PHYSICS 210A : STATISTICAL PHYSICS
FINAL EXAMINATION SOLUTIONS
All parts are worth 5 points each

(1) [40 points total] Consider a noninteracting gas of bosons in d dimensions. Let the single particle dispersion be $\varepsilon(\boldsymbol{k}) = A\,|\boldsymbol{k}|^{\sigma}$, where $\sigma > 0$.

(a) Find the single particle density of states per unit volume $g(\varepsilon)$. Show that $g(\varepsilon) = C\,\varepsilon^{p-1}\,\Theta(\varepsilon)$, and find C and p in terms of A, d, and σ. You may abbreviate the total solid angle in d dimensions as $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$.

We have

$$g(\varepsilon)\,d\varepsilon = \frac{d^d k}{(2\pi)^d} = (2\pi)^{-d}\,\Omega_d\,k^{d-1}\,dk$$

and hence

$$g(\varepsilon) = (2\pi)^{-d}\,\Omega_d\,k^{d-1}\,\frac{dk}{d\varepsilon} = C\,\varepsilon^{p-1}\ ,$$

where $p = d/\sigma$ and

$$C = \frac{\Omega_d\,A^{-d/\sigma}}{\sigma(2\pi)^d} = \frac{A^{-d/\sigma}}{2^{d-1}\pi^{d/2}\,\Gamma(d/2)\,\sigma}\ .$$

(b) Under what conditions will there be a finite temperature $T_{\rm c}$ for Bose condensation?

The number density is

$$n(T,z) = \int\limits_0^\infty d\varepsilon\ \frac{g(\varepsilon)}{z^{-1}\,e^{\beta\varepsilon}-1} = C\,\Gamma(p)\,\beta^{-p}\,\mathsf{Li}_p(z)\ .$$

The RHS is a monotonically increasing function of the fugacity z. It vanishes for $z = 0$. In the limit $z \to 1^-$, the RHS diverges for $p \le 1$. In this case, we can invert this equation to obtain a unique solution for $z(T,n)$. In this case, there is no Bose condensation. If $p > 1$, the RHS is finite for $z = 1$, which establishes a maximum density $n_{\rm max}(T)$ at each temperature, above which the system must be in a condensed phase. Thus, the criterion for a finite $T_{\rm c}$ is $p > 1$, *i.e.* $d > \sigma$.

(c) For $T > T_{\rm c}$, find an expression for the number density $n(T,z)$. You may find the following useful:

$$\int\limits_0^\infty d\varepsilon\ \frac{\varepsilon^{q-1}}{z^{-1}e^{\beta\varepsilon}-1} = \Gamma(q)\,\beta^{-q}\,\mathsf{Li}_q(z)\ ,$$

where $\mathsf{Li}_q(z) = \sum_{j=1}^\infty z^j/j^q$ is the polylogarithm function. Note that $\mathsf{Li}_q(1) = \zeta(q)$.

This has been computed in part (b) above: $n(T,z) = C\,\Gamma(p)\,(k_{\rm B}T)^p\,\mathsf{Li}_p(z)$.

(d) Assuming $T_{\rm c} > 0$, find an expression for $T_{\rm c}(n)$.

Set $z = 1$ and $T = T_{\rm c}$. We then have

$$k_{\rm B} T_{\rm c} = \left(\frac{n}{C \, \Gamma(p) \, \zeta(p)} \right)^{1/p} .$$

(e) For $T < T_{\rm c}$, find an expression for the condensate number density $n_0(T, n)$.

We set $z = 1$. Then $n_0 = n - n_{\rm max}(T)$, *i.e.*

$$n_0(T) = n \cdot \left\{ 1 - \left(\frac{T}{T_{\rm c}(n)} \right)^p \right\} .$$

where $T_{\rm c}(n)$ is given in part (d).

(f) For $T < T_{\rm c}$, compute the molar heat capacity at constant volume and particle number $c_{V,N}(T, n)$. Recall that $c_{V,N} = \frac{N_{\rm A}}{N} \left(\frac{\partial E}{\partial T} \right)_{V,N}$.

The energy density is

$$E = V \int_0^\infty d\varepsilon \, \frac{\varepsilon \, g(\varepsilon)}{e^{\beta \varepsilon} - 1} = C \, V \, \Gamma(p+1) \, \zeta(p+1) \, (k_{\rm B} T)^{p+1} .$$

Thus,

$$C_{V,N} = \left(\frac{\partial E}{\partial T} \right)_{V,N} = C \, k_{\rm B} \, V \, \Gamma(p+2) \, \zeta(p+1) \, (k_{\rm B} T)^p .$$

As we have derived above, the particle number is related to the critical temperature by

$$N = C \, V \, \Gamma(p) \, \zeta(p) \, (k_{\rm B} T_{\rm c})^p .$$

Therefore the molar heat capacity is

$$c_{V,N}(T, n) = \frac{N_{\rm A}}{N} \cdot C_{V,N} = R \cdot \frac{p(p+1) \, \zeta(p+1)}{\zeta(p)} \cdot \left(\frac{T}{T_{\rm c}(n)} \right)^p .$$

where $R = N_{\rm A} k_{\rm B}$ is the gas constant.

(g) For $T > T_{\rm c}$, compute the molar heat capacity at constant volume and particle number $c_{V,N}(T, z)$.

In this regime,

$$N(T, V, z) = V \int_0^\infty d\varepsilon \, \frac{g(\varepsilon)}{z^{-1} e^{\beta \varepsilon} - 1} = C \, V \, \Gamma(p) \, (k_{\rm B} T)^p \, \mathsf{Li}_p(z)$$

$$E(T, V, z) = V \int_0^\infty d\varepsilon \, \frac{\varepsilon \, g(\varepsilon)}{z^{-1} e^{\beta \varepsilon} - 1} = C \, V \, \Gamma(p+1) \, (k_{\rm B} T)^{p+1} \, \mathsf{Li}_{p+1}(z) .$$

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Now take the differentials:

$$dN = C\,V\,\Gamma(p)\,(k_{\mathrm{B}}T)^p \cdot \left\{ p\,\mathsf{Li}_p(z)\,\frac{dT}{T} + \mathsf{Li}_{p-1}(z)\,\frac{dz}{z} \right\}$$

$$dE = C\,V\,\Gamma(p+1)\,(k_{\mathrm{B}}T)^{p+1} \cdot \left\{ (p+1)\,\mathsf{Li}_{p+1}(z)\,\frac{dT}{T} + \mathsf{Li}_p(z)\,\frac{dz}{z} \right\}.$$

Since $dN = 0$, we can use the first of these to solve for dz in terms of dT:

$$\left.\frac{dz}{z}\right|_N = -\frac{p\,\mathsf{Li}_p(z)}{\mathsf{Li}_{p-1}(z)} \cdot \frac{dT}{T}.$$

Inserting this into the equation for dE, we have

$$dE\big|_N = C\,V\,\Gamma(p+1)\,(k_{\mathrm{B}}T)^{p+1} \cdot \left\{ (p+1)\,\mathsf{Li}_{p+1}(z) - \frac{p\,\mathsf{Li}_p^2(z)}{\mathsf{Li}_{p-1}(z)} \right\} \cdot \frac{dT}{T}$$

$$= pNk_{\mathrm{B}}T \cdot \left\{ \frac{(p+1)\,\mathsf{Li}_{p+1}(z)}{\mathsf{Li}_p(z)} - \frac{p\,\mathsf{Li}_p(z)}{\mathsf{Li}_{p-1}(z)} \right\} \cdot \frac{dT}{T},$$

and hence

$$c_{V,N}(T,z) = pR \cdot \left\{ \frac{(p+1)\,\mathsf{Li}_{p+1}(z)}{\mathsf{Li}_p(z)} - \frac{p\,\mathsf{Li}_p(z)}{\mathsf{Li}_{p-1}(z)} \right\}.$$

(h) Show that under certain conditions the heat capacity is discontinuous at T_{c}, and evaluate $c_{V,N}(T_{\mathrm{c}}^{\pm})$ just above and just below the transition.

Setting $z = 1$ and $T = T_{\mathrm{c}}$, the results from parts (f) and (g) yield

$$c_{V,N}(T_{\mathrm{c}}^-) = \frac{p(p+1)\,\zeta(p+1)R}{\zeta(p)}$$

$$c_{V,N}(T_{\mathrm{c}}^+) = \frac{p(p+1)\,\zeta(p+1)R}{\zeta(p)} - \frac{p^2\zeta(p)R}{\zeta(p-1)}.$$

Subtracting these values we obtain the discontinuity at the transition,

$$\Delta c \equiv c_{V,N}(T_{\mathrm{c}}^+) - c_{V,N}(T_{\mathrm{c}}^-) = -\frac{p^2\,\zeta(p)\,R}{\zeta(p-1)}.$$

For $1 < p < 2$ we have $T_{\mathrm{c}} > 0$ and $\Delta c = 0$, since $\zeta(p-1) = \infty$. For $p > 2$, however, there is a finite discontinuity in the specific heat at the transition.

(2) [30 points total] Consider the following model Hamiltonian,

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

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where each σ_i may take on one of three possible values, and

$$E(\sigma, \sigma') = \begin{pmatrix} -J & +J & 0 \\ +J & -J & 0 \\ 0 & 0 & +K \end{pmatrix} ,$$

with $J > 0$ and $K > 0$. Consider a variational density matrix $\varrho_{\mathrm{v}}(\sigma_1, \ldots, \sigma_N) = \prod_i \tilde{\varrho}(\sigma_i)$, where the normalized single site density matrix has diagonal elements

$$\tilde{\varrho}(\sigma) = \left(\frac{n+m}{2}\right)\delta_{\sigma,1} + \left(\frac{n-m}{2}\right)\delta_{\sigma,2} + (1-n)\,\delta_{\sigma,3} .$$

(a) What is the global symmetry group for this Hamiltonian?

The global symmetry group is $\mathbb{Z}_2$. If we label the spin values as $\sigma \in \{1,2,3\}$, then the group elements can be written as permutations, $1 = \binom{123}{123}$ and $\mathcal{J} = \binom{123}{213}$, with $\mathcal{J}^2 = 1$.

(b) Evaluate $E = \mathsf{Tr}\,(\varrho_{\mathrm{v}}\,\hat{H})$.

For each nearest neighbor pair (ij), the distribution of $\{\sigma_i \sigma_j\}$ is according to the product $\tilde{\varrho}(\sigma_i)\,\tilde{\varrho}(\sigma_j)$. Thus, we have

$$E = \tfrac{1}{2}NzJ \sum_{\sigma, \sigma'} \tilde{\varrho}(\sigma)\,\tilde{\varrho}(\sigma')\,\varepsilon(\sigma, \sigma')$$

$$= \tfrac{1}{2}NzJ \cdot \left\{ \overbrace{\left(\frac{n+m}{2}\right)^2}^{\tilde{\varrho}^2(1)}(-J) + \overbrace{\left(\frac{n-m}{2}\right)^2}^{\tilde{\varrho}^2(2)}(-J) + \overbrace{2\left(\frac{n+m}{2}\right)\left(\frac{n-m}{2}\right)}^{2\,\tilde{\varrho}(1)\,\tilde{\varrho}(2)}(+J) + \overbrace{(1-n)^2}^{\tilde{\varrho}^2(3)}(+K) \right\}$$

$$= -\tfrac{1}{2}Nz\left[Jm^2 - K(1-n)^2\right] .$$

(c) Evaluate $S = -k_{\mathrm{B}}\,\mathsf{Tr}\,(\varrho_{\mathrm{v}}\ln\varrho_{\mathrm{v}})$.

The entropy is

$$S = -Nk_{\mathrm{B}}\,\mathsf{Tr}\,(\tilde{\varrho}\ln\tilde{\varrho})$$

$$= -Nk_{\mathrm{B}}\left\{\left(\frac{n+m}{2}\right)\ln\left(\frac{n+m}{2}\right) + \left(\frac{n-m}{2}\right)\ln\left(\frac{n-m}{2}\right) + (1-n)\ln(1-n)\right\} .$$

(d) Adimensionalize by writing $\theta = k_{\mathrm{B}}T/zJ$ and $c = K/J$, where z is the lattice coordination number. Find $f(n,m,\theta,c) = F/NzJ$.

This can be solved by inspection from the results of parts (b) and (c):

$$f = -\tfrac{1}{2}m^2 + \tfrac{1}{2}c\,(1-n)^2 + \theta\left[\left(\frac{n+m}{2}\right)\ln\left(\frac{n+m}{2}\right) + \left(\frac{n-m}{2}\right)\ln\left(\frac{n-m}{2}\right) + (1-n)\ln(1-n)\right] .$$

(e) Find all the mean field equations.

There are two mean field equations, obtained by extremizing with respect to n and to m, respectively:

$$\frac{\partial f}{\partial n} = 0 = c\,(n-1) + \tfrac{1}{2}\theta\,\ln\!\left(\frac{n^2 - m^2}{4\,(1-n)^2}\right)$$

$$\frac{\partial f}{\partial m} = 0 = -m + \tfrac{1}{2}\theta\,\ln\!\left(\frac{n-m}{n+m}\right).$$

These may be recast as

$$n^2 = m^2 + 4\,(1-n)^2\,e^{-2c(n-1)/\theta}$$
$$m = n\,\tanh(m/\theta)\,.$$

(f) Find an equation for the critical temperature θ_{c}, and show graphically that it has a unique solution.

To find θ_{c}, we take the limit $m \to 0$. The second mean field equation then gives $n = \theta$. Substituting this into the first mean field equation yields

$$\theta = 2\,(1-\theta)\,e^{-2c(\theta-1)/\theta}\,.$$

If we define $u \equiv \theta^{-1} - 1$, this equation becomes

$$2u = e^{-cu}\,.$$

It is clear that for $c > 0$ this equation has a unique solution, since the LHS is monotonically increasing and the RHS is monotonically decreasing, and the difference changes sign for some $u > 0$. The low temperature phase is the ordered phase, which spontaneously breaks the aforementioned $\mathbb{Z}_2$ symmetry. In the high temperature phase, the $\mathbb{Z}_2$ symmetry is unbroken.

(3) [30 points total] Provide clear, accurate, and brief answers for each of the following:

(a) Explain what is meant by (i) recurrent, (ii) ergodic, and (iii) mixing phase flows.

(i) In a recurrent system, for every neighborhood $\mathcal{N}$ of phase space there exists a point $\varphi_0 \in \mathcal{N}$ which will return to $\mathcal{N}$ after a finite number of application of the τ-advance map g_τ, where τ is finite. (ii) An ergodic system is one in which time averages may be replaced by phase space averages. (iii) A mixing system is one for which, as $t \to \infty$, the *instantaneous* time average of a quantity may be replaced by its phase space average.

(b) Why is it more accurate to compute response functions $\chi_{ij} = \partial m_i/\partial H_j$ rather than correlation functions $C_{ij} = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$ in mean field theory? What is the exact thermodynamic relationship between χ_{ij} and C_{ij}?

Within the conventional mean field theory approach we have discussed, $C_{ij} = 0$ because each site is independent, as the trial density matrix is a direct product of individual single site density matrices. Extremizing the free energy, though yields a set of coupled nonlinear equations for m_i in terms of all the local fields $\{H_j\}$, so χ_{ij} is nonzero. Another way to look at it is that $\chi_{ij} = -\partial^2 F/\partial H_i \, \partial H_j$, and the variational approach assures us that F is accurate up to terms of order $(\delta\rho)^2$, where $\rho = \rho_{\mathrm{v}} + \delta\rho$. Using this expression, we see that C_{ij} is only accurate up to terms of order $\delta\rho$. The exact relation between correlation and response functions is $C_{ij} = k_{\mathrm{B}} T \chi_{ij}$.

(c) What is a tricritical point?

A critical point T_{c} may be extended to a critical *curve* in an extended parameter space (T, λ), where λ is an additional parameter which does not explicitly break the symmetry group G which is spontaneously broken in the ordered phase. At a specific point $(T_{\mathrm{t}}, \lambda_{\mathrm{t}})$ along this critical curve, the transition may change from first to second order. The confluence of the first and second order boundaries lies at a *tricritical point*.

(d) Sketch what the radial distribution function $g(r)$ looks like for a simple fluid like liquid Argon. Identify any relevant length scales, as well as the proper limiting value for $g(r \to \infty)$.

See Fig. 6.13 of the Lecture Notes. Note that $g(\infty) = 1$, and $g(r) = 0$ for $r < a$, where a is the hard sphere core diameter.

(e) Discuss the First Law of Thermodynamics from the point of view of statistical mechanics.

The thermodynamic energy is $E = \sum_n P_n E_n$, where $P_n = Z^{-1} e^{-E_n/k_{\mathrm{B}}T}$. Thus $dE = \dj Q = \dj W$, with $\dj Q = \sum_n E_n \, dP_n$ and $\dj W = -\sum_n P_n \, dE_n$. The differential heat is due to changes in the probability distribution P_n, while the differential work is due to changes in the energy eigenvalues E_n.

(f) Explain what is meant by the Dulong-Petit limit of the heat capacity of a solid.

In the high temperature limit (but below the melting point), the ion cores of any solid behave classically. Each of the N ion cores has $2d$ degrees of freedom: d coordinates and d momenta. The potential energy can be modeled as a harmonic potential (in all the coordinates), and the kinetic energy is the usual ballistic expression. Thus, from equipartition, the energy is $N \times 2d \times \frac{1}{2}k_{\mathrm{B}}T = Ndk_{\mathrm{B}}T$, and the heat capacity in this limit is $C_{V,N} = Ndk_{\mathrm{B}}$.