PHYSICS 210A : STATISTICAL PHYSICS
FINAL EXAM SOLUTIONS

(1) Provide clear, accurate, and brief answers for each of the following:

(a) For the free energy density $f = \frac{1}{2}am^2 - \frac{1}{3}ym^3 + \frac{1}{4}bm^4$, what does it mean to say that 'a first order transition preempts the second order transition'?

(b) A system of noninteracting bosons has a power law dispersion $\varepsilon(\boldsymbol{k}) = A\,k^\sigma$. What is the condition on the power σ and the dimension d of space such that Bose condensation will occur at some finite temperature?

(c) Sketch what the pair distribution function $g(r)$ should look like for a fluid composed of infinitely hard spheres of diameter a. How does $g(r)$ change with temperature?

(d) For the cluster γ shown in Fig. 1, identify the symmetry factor s_γ, the lowest order virial oefficient B_j to which this contributes, and write an expression for the cluster integral $b_\gamma(T)$ in terms of the Mayer function.

(e) Explain the following terms in the context of dynamical systems: *recurrent*, *ergodic*, and *mixing*. How are these classifications arranged hierarchically?

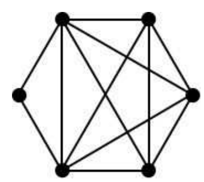

Figure 1: The connected cluster γ for problem (1d).

Solution:

(a) In the absence of a cubic term (*i.e.* when $y = 0$), there is a second order transition at $a = 0$, assuming $b > 0$ for stability. The ordered phase, for $a < 0$, has a spontaneous moment $m \neq 0$. When the cubic term is present, a *first order* (*i.e.* discontinuous) transition takes place at $a = \frac{2y^2}{9b}$, which is positive. Thus, as a is decreased from large positive values, the first order transition takes place before a reaches $a = 0$, hence we say that the second order transition that *would have* occurred at $a = 0$ is *preempted*. Typically $a(T) \propto T - T_c$, where T_c is what the second order transition temperature would be in the case $y = 0$.
`[5 points]`

(b) At $T = T_c$, we have the relation

$$n = \int \frac{d^d\!k}{(2\pi)^d}\,\frac{1}{e^{\varepsilon(\boldsymbol{k})/k_B T_c} - 1}\,.$$

If the integral fails to converge, then there is no finite temperature solution and no Bose condensation. For small k, we may expand the exponential in the denominator, and we

find the occupancy function behaves as $k_{\rm B}T_{\rm c}/\varepsilon(\boldsymbol{k}) \propto k^{-\sigma}$. From the integration metric, in d-dimensional polar coordinates, we have $d^d\!k = \Omega_d\, k^{d-1}\, dk$, where Ω_d is the surface area of the d-dimensional unit sphere. Thus, the integrand is proportional to $k^{d-\sigma-1}$. For convergence, then, we require $d > \sigma$. This is the condition for finite temperature Bose condensation.
[5 points]

(c) The pdf for a hard sphere gas is shown in Fig. 2 below. The main features are $g(r=0)$ for $r < a$, and a decaying oscillation for $r > a$. Since the potential is either $U = 0$ (no two spheres overlapping), or $U = \infty$ (overlap of at least two spheres), temperature has no effect, because $U/k_{\rm B}T$ is also either 0 or ∞. The hard sphere gas is a reasonable model for the physics of liquid argon (see figure).
[5 points]

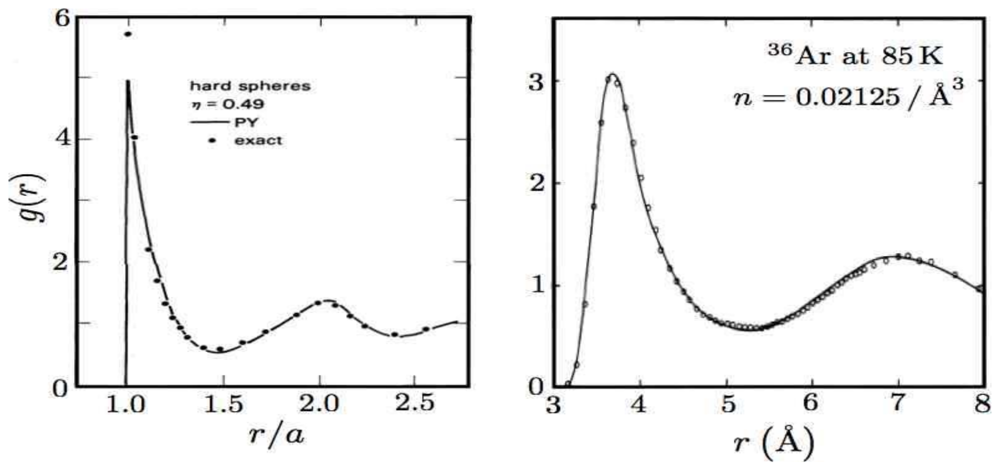

Figure 2: (1c) Pair distribution functions (PDF) for hard spheres of diameter a at filling fraction $\eta = \frac{\pi}{6}a^3 n = 0.49$ (left) and for liquid argon at $T = 85\,$K (right). Molecular dynamics data for hard spheres (points) is compared with the result of the Percus-Yevick approximation. Experimental data on liquid argon are from the neutron scattering work of Yarnell *et al.* (1973). The data (points) are compared with molecular dynamics calculations by Verlet (1967) for a Lennard-Jones fluid. See fig. 5.8 of the lecture notes.

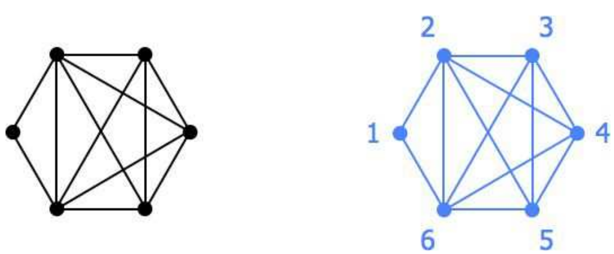

Figure 3: Left: the connected cluster γ for problem (1d). Right: a labeled version of this cluster used in expressing the cluster integral b_γ.

(d) The symmetry factor is $2!\cdot 3! = 12$, because, consulting the right panel of Fig. 3, vertices

2 and 6 can be exchanged, and vertices 3, 4, and 5 can be permuted in any way. There are six vertices, hence the lowest order virial coefficient to which this cluster contributes is B_6. The cluster integral is

$$b_\gamma = \frac{1}{12\,V}\int\!d^dx_1\!\int\!d^dx_2\!\int\!d^dx_3\!\int\!d^dx_4\!\int\!d^dx_5\!\int\!d^dx_6\; f_{12}\, f_{16}\, f_{23}\, f_{24}\, f_{25}\, f_{26}\, f_{34}\, f_{35}\, f_{36}\, f_{45}\, f_{46}\, f_{56}\ ,$$

where $f_{ij} = e^{-u(r_{ij})/k_\mathrm{B}T} - 1$. See Fig. 3 for the labels.
[5 points]

(e) A recurrent dynamical system exhibits the property that within any finite region of phase space one can find a point which will return to that region in a finite time. Poincaré recurrence is guaranteed whenever the dynamics are invertible and volume-preserving on a finite phase space. An ergodic system is one where time averages are equal to phase space averages. For the dynamical system $\dot{\boldsymbol{\varphi}} = \boldsymbol{V}(\boldsymbol{\varphi})$, ergodicity means

$$\big\langle f(\boldsymbol{\varphi})\big\rangle_T = \lim_{T\to\infty}\frac{1}{T}\int\limits_0^T\!dt\; f\big(\boldsymbol{\varphi}(t)\big) = \frac{\mathsf{Tr}\, f(\boldsymbol{\varphi})\,\delta\big(E - H(\boldsymbol{\varphi})\big)}{\mathsf{Tr}\,\delta\big(E - H(\boldsymbol{\varphi})\big)} = \big\langle f(\boldsymbol{\varphi})\big\rangle_S\ ,$$

where $f(\boldsymbol{\varphi})$ is any smooth function on phase space. A mixing system is one where any smooth normalized distribution $\varrho(\boldsymbol{\varphi},t)$ satisfies

$$\lim_{t\to\infty}\mathsf{Tr}\,\varrho(\boldsymbol{\varphi},t)\, f(\boldsymbol{\varphi}) = \big\langle f(\boldsymbol{\varphi})\big\rangle_S\ .$$

Thus, the distribution spreads out 'evenly' over the entire energy surface. The hierarchy is

$$\text{mixing} \subset \text{ergodic} \subset \text{recurrent}\ .$$

[5 points]

(2) Consider a gas of spinless bosons in $d = 3$ dimensions with dispersion $\varepsilon(\boldsymbol{p}) = \boldsymbol{p}^2/2m$ and bulk number density n. The gas is in equilibrium with a $d = 2$ surface, and the surface bosons have dispersion $\varepsilon_{2\mathrm{d}}(p_x, p_y) = (p_x^2 + p_y^2)/2m + \Delta$ with $\Delta > 0$. Note that $\mathsf{Li}_1(z) = -\log(1-z)$.

(a) For $T > T_\mathrm{c}$, where T_c is the bulk critical temperature for Bose-Einstein condensation, write down relations between (i) the bulk density n, temperature T, and fugacity z, and (ii) the surface density $n_{2\mathrm{d}}$, T, and z. Your expressions may also involve m, Δ, and numeral and physical constants.

(b) For $T < T_\mathrm{c}$, write down relations between (i) the bulk density n, temperature T, and bulk condensate density n_0, and (ii) the surface density $n_{2\mathrm{d}}$, T, and n_0. Your expressions may also involve m, Δ, and numeral and physical constants.

(c) What is T_c? Find an equation relating $n_{2\mathrm{d}}(T_\mathrm{c})$ to n, Δ, m, and physical constants.

(d) What is the $T \to 0$ limit of the surface density $n_{2\mathrm{d}}$? Interpret your result. Do the surface bosons ever condense? Why or why not? What do you think happens if $\Delta < 0$?

Important: You may regard the bulk number density to be fixed at n regardless of the surface number density n_{2d} because in the thermodynamic limit the bulk contains vastly more particles than the surface.

Solution:

(a) The derivation may be found in ch. 5 of the lecture notes:

$$n = \lambda_T^{-3}\,\mathrm{Li}_{3/2}(z) \qquad , \qquad n_{2d} = \lambda_T^{-2}\,\mathrm{Li}_1\big(z\,e^{-\Delta/k_B T}\big) = -\lambda_T^{-2}\log\big(1 - z\,e^{-\Delta/k_B T}\big) \quad .$$

`[5 points]`

(b) When the bulk is condensed, $\mu = 0$ and $z = 1$, hence

$$n = n_0 + \zeta\big(\tfrac{3}{2}\big)\lambda_T^{-3} \qquad , \qquad n_{2d} = -\lambda_T^{-2}\log\big(1 - e^{-\Delta/k_B T}\big) \quad .$$

`[10 points]`

(c) When $T = T_c = (2\pi\hbar^2/m)\big(n/\zeta(\frac{3}{2})\big)^{2/3}$, we have

$$n_{2d}(T_c) = -\big(n/\zeta(\tfrac{3}{2})\big)^{2/3}\log\left[1 - \exp\left(-\frac{m\Delta}{2\pi\hbar^2\big(n/\zeta(\frac{3}{2})\big)^{2/3}}\right)\right]$$

`[5 points]`

(d) As $T \to 0$ we have from (b) that $n_{2d} = \lambda_T^{-2}\exp(-\Delta/k_B T) \to 0$. In this limit all the bosons are in the bulk and condensed into their lowest energy state, $\varepsilon(\boldsymbol{p} = \boldsymbol{0}) = 0$. Since $\Delta > 0$, the lowest energy surface state has $\varepsilon_{2d} = \Delta > 0$ and is unoccupied. The surface bosons never condense because there is no 2D Bose condensation of ballistic particles. This would be the case even if Δ were negative. If $\Delta < 0$, the maximum value of the fugacity is $z = e^{-|\Delta|/k_B T}$. In this case as $T \to 0$ the bosons all crowd onto the surface., which is unphysical if the bosons have a hard core.
`[5 points]`

(3) The Hamiltonian for the one-dimensional p-state clock model is

$$\hat{H} = -J\sum_i \cos\left(\frac{2\pi(n_i - n_{i+1})}{p}\right) = \sum_i E_{n_i,n_{i+1}} \quad ,$$

where on each site one has $n_i \in \{0, 1, \ldots, p-1\}$. Here you are invited to consider the case $p = 4$. The interaction energy between neighboring clock spins with values n and n' is then

$$E_{n,n'} = \begin{pmatrix} -J & 0 & J & 0 \\ 0 & -J & 0 & J \\ J & 0 & -J & 0 \\ 0 & J & 0 & -J \end{pmatrix} \quad .$$

(a) Write down the transfer matrix $T_{n,n'}$ at temperature T.

(b) Find the eigenvalues of T. As a helpful hint, note that the (normalized) eigenvectors of the matrix

$$M = \begin{pmatrix} a & 1 & b & 1 \\ 1 & a & 1 & b \\ b & 1 & a & 1 \\ 1 & b & 1 & a \end{pmatrix}$$

are

$$\psi_1 = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \quad , \quad \psi_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix} \quad , \quad \psi_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix} \quad , \quad \psi_4 = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} \quad .$$

(c) Find the free energy per site in the thermodynamic limit.

(d) Let $\phi_i = \delta_{n_i,1} - \frac{1}{4}$. This serves as an order parameter since $\langle \phi_i \rangle = 0$ in the disordered phase where each n value is equally likely and hence $\langle \delta_{n_i,1} \rangle = \frac{1}{4}$. Using the transfer matrix formalism, find the correlator $C(m) = \langle \phi_1 \, \phi_{1+m} \rangle$. What is the correlation length $\xi(T)$?

Solution:

(a) The transfer matrix is

$$T_{n,n'} = e^{-\beta E_{n,n'}} = \begin{pmatrix} e^{\beta J} & 1 & e^{-\beta J} & 1 \\ 1 & e^{\beta J} & 1 & e^{-\beta J} \\ e^{-\beta J} & 1 & e^{\beta J} & 1 \\ 1 & e^{-\beta J} & 1 & e^{\beta J} \end{pmatrix} \quad .$$

[9 points]

(b) Applying M to each of the given mutually orthogonalnnormalized eigenvectors, we find $\lambda_1 = a + b + 2$, $\lambda_2 = \lambda_3 = a - b$, and $\lambda_4 = a + b - 2$. For our purposes, we have $a = \exp(\beta J)$ and $b = \exp(-\beta J)$. Thus, the four eigenvalues of T are

$$\lambda_1 = 2\cosh(\beta J) + 2 \quad , \quad \lambda_2 = \lambda_3 = 2\sinh(\beta J) \quad , \quad \lambda_4 = 2\cosh(\beta J) - 2 \quad ,$$

with $\lambda_1 > \lambda_2 = \lambda_3 \geq \lambda_4$.
[8 points]

(c) In the thermodynamic limit $L \to \infty$ the maximum eigenvalue λ_1 dominates and we have $Z = \lambda_1^L$, hence

$$f = \frac{F}{L} = -k_{\mathrm{B}} T \log \lambda_1 = -k_{\mathrm{B}} T \log\big(2\cosh(J/k_{\mathrm{B}} T) + 2\big) \quad .$$

[8 points]

(d) The correlator is

$$C(m) = \frac{\mathsf{Tr}\left(\Phi \, T^m \, \Phi \, T^{L-m}\right)}{\mathsf{Tr}\, T^L} = \frac{\sum_{\alpha,\beta=1}^{4} \big|\langle \, \psi_\alpha \, | \, \Phi \, | \, \psi_\beta \, \rangle\big|^2 \, \lambda_\beta^m \, \lambda_\alpha^{L-m}}{\sum_{\gamma=1}^{4} \lambda_\gamma^L}$$

where

$$\Phi = \begin{pmatrix} \frac{3}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 & 0 \\ 0 & 0 & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & -\frac{1}{4} \end{pmatrix} \quad .$$

Note that $\langle\, \psi_1 \,|\, \Phi \,|\, \psi_1 \,\rangle = \langle\, \psi_3 \,|\, \Phi \,|\, \psi_1 \,\rangle = 0$, $\langle\, \psi_2 \,|\, \Phi \,|\, \psi_1 \,\rangle = 2^{-3/2}$, and $\langle\, \psi_4 \,|\, \Phi \,|\, \psi_1 \,\rangle = \frac{1}{4}$. Thus, we have

$$\begin{aligned} C(m) &= \big|\langle\, \psi_2 \,|\, \Phi \,|\, \psi_1 \,\rangle\big|^2 \left(\frac{\lambda_2}{\lambda_1}\right)^m + \big|\langle\, \psi_4 \,|\, \Phi \,|\, \psi_1 \,\rangle\big|^2 \left(\frac{\lambda_4}{\lambda_1}\right)^m \\ &= \tfrac{1}{8}\big[\tanh(J/2k_{\rm B}T)\big]^{|m|} + \tfrac{1}{6}\big[\tanh(J/2k_{\rm B}T)\big]^{2\,|m|} \quad , \end{aligned}$$

since

$$\frac{\lambda_{2,3}}{\lambda_1} = \frac{\sinh(\beta J)}{1+\cosh(\beta J)} = \tanh(\tfrac{1}{2}\beta J) \qquad , \qquad \frac{\lambda_4}{\lambda_1} = \frac{\cosh(\beta J) - 1}{\cosh(\beta J) + 1} = \tanh^2(\tfrac{1}{2}\beta J) \quad .$$

The correlation length is obtained by setting $\exp(-1/\xi) = \tanh(\frac{1}{2}\beta J)$, yielding

$$\xi(T) = \frac{1}{\log\,{\rm ctnh}\,(J/2k_{\rm B}T)} \quad .$$

[100 quatloos extra credit]

(4) Now consider the mean field phase transition of the $p = 4$ clock model, with

$$\hat{H} = -J \sum_{\langle ij \rangle} \cos\!\left(\frac{2\pi(n_i - n_j)}{4}\right) - H \sum_i \big(\delta_{n_i,0} - \tfrac{1}{4}\big) \quad ,$$

with $n_i \in \{0,1,2,3\}$ on each site i. Find the variational free energy from the normalized single site density matrix

$$\begin{aligned} \varrho(n) &= \frac{e^{u\cos(2\pi n/4)}}{2 + 2\cosh u} \\ &= \frac{e^{u}}{2+2\cosh u}\,\delta_{n,0} + \frac{1}{2+2\cosh u}\,\delta_{n,1} + \frac{e^{-u}}{2+2\cosh u}\,\delta_{n,2} + \frac{1}{2+2\cosh u}\,\delta_{n,3} \quad . \end{aligned}$$

(a) Find $E = {\sf Tr}\,(\hat{H}\,\varrho_N^{\rm var})$, where $\varrho_N = \prod_{i=1}^N \varrho(n_i)$. You should assume a Bravais lattice with of coordination number z with nearest neighbor interactions only.

(b) Find $S = -k_{\rm B}\,{\sf Tr}\,\big(\varrho_N^{\rm var} \log \varrho_N^{\rm var}\big)$

(c) Find the dimensionless free energy per site $f(u,\theta,h) = F/NzJ$, with $\theta = k_{\rm B}T/zJ$ and $h = H/zJ$ the dimensionless temperature and symmetry-breaking external field.

(d) Find $\theta_{\rm c}$ and $\phi(h)$ above $\theta_{\rm c}$, where $\phi = \langle \delta_{n_i,1} - \frac{1}{4}\rangle$ is the order parameter.

Solution:

(a) We have

$$
\begin{aligned}
E &= -\tfrac{1}{2} N z J \sum_{n=1}^{4} \sum_{n'=1}^{4} E_{n,n'}\, \varrho(n)\, \varrho(n') - H\big(\varrho(0) - \tfrac{1}{4}\big) \\
&= -\tfrac{1}{2} N z J \big[\varrho(0) - \varrho(2)\big]^2 - \tfrac{1}{2} N z J \big[\varrho(1) - \varrho(3)\big]^2 - H\big(\varrho(0) - \tfrac{1}{4}\big) \\
&= -\tfrac{1}{2} N z J \tanh^2(\tfrac{1}{2}u) - H\left(\frac{e^u}{2 + 2\cosh u} - \tfrac{1}{4}\right) \quad .
\end{aligned}
$$

[6 points]

(b) The entropy is

$$
\begin{aligned}
S &= -N k_{\rm B} \sum_{n=1}^{4} \varrho(n) \log \varrho(n) \\
&= -N k_{\rm B} \left[\frac{u \sinh u}{1 + \cosh u} - \log(2 + 2\cosh u) \right] \quad .
\end{aligned}
$$

[6 points]

(c) The dimensionless free energy is

$$
\begin{aligned}
f(u, \theta, h) &= -\tfrac{1}{2} \tanh^2(u/2) - \frac{h\, e^u}{2 + 2\cosh u} + \tfrac{1}{4} h + \theta \left[\frac{u \sinh u}{1 + \cosh u} - \log(2 + 2\cosh u) \right] \\
&= -\theta \log 4 - \tfrac{1}{4} h u + \tfrac{1}{4}\left(\theta - \tfrac{1}{2}\right) u^2 + \tfrac{1}{32}\left(\tfrac{2}{3} - \theta\right) u^4 + \ldots \quad .
\end{aligned}
$$

The expansion to order u^2 is straightforward.
[6 points]

(d) From the above Landau expansion to order u^2 we have $\theta_{\rm c} = \frac{1}{2}$. The order parameter is $\phi = -\partial f/\partial h = \frac{1}{4} u$, and setting $\partial f/\partial u = 0$ yields $(\theta - \theta_{\rm c}) u = \frac{1}{2} h$, whence

$$
\phi = \tfrac{1}{8} (\theta - \theta_{\rm c})^{-1} \quad .
$$

Nota bene: The coefficient of the quartic term in the expansion from part (c), which you were not expected to derive, might elicit some concern - what happens when $\theta > \frac{2}{3}$? Is there a first order transition for $h = 0$? There is not. One obtains

$$
\frac{\partial f(u, \theta, h = 0)}{\partial u} = \frac{\theta u - \tanh(u/2)}{2 \cosh^2(u/2)} \quad .
$$

Thus there are at most three stationary points at finite values of u: $u = 0$ and, for $\theta < \frac{1}{2}$, the two equal and opposite solutions to $\theta u = \tanh(u/2)$. Thus, the transition is second order.
[7 points]