mathcal{O}(x^6).$$

[10 points]

We have

$$f(\theta, m_A, m_B) = f_0 + \frac{1}{2} m_A m_B - \frac{m_A^2}{4\theta} - \frac{m_B^2}{6\theta} + \frac{m_A^4}{24\theta^3} + \frac{m_B^4}{72\theta^3} + \dots,$$

with $f_0 = -\frac{1}{2}\theta \ln 6$.

(d) Show that the part of $f(\theta, m_A, m_B)$ which is quadratic in m_A and m_B may be written as a quadratic form, *i.e.*

$$f(\theta, m_A, m_B) = f_0 + \frac{1}{2} \begin{pmatrix} m_A & m_B \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} m_A \\ m_B \end{pmatrix} + \mathcal{O}(m_A^4, m_B^4),$$

where the matrix M is symmetric, with components $M_{aa'}$ which depend on θ . The critical temperature θ_c is identified as the largest value of θ for which $\det M(\theta) = 0$. Find θ_c and explain why this is the correct protocol to determine it. [5 points]

From the answer to part (c), we read off

$$M(\theta) = \begin{pmatrix} -\frac{1}{2\theta} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{3\theta} \end{pmatrix},$$

from which we obtain $\det M = \frac{1}{6}\theta^{-2} - \frac{1}{4}$. Setting $\det M = 0$ we obtain $\theta_c = \sqrt{\frac{2}{3}}$.

(2) Consider a two-dimensional gas of particles with dispersion $\varepsilon(\mathbf{k}) = J\mathbf{k}^2$, where \mathbf{k} is the wavevector. The particles obey photon statistics, so $\mu = 0$ and the equilibrium distribution is given by

$$f^0(\mathbf{k}) = \frac{1}{e^{\varepsilon(\mathbf{k})/k_B T} - 1}.$$

- (a) Writing $f = f^0 + \delta f$, solve for $\delta f(\mathbf{k})$ using the steady state Boltzmann equation in the relaxation time approximation,

$$\mathbf{v} \cdot \frac{\partial f^0}{\partial \mathbf{r}} = -\frac{\delta f}{\tau}.$$

Work to lowest order in ∇T . Remember that $\mathbf{v} = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}}$ is the velocity. [15 points]

We have

$$\begin{aligned} \delta f &= -\tau \mathbf{v} \cdot \frac{\partial f^0}{\partial \mathbf{r}} = -\tau \mathbf{v} \cdot \nabla T \frac{\partial f^0}{\partial T} \\ &= -\frac{2\tau}{\hbar} \frac{J^2 k^2}{k_B T^2} \frac{e^{\varepsilon(\mathbf{k})/k_B T}}{(e^{\varepsilon(\mathbf{k})/k_B T} - 1)^2} \mathbf{k} \cdot \nabla T \end{aligned}$$

- (b) Show that $\mathbf{j} = -\lambda \nabla T$, and find an expression for λ . Represent any integrals you cannot evaluate as dimensionless expressions. [10 points]

The particle current is

$$\begin{aligned} j^\mu &= \frac{2J}{\hbar} \int \frac{d^2 k}{(2\pi)^2} k^\mu \delta f(\mathbf{k}) = -\lambda \frac{\partial T}{\partial x^\mu} \\ &= -\frac{4\tau}{\hbar^2} \frac{J^3}{k_B T^2} \frac{\partial T}{\partial x^\nu} \int \frac{d^2 k}{(2\pi)^2} k^2 k^\mu k^\nu \frac{e^{Jk^2/k_B T}}{(e^{Jk^2/k_B T} - 1)^2} \end{aligned}$$

We may now send $k^\mu k^\nu \rightarrow \frac{1}{2} k^2 \delta^{\mu\nu}$ under the integral. We then read off

$$\begin{aligned} \lambda &= \frac{2\tau}{\hbar^2} \frac{J^3}{k_B T^2} \int \frac{d^2 k}{(2\pi)^2} k^4 \frac{e^{Jk^2/k_B T}}{(e^{Jk^2/k_B T} - 1)^2} \\ &= \frac{\tau k_B^2 T}{\pi \hbar^2} \int_0^\infty ds \frac{s^2 e^s}{(e^s - 1)^2} = \frac{\zeta(2)}{\pi} \frac{\tau k_B^2 T}{\hbar^2}. \end{aligned}$$

Here we have used

$$\int_0^\infty ds \frac{s^\alpha e^s}{(e^s - 1)^2} = \int_0^\infty ds \frac{\alpha s^{\alpha-1}}{e^s - 1} = \Gamma(\alpha + 1) \zeta(\alpha).$$

- (c) Show that $\mathbf{j}_\varepsilon = -\kappa \nabla T$, and find an expression for κ . Represent any integrals you cannot evaluate as dimensionless expressions. [10 points]

The energy current is

$$j_\varepsilon^\mu = \frac{2J}{\hbar} \int \frac{d^2 k}{(2\pi)^2} J k^2 k^\mu \delta f(\mathbf{k}) = -\kappa \frac{\partial T}{\partial x^\mu}.$$

We therefore repeat the calculation from part (c), including an extra factor of Jk^2 inside the integral. Thus,

$$\begin{aligned} \kappa &= \frac{2\tau}{\hbar^2} \frac{J^4}{k_B T^2} \int \frac{d^2k}{(2\pi)^2} k^6 \frac{e^{Jk^2/k_B T}}{(e^{Jk^2/k_B T} - 1)^2} \\ &= \frac{\tau k_B^3 T^2}{\pi \hbar^2} \int_0^\infty ds \frac{s^3 e^s}{(e^s - 1)^2} = \frac{6 \zeta(3)}{\pi} \frac{\tau k_B^3 T^2}{\hbar^2}. \end{aligned}$$

(3) Provide clear, accurate, and substantial answers for each of the following:

- (a) For the cluster γ shown in Fig. ??, identify the symmetry factor s_γ , the lowest order virial coefficient B_j to which γ contributes, and write an expression for the cluster integral $b_\gamma(T)$ in terms of the Mayer function $f(r)$. [6 points]

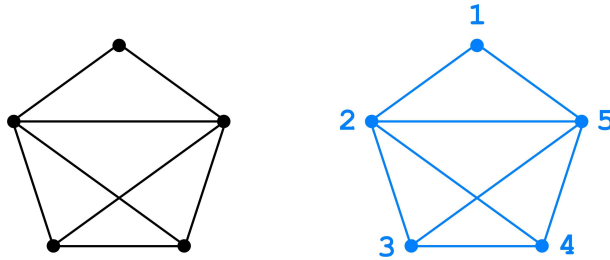


Figure 2: Left: the connected cluster γ for problem 3a. Right: the same cluster, with labels.

The symmetry factor is $2! \cdot 2! = 4$, because, consulting the right panel of Fig. 2, vertices 2 and 5 can be exchanged, and vertices 3 and 4 can be exchanged. There are five vertices, hence the lowest order virial coefficient to which this cluster contributes is B_4 . The cluster integral is

$$b_\gamma = \frac{1}{4V} \int d^d x_1 \int d^d x_2 \int d^d x_3 \int d^d x_4 \int d^d x_5 f_{12} f_{15} f_{23} f_{25} f_{34} f_{35} f_{45},$$

where $f_{ij} = e^{-u(r_{ij})/k_B T} - 1$. See Fig. 2 for the labels.

- (b) Sketch what the pair distribution function $g(r)$ should look like for a gas of hard spheres of diameter a , and discuss its salient features. [6 points]

The pair distribution function $g(r)$ is

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

where n is the bulk density. This may be interpreted as the scaled probability density for simultaneously finding a particle at the origin and a particle at a position \mathbf{r} .

Isotropy means it is a function of $r = |\mathbf{r}|$ alone. As $r \rightarrow \infty$, there is no correlation between these two events, hence $g(\infty) = 1$. For hard spheres, it is impossible for r to be less than the sphere diameter a . Thus, there is a discontinuity in $g(r)$ at $r = a$. There is a characteristic damped oscillation in $g(r)$ with a wavevector corresponding to the inverse average interparticle spacing, which is proportional to $n^{1/3}$. All these features are evident in Fig. 3.

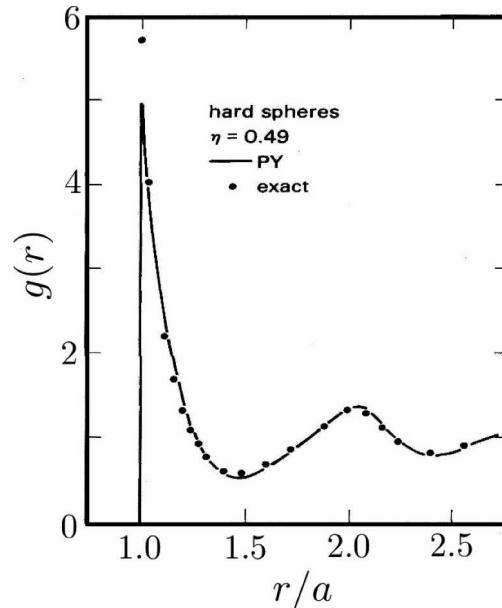


Figure 3: Pair distribution function $g(r)$ for a gas of hard spheres with diameter a , at a density $n \approx 3\pi/a^3$ ($\eta \equiv \frac{\pi}{6}na^3 = 0.49$), showing a comparison of exact (Monte Carlo) results (dots) and results within the Percus-Yevick approximation (curve).

(c) What is the Maxwell construction? [6 points]

The Maxwell construction is a fix for the van der Waals system and other related phenomenological equations of state $p = p(T, v)$ in which, throughout a region of temperature T , the pressure as a function of volume $p(v)$ is nonmonotonic. This is unphysical since the isothermal compressibility $\kappa_T = -\frac{1}{v} \frac{\partial v}{\partial p}$ becomes negative, which signals an absolute thermal instability, known as *spinodal decomposition*. The regime of instability is even larger than this, however, because of the possibility of *phase separation* into regions of different bulk density. The situation is depicted in Fig. 4. To remedy these defects, one replaces the unstable part of the $p(v)$ curve with a flat line extending from $v = v_1$ to $v = v_2$ at each temperature T in the unstable region, such that

$$p(T, v_1) = p(T, v_2)$$

$$\int_{v_1}^{v_2} dv p(T, v) = (v_2 - v_1) p(T, v_1) .$$

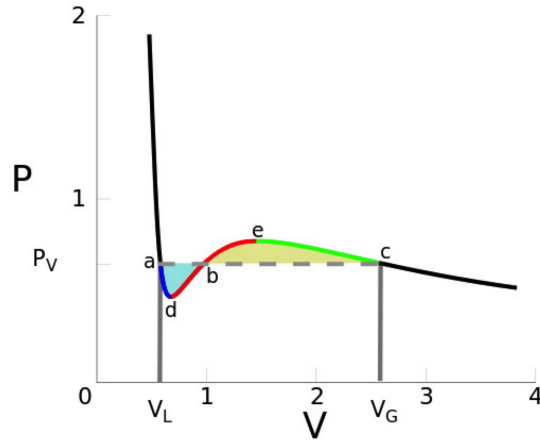


Figure 4: The Maxwell construction corrects a nonmonotonic $p(v)$ to include a flat section, known as the coexistence region, which guarantees that the Helmholtz free energy of the system is at a true minimum. The system is absolutely unstable between volumes v_d and v_e . For $v \in [v_a, v_d]$ or $v \in [v_e, v_c]$, the solution is unstable with respect to phase separation. Source: *Wikipedia*.

- (d) Provide explicit examples of models which have a discrete and a continuous global symmetry, and identify the respective symmetry groups. [6 points]

The parade example of a model with a discrete global symmetry is the Ising model,

$$\hat{H}_{\text{Ising}} = -\frac{1}{2} \sum_{i,j} J_{ij} \sigma_i \sigma_j ,$$

where $\sigma_i \in \{-1, 1\}$ for each i . The global symmetry group here is \mathbb{Z}_2 , which has two elements: identity (1) and inversion (-1). Under multiplication, these two operations form a group in the mathematical sense. Under inversion, we have $\sigma_i \rightarrow -\sigma_i$ for all sites i . The Hamiltonian is invariant under any group operation.

As an example of a model with a continuous global symmetry, consider the $O(2)$, or XY , model,

$$\hat{H}_{O(2)} = -\frac{1}{2} \sum_{i,j} J_{ij} \cos(\phi_i - \phi_j) ,$$

where $\phi_i \in [0, 2\pi)$ for each i . This Hamiltonian is invariant under global $O(2)$ rotations, $\phi_i \rightarrow \phi_i + \alpha$.

- (e) Explain the principle of detailed balance. [6 points]

Detailed balance says that under equilibrium conditions, there is a perfect balance between the number of scattering events between any two regions of phase space. Thus, if $w(\Gamma' \Gamma'_1 | \Gamma \Gamma_1) d\Gamma' d\Gamma'_1$ is a scattering rate from $|\Gamma \Gamma_1\rangle$ to a region of volume $d\Gamma' d\Gamma'_1$ containing $|\Gamma' \Gamma'_1\rangle$, then we must have

$$w(\Gamma' \Gamma'_1 | \Gamma \Gamma_1) d\Gamma' d\Gamma'_1 \times f^0(\Gamma) f^0(\Gamma') d\Gamma d\Gamma' = w(\Gamma \Gamma_1 | \Gamma' \Gamma'_1) d\Gamma d\Gamma' \times f^0(\Gamma') f^0(\Gamma'_1) d\Gamma' d\Gamma'_1 .$$

Thus,

$$\frac{f^0(\Gamma')f^0(\Gamma_1)}{f^0(\Gamma)f^0(\Gamma_1)} = \frac{w(\Gamma'\Gamma_1|\Gamma\Gamma_1)}{w(\Gamma\Gamma_1|\Gamma'\Gamma_1)}.$$

For the master equation,

$$\frac{dP_i}{dt} = \sum_k (W_{ji}P_j - W_{ij}P_i),$$

detailed balance means

$$\frac{P_i^0}{P_j^0} = \frac{W_{ji}}{W_{ij}},$$

where P_i^0 is the equilibrium distribution.

(4) Which two of Gustav Mahler's symphonies open in the key of D major?

[1000 quatloos extra credit]

Keys for Mahler's symphonies:

Symphony No. 1 in D (1887-88)

Symphony No. 2 in c (1888-94)

Symphony No. 3 in d (1893-96)

Symphony No. 4 in G (1899-1901)

Symphony No. 5 in c[#] (1901-02)

Symphony No. 6 in a (1903-04, rev. 1906)

Symphony No. 7 in e (1904-05)

Symphony No. 8 in E^b (1906)

Symphony No. 9 in D (1909-10; ends in D^b)

Symphony No. 10 in F[#] (1910; unfinished)