

**PHYSICS 210A : STATISTICAL PHYSICS
FINAL EXAMINATION**

(1) Consider a lattice of noninteracting spin dimers, where the dimer Hamiltonian is

$$\hat{H} = -H^\sigma \sigma - H^\tau \tau - K \sigma \tau ,$$

where H^σ and H^τ are magnetic fields acting on the σ and τ spins, respectively. Each spin is a two-state Ising variable, *i.e.* $\sigma = \pm 1$ and $\tau = \pm 1$.

(a) Compute the partition function ξ for a single dimer. [5 points]

The single dimer partition function is

$$\xi = 2 \cosh\left(\frac{H^\sigma + H^\tau}{k_B T}\right) e^{K/k_B T} + 2 \cosh\left(\frac{H^\sigma - H^\tau}{k_B T}\right) e^{-K/k_B T} .$$

(b) Find $m \equiv \langle \sigma \rangle$. [5 points]

$$\langle \sigma \rangle = -\frac{\partial F}{\partial H^\sigma} = \frac{k_B T}{\xi} \frac{\partial \xi}{\partial H^\sigma} = \frac{\sinh\left(\frac{H^\sigma + H^\tau}{k_B T}\right) e^{K/k_B T} + 2 \sinh\left(\frac{H^\sigma - H^\tau}{k_B T}\right) e^{-K/k_B T}}{\cosh\left(\frac{H^\sigma + H^\tau}{k_B T}\right) e^{K/k_B T} + 2 \cosh\left(\frac{H^\sigma - H^\tau}{k_B T}\right) e^{-K/k_B T}} .$$

Now consider an interacting model,

$$\hat{H} = -\frac{1}{2} \sum_{i,j} J_{ij}^\sigma \sigma_i \sigma_j - \frac{1}{2} \sum_{i,j} J_{ij}^\tau \tau_i \tau_j - K \sum_i \sigma_i \tau_i .$$

Treat the first two terms by mean field theory, writing $\sigma_i = m + \delta\sigma_i$ and $\tau_i = n + \delta\tau_i$, with $m = \langle \sigma_i \rangle$ and $n = \langle \tau_i \rangle$ are presumed to be independent of i . You may assume that all interactions are ferromagnetic. *Treat the third term exactly and do not make the mean field approximation for this term.*

(c) What is the mean field H_{eff}^σ for the σ spins? [5 points]

The mean fields are

$$H_{\text{eff}}^\sigma = \hat{J}^\sigma(0) m \quad , \quad H_{\text{eff}}^\tau = \hat{J}^\tau(0) n ,$$

where $\hat{J}^\sigma(0) = \sum_j J_{ij}^\sigma$ and $\hat{J}^\tau(0) = \sum_j J_{ij}^\tau$.

(d) What is the mean field free energy per site F/N ? *Hint : Once you have the mean fields H^σ and H^τ , you can make use of the results of part (a).* [5 points]

$$F = \frac{1}{2} N \hat{J}^\sigma(0) m^2 + \frac{1}{2} N \hat{J}^\tau(0) n^2 - N k_B T \left\{ 2 \cosh\left(\frac{\hat{J}^\sigma(0) m + \hat{J}^\tau(0) n}{k_B T}\right) e^{K/k_B T} + 2 \cosh\left(\frac{\hat{J}^\sigma(0) m - \hat{J}^\tau(0) n}{k_B T}\right) e^{-K/k_B T} \right\} .$$

(e) Find the mean field equations. [5 points]

Setting the variation of F with respect to m and n to zero, we find

$$m = \frac{\sinh\left(\frac{mT_\sigma + nT_\tau}{T}\right) e^{T_K/T} + \sinh\left(\frac{mT_\sigma - nT_\tau}{T}\right) e^{-T_K/T}}{\cosh\left(\frac{mT_\sigma + nT_\tau}{T}\right) e^{T_K/T} + \cosh\left(\frac{mT_\sigma - nT_\tau}{T}\right) e^{-T_K/T}}$$

and

$$n = \frac{\sinh\left(\frac{mT_\sigma + nT_\tau}{T}\right) e^{T_K/T} - \sinh\left(\frac{mT_\sigma - nT_\tau}{T}\right) e^{-T_K/T}}{\cosh\left(\frac{mT_\sigma + nT_\tau}{T}\right) e^{T_K/T} + \cosh\left(\frac{mT_\sigma - nT_\tau}{T}\right) e^{-T_K/T}},$$

where $k_B T_\sigma \equiv \hat{J}^\sigma(0)$, $k_B T_\tau \equiv \hat{J}^\tau(0)$, and $k_B T_K \equiv K$.

(f) The mean field free energy has a Landau expansion of the form

$$f(m, n) = f_0 + \frac{1}{2} a_{\sigma\sigma} m^2 + \frac{1}{2} a_{\tau\tau} n^2 + a_{\sigma\tau} mn + \mathcal{O}(m^4, m^3 n, m^2 n^2, mn^3, n^4).$$

Focusing only on the quadratic terms, find an equation for the temperature where the curvature of the free energy first changes sign as T is decreased from infinity. If there is no preempting first order transition, this gives you the critical temperature T_c . *You will need to first find the coefficients $a_{\sigma\sigma}$, $a_{\tau\tau}$, and $a_{\sigma\tau}$.* [10 points]

Expanding $f = F/N$ in powers of m and n , we must go to work on the log, expanding the hyperbolic cosine terms each to fourth order in their arguments, and then using the power series for the logarithm itself. This is tedious, but you were only asked to go to the lowest nontrivial order, which isn't so difficult. Here I will show how to obtain the Landau coefficients up to fourth order. We have

$$f = k_B T \ln [4 \cosh(T_K/T)] + \frac{1}{2} k_B T_\sigma m^2 + \frac{1}{2} k_B T_\tau n^2 + \Delta f$$

where

$$\Delta f = -k_B T \ln \left[\frac{\cosh\left(\frac{mT_\sigma + nT_\tau}{T}\right) e^{T_K/T} + \cosh\left(\frac{mT_\sigma - nT_\tau}{T}\right) e^{-T_K/T}}{2 \cosh(T_K/T)} \right].$$

Working on the log term,

$$\Delta f = -k_B T \ln \left[1 + \frac{m^2 T_\sigma^2 + n^2 T_\tau^2 + 2 m n T_\sigma T_\tau \tanh(T_K/T)}{2 T^2} + \frac{m^4 T_\sigma^4 + 6 m^2 n^2 T_\sigma^2 T_\tau^2 + n^4 T_\tau^4 + 4 (m^2 T_\sigma^2 + n^2 T_\tau^2) m n T_\sigma T_\tau \tanh(T_K/T)}{24 T^3} + \dots \right].$$

To carry out the Landau expansion to quadratic order, as you were asked, one needs only the first nontrivial term inside the big brackets. To go to fourth order, however, we must

invoke $\ln(1 + \varepsilon) = \varepsilon - \frac{1}{2}\varepsilon^2 + \mathcal{O}(\varepsilon^3)$ and then combine the square of the second term and the third term inside the big brackets. The result to fourth order is

$$f = k_B T \ln [4 \cosh(T_K/T)] + \frac{1}{2} k_B T_\sigma \left(1 - \frac{T_\sigma}{T}\right) m^2 + \frac{1}{2} k_B T_\tau \left(1 - \frac{T_\tau}{T}\right) n^2 - \frac{k_B T_\sigma T_\tau}{T} \tanh(T_K/T) m n \\ + \frac{k_B T_\sigma^4}{12 T^3} m^4 + \frac{k_B T_\tau^4}{12 T^3} n^4 + \frac{k_B T_\sigma^2 T_\tau^2}{4 T^3} \tanh^2(T_K/T) m^4 + \frac{k_B (m^2 T_\sigma^2 + n^2 T_\tau^2) T_\sigma T_\tau m n}{3 T^3} \tanh(T_K/T) + \dots$$

At any rate, the coefficients of the quadratic form are

$$a_{\sigma\sigma} = k_B T_\sigma \left(1 - \frac{T_\sigma}{T}\right) \quad , \quad a_{\tau\tau} = k_B T_\tau \left(1 - \frac{T_\tau}{T}\right) \quad , \quad a_{\sigma\tau} = -\frac{k_B T_\sigma T_\tau}{T} \tanh(T_K/T) \quad .$$

If $K = 0$, the model decomposes into two independent Landau theories, with critical temperatures T_σ and T_τ , respectively. When $K \neq 0$, we need to find the eigenvalues of the matrix

$$M = \begin{pmatrix} a_{\sigma\sigma} & a_{\sigma\tau} \\ a_{\sigma\tau} & a_{\tau\tau} \end{pmatrix} \quad ,$$

which are

$$\lambda_\pm = \frac{1}{2}(a_{\sigma\sigma} + a_{\tau\tau}) \pm \sqrt{\frac{1}{4}(a_{\sigma\sigma} - a_{\tau\tau})^2 + a_{\sigma\tau}^2}$$

Setting the lower of the two eigenvalues to zero, we obtain the equation $a_{\sigma\sigma} a_{\tau\tau} = a_{\sigma\tau}^2$. This gives rise to the transcendental equation

$$T^2 - (T_\sigma + T_\tau) T + T_\sigma T_\tau \operatorname{sech}^2(T_K/T) = 0 \quad ,$$

the solution of which is the critical temperature T_C .

This is as far as you were asked to go. Proceeding further, let us adimensionalize by defining $\theta \equiv T/\sqrt{T_\sigma T_\tau}$, $\theta_K \equiv T_K/\sqrt{T_\sigma T_\tau}$, and $\varepsilon \equiv \sqrt{T_\tau/T_\sigma}$. We may, without loss of generality, assume $0 \leq \varepsilon \leq 1$. We then have

$$\theta (\varepsilon + \varepsilon^{-1} - \theta) = \operatorname{sech}^2(\theta_K/\theta) \quad .$$

In the top panel of Fig. 1 we plot the left hand side (LHS) of this equation in black and the right hand side in different colors corresponding to three different values of θ_K , all for $\varepsilon = 0.7$. Defining $D(\theta) \equiv \theta^2 - (\varepsilon + \varepsilon^{-1})\theta + \operatorname{sech}^2(\theta_K/\theta)$, the determinant $\det(M)$ is proportional to $D(\theta)/\theta^2$. For high temperatures, $D(\theta) > 0$ and both eigenvalues λ_\pm of M are positive. What happens as we lower θ then depends on the value of θ_K . If $\theta_K > \theta^*(\varepsilon)$, then there is a single second order phase transition at the unique root of the equation $D(\theta) = 0$. As we pass through this temperature, the lower eigenvalue λ_- passes through zero and becomes negative. The low temperature phase exhibits a spontaneous moment, where both m and n are nonzero. As θ is further decreased toward $\theta = 0$, we still have $\lambda_- < 0 < \lambda_+$ and no additional transitions are encountered.

If $\theta_K < \theta^*(\varepsilon)$, then $D(\theta) = 0$ has three roots, $\theta_A > \theta_B > \theta_C$. For $\theta > \theta_A$, we have $0 < \lambda_- < \lambda_+$. For $\theta_B < \theta < \theta_A$, we have $\lambda_- < 0 < \lambda_+$. At $\theta = \theta_B$, the upper eigenvalue λ_+ changes sign, and for $\theta_C < \theta < \theta_B$, we have $\lambda_- < \lambda_+ < 0$, *i.e.* both eigenvalues are negative.

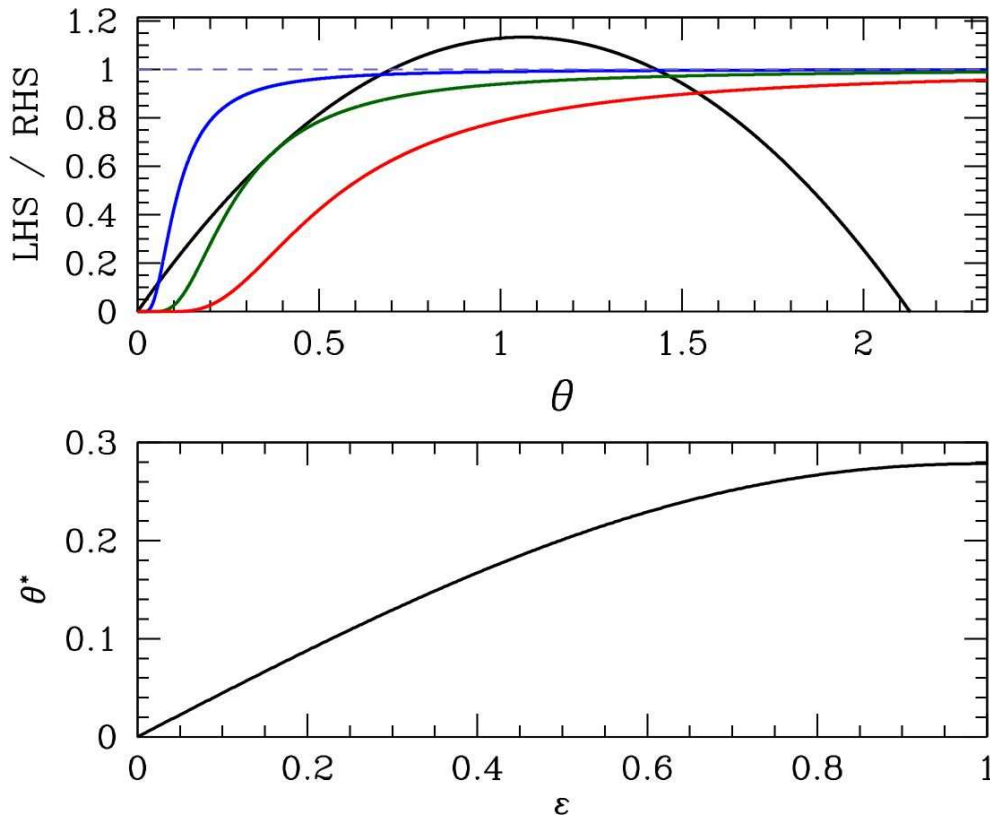


Figure 1: Top panel: Graphical solution to the transcendental equation from problem (1)(f) for $\epsilon = 0.7$. Blue curve: $\theta_K = 0.1$; green curve: $\theta_K = \theta^*(\epsilon) = 0.2514$; red curve: $\theta_K = 0.5$. Bottom panel: Critical value of θ_K below which there are three solutions to $\det(M) = 0$.

Finally, at $\theta = \theta_C$, the upper eigenvalue changes sign once again, and for $\theta < \theta_C$, we have $\lambda_- < 0 < \lambda_+$ once more. Throughout the entire region $\theta < \theta_A$ the system is ordered and there is a spontaneous moment in which both m and n are nonzero.

Despite the additional roots of $D(\theta) = 0$ when $\theta_K < \theta^*(\epsilon)$, there are no additional phase transitions. It is worth emphasizing two things that are *not* happening here. The first thing is a spontaneous breaking of an additional symmetry. For $K \neq 0$, there is only one global symmetry in this problem, which is the \mathbb{Z}_2 Ising symmetry under which $\sigma_i \rightarrow -\sigma_i$ and $\tau_i \rightarrow -\tau_i$ for every spin. Many systems in Nature exhibit a cascade of symmetry breaking transitions. Not this one. As soon as the σ spins develop a spontaneous moment, this acts, through the K term, as an external field which immediately polarizes the τ spins, and there is no phase where $m \neq 0$ and $n = 0$ (and *vice versa*). The second thing which isn't happening is a reentrant transition. If the *lower* eigenvalue λ_- were to change sign at θ_B and θ_C , as well as at θ_A , then throughout the range $\theta_C < \theta < \theta_B$ we would have both eigenvalues again positive, and the minimum of $f(m, n)$ would again lie at $m = n = 0$ as it does in the high temperature phase. As θ finally passed through θ_C , the moment would spontaneously reappear. The sign change of λ_+ at $\theta = \theta_B$ however is inconsequential, since λ_- is negative and the minimum of $f(m, n)$ already lies away from the origin for $\theta < \theta_A$.

(2) A three-dimensional gas of particles obeys the dispersion $\varepsilon(\mathbf{k}) = A k^{5/2}$. There are no internal degrees of freedom (*i.e.* the degeneracy factor is $g = 1$). The number density is n . We will solve the problem for the more general dispersion $\varepsilon(k) = A k^\sigma$ and then indicate the result for $\sigma = \frac{5}{2}$.

(a) Compute the single particle density of states $g(\varepsilon)$. [5 points]

With $\varepsilon = A k^\sigma$ we have $k(\varepsilon) = (\varepsilon/A)^{1/\sigma}$, and

$$g(\varepsilon) = \frac{1}{2\pi^2} \frac{k^2}{\varepsilon'(k)} \Big|_{k=k(\varepsilon)} = \frac{\varepsilon^{\frac{3}{\sigma}-1}}{2\pi^2 \sigma A^{3/\sigma}} = \frac{\varepsilon^{1/5}}{5\pi^2 A^{6/5}} .$$

(b) For bosons, compute the condensation temperature $T_{\text{BEC}}(n)$. [5 points]

The number density $n(T, z, n_0)$ for bosons, in the grand canonical ensemble, is

$$n(T, z, n_0) = \int_0^\infty d\varepsilon \frac{g(\varepsilon)}{z^{-1} e^{\varepsilon/k_B T} - 1} + n_0 ,$$

where n_0 is the condensate density. For $T < T_{\text{BEC}}$, we have $z = 1$ and $n_0 > 0$. For $T > T_{\text{BEC}}$, we have $z < 1$ and $n_0 = 0$. Precisely at $T = T_{\text{BEC}}$, both conditions apply: $z = 1$ and $n_0 = 0$. Thus,

$$n = \int_0^\infty d\varepsilon \frac{g(\varepsilon)}{e^{\varepsilon/k_B T_c} - 1} = \frac{\Gamma(\frac{3}{\sigma}) \zeta(\frac{3}{\sigma})}{2\pi^2 \sigma} \left(\frac{k_B T_c}{A} \right)^{3/\sigma} = \frac{\Gamma(\frac{6}{5}) \zeta(\frac{6}{5})}{5\pi^2} \left(\frac{k_B T_c}{A} \right)^{6/5} .$$

Thus,

$$T_{\text{BEC}}(n) = \left(\frac{2\pi^2 \sigma n}{\Gamma(\frac{3}{\sigma}) \zeta(\frac{3}{\sigma})} \right)^{\sigma/3} \cdot \frac{A}{k_B} = \left(\frac{5\pi^2 n}{\Gamma(\frac{6}{5}) \zeta(\frac{6}{5})} \right)^{5/6} \cdot \frac{A}{k_B} .$$

(c) For fermions, compute the ground state energy density $e_0(n)$. [5 points]

The ground state energy density for spinless (*i.e.* $g = 1$) fermions is

$$\varepsilon_0 = \frac{E_0}{V} = \int \frac{d^3k}{(2\pi)^3} A k^\sigma \Theta(k_F - k) = \frac{A}{2\pi^2} \frac{k_F^{3+\sigma}}{3+\sigma} .$$

The number density is

$$n = \frac{N}{V} = \int \frac{d^3k}{(2\pi)^3} \Theta(k_F - k) = \frac{k_F^3}{6\pi^2} \implies k_F = (6\pi^2 n)^{1/3} .$$

Thus,

$$\varepsilon_0(n) = \frac{(6\pi^2)^{\sigma/3}}{1 + \frac{\sigma}{3}} \cdot A n^{1 + \frac{\sigma}{3}} = \frac{6}{11} (6\pi^2)^{5/6} \cdot A n^{11/6} .$$

(d) For photon statistics, compute the temperature $T(n)$. [5 points]

The photon density is

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

which is the same expression as in part (b) above! Thus,

$$T(n) = \left(\frac{2\pi^2 \sigma n}{\Gamma(\frac{3}{\sigma}) \zeta(\frac{3}{\sigma})} \right)^{\sigma/3} \cdot \frac{A}{k_B} = \left(\frac{5\pi^2 n}{\Gamma(\frac{6}{5}) \zeta(\frac{6}{5})} \right)^{5/6} \cdot \frac{A}{k_B}.$$

(e) For photon statistics, compute the entropy density $s(n) = S/V$. [5 points]

The grand potential is

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

where $g(\varepsilon) = H'(\varepsilon)$. Integrating $g(\varepsilon)$ to obtain $H(\varepsilon)$, we have

$$\Omega(T, V) = -\frac{V}{6\pi^2 A^{3/\sigma}} \int_0^{\infty} d\varepsilon \frac{\varepsilon^{3/\sigma}}{e^{\varepsilon/k_B T} - 1} = -\frac{\Gamma(\frac{3}{\sigma} + 1) \zeta(\frac{3}{\sigma})}{6\pi^2 A^{3/\sigma}} V (k_B T)^{1+\frac{3}{\sigma}}$$

The entropy density is then

$$s(T) = -\frac{1}{V} \frac{\partial \Omega}{\partial T} = \frac{\Gamma(\frac{3}{\sigma} + 2) \zeta(\frac{3}{\sigma} + 1)}{6\pi^2} \left(\frac{k_B T}{A} \right)^{3/\sigma} k_B,$$

The number density, as we have seen, is

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

hence

$$s(n) = \frac{\zeta(\frac{3}{\sigma} + 1)}{\zeta(\frac{3}{\sigma})} \cdot (\frac{3}{\sigma} + 1) n k_B = \frac{\zeta(\frac{11}{5})}{\zeta(\frac{6}{5})} \cdot \frac{11}{5} n k_B.$$

On dimensionful grounds, we knew *a priori* that $s(n) \propto n k_B$.

(f) For bosons and fermions, compute the second virial coefficient $B_2(T)$. [5 points]

We have

$$n = \int_0^{\infty} d\varepsilon \frac{g(\varepsilon)}{z^{-1} e^{\varepsilon/k_B T} - 1} = \pm \frac{\Gamma(\frac{3}{\sigma})}{2\pi^2 \sigma} \left(\frac{k_B T}{A} \right)^{3/\sigma} \zeta_{\frac{3}{\sigma}}(\pm z)$$

$$\frac{p}{k_B T} = \int_0^{\infty} d\varepsilon \frac{H(\varepsilon)}{z^{-1} e^{\varepsilon/k_B T} - 1} = \pm \frac{\Gamma(\frac{3}{\sigma})}{2\pi^2 \sigma} \left(\frac{k_B T}{A} \right)^{3/\sigma} \zeta_{\frac{3}{\sigma}+1}(\pm z),$$

where the top sign is for bosons and the bottom for fermions. It helps to define the thermal wavelength

$$\lambda_T \equiv \left(\frac{2\pi^2\sigma}{\Gamma(\frac{3}{\sigma})} \right)^{1/3} \cdot \left(\frac{k_B T}{A} \right)^{1/\sigma} = \left(\frac{5\pi^2}{\Gamma(\frac{6}{5})} \right)^{1/3} \left(\frac{A}{k_B T} \right)^{2/5},$$

so

$$\begin{aligned} n\lambda_T^3 &= \pm \zeta_{\frac{3}{\sigma}}(\pm z) = z \pm 2^{-3/\sigma} z^2 + \mathcal{O}(z^3) \\ \frac{p\lambda_T^3}{k_B T} &= \pm \zeta_{\frac{3}{\sigma}+1}(\pm z) = z \pm 2^{-1-(3/\sigma)} z^2 + \mathcal{O}(z^3). \end{aligned}$$

From the first of these, we have

$$z = n\lambda_T^3 \mp 2^{-3/\sigma} n^2 \lambda_T^6 + \mathcal{O}(n^3 \lambda_T^9).$$

Substituting this into the second equation, we obtain the lowest nontrivial term in the virial expansion of the equation of state:

$$\frac{p}{k_B T} = n \mp 2^{-1-(3/\sigma)} n^2 \lambda_T^3 + \mathcal{O}(n^3 \lambda_T^6).$$

The second virial coefficient is then

$$B_2(T) = \mp 2^{-1-(3/\sigma)} \lambda_T^3 = \mp \frac{5\pi^2}{2^{11/5} \Gamma(\frac{6}{5})} \left(\frac{A}{k_B T} \right)^{6/5}.$$

(3) 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’? [5 points]

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 we write $a \propto T - T_c$, where T_c is what the second order transition temperature would be in the case $y = 0$.

(b) A system of noninteracting bosons has a power law dispersion $\varepsilon(\mathbf{k}) = Ak^\sigma$. What is the condition on the power σ and the dimension d of space such that Bose condensation will occur at some finite temperature? [5 points]

At $T = T_{\text{BEC}}$, we have the relation

$$n = \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\varepsilon(\mathbf{k})/k_B T_{\text{BEC}}} - 1}.$$

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 $k_B T_{\text{BEC}}/\varepsilon(\mathbf{k}) \propto k^{-\sigma}$. 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.

(c) Which has a longer Thomas-Fermi screening length: a metal with a high density of states at the Fermi level, or a metal with a low density of states? Explain why. [5 points]

A small electrical potential $\phi(\mathbf{r})$ will induce a local density change $\delta n(\mathbf{r}) = e\phi(\mathbf{r})g(\varepsilon_F)$ in a metal, where $g(\varepsilon_F)$ is the density of states at the Fermi energy. We assume $k_B T \ll \varepsilon_F$, which is very much the case for most metals at room temperature. Then from Poisson's equation we derive $\nabla^2 \phi = 4\pi e \delta n = \lambda_{\text{TF}}^{-2} \phi$, where $\lambda_{\text{TF}} = 1/\sqrt{4\pi e^2 g(\varepsilon_F)}$ is the Thomas-Fermi screening length. Thus, high density of states is associated with a shorter screening length – there are more electrons present per unit volume to participate in screening. The metal with the lower density of states has the longer TF screening length.

(d) 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? [5 points]

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 $U/k_B T$ is also either 0 or ∞ . The hard sphere gas is a reasonable model for the physics of liquid Argon (see figure).

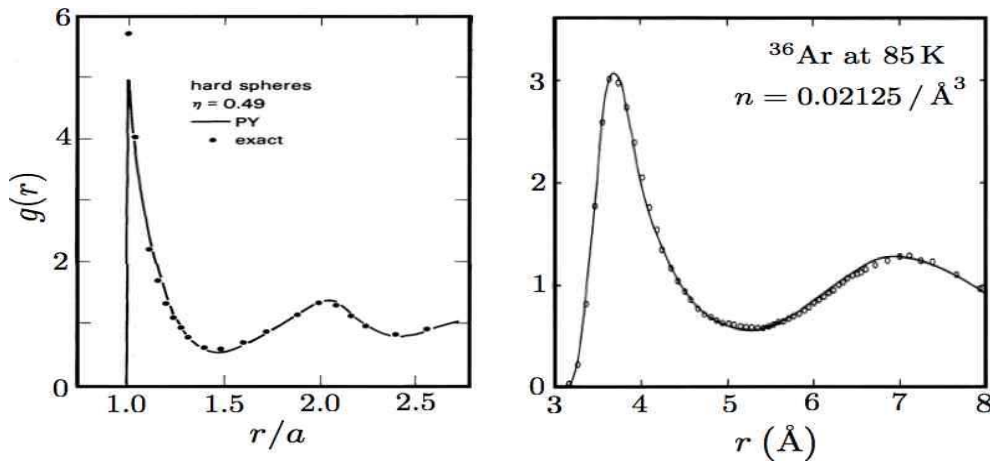


Figure 2: (3)(d) Pair distribution functions (PDF) for hard spheres of diameter a at filling fraction $\eta = \frac{\pi}{6} a^3 n = 0.49$ (left) and for liquid Argon at $T = 85\text{ K}$ (right). Molecular dynamics data for hard spheres (points) is compared with the result of the Percus-Yevick approximation. 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.

(e) For the cluster γ shown in Fig. 3, identify the symmetry factor s_γ , the lowest order virial coefficient B_j to which this contributes, and write an expression for the cluster integral $b_\gamma(T)$ in terms of the Mayer function. [5 points]

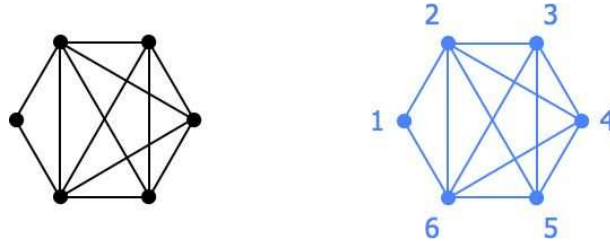


Figure 3: Left: the connected cluster γ for problem (3)(e). Right: a labeled version of this cluster used in expressing the cluster integral b_γ .

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

$$b_\gamma = \frac{1}{12V} \int d^d x_1 \int d^d x_2 \int d^d x_3 \int d^d x_4 \int d^d x_5 \int d^d x_6 f_{12} f_{16} f_{23} f_{24} f_{25} f_{26} f_{34} f_{35} f_{36} f_{45} f_{46} f_{56} ,$$

where $f_{ij} = e^{-u(r_{ij})/k_B T} - 1$. See Fig. 3 for the labels. Whee!

(f) Explain the following terms in the context of dynamical systems: *recurrent*, *ergodic*, and *mixing*. How are these classifications arranged hierarchically? [5 points]

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 $\dot{\varphi} = \mathbf{V}(\varphi)$, ergodicity means

$$\langle f(\varphi) \rangle_T = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt f(\varphi(t)) = \frac{\text{Tr} f(\varphi) \delta(E - H(\varphi))}{\text{Tr} \delta(E - H(\varphi))} = \langle f(\varphi) \rangle_S ,$$

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

$$\lim_{t \rightarrow \infty} \text{Tr} \varrho(\varphi, t) f(\varphi) = \langle f(\varphi) \rangle_S .$$

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

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

(g) What is the significance of the Ginzburg criterion? [5 points]

The Ginzburg criterion tells how close we can come to a second order phase transition before fluctuation effects start to overwhelm the mean field contribution to the heat capacity. The criterion for the sufficiency of mean field theory is $|t| \gg t_G$, where $t = (T - T_c)/T_c$ is the reduced temperature and $t_G = (a/R_*)^{\frac{2d}{4-d}}$, where a is the lattice spacing and R_* is a length scale set by the interactions. For most magnetic transitions, R_* is on the order of the lattice spacing, $t_G \sim 1$, and mean field theory breaks down rapidly. For most superconductors, R_* is on the order of the coherence length, which is large on the scale of the lattice spacing, and $t_G \sim 10^{-18} - 10^{-12}$, and mean field exponents are quantitatively accurate essentially all the way up to the transition.

Some useful formulas:

$$\zeta_\alpha(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^\alpha}$$
$$\int_0^{\infty} d\varepsilon \frac{\varepsilon^{\alpha-1}}{z^{-1}e^{\beta\varepsilon} - 1} = \Gamma(\alpha) \zeta_\alpha(z) (k_B T)^\alpha$$
$$\ln(1+x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 - \frac{1}{4}x^4 + \dots$$
$$\cosh(x) = 1 + \frac{1}{2!}x^2 + \frac{1}{4!}x^4 + \dots$$