1.

Fall 2014 Comp Stat Mech

1. Spinless fermions populating two degenerate levels

Consider a system with two energy levels, one with energy 0, and the other with energy $\Delta > 0$. Both levels are N-fold degenerate, and the system is in equilibrium at temperature T. There are N non-interacting and effectively spinless fermions in the system.

a) Assume the grand canonical ensemble with chemical potential μ to describe the system. Write down the condition that determines μ, solve it for μ, and find the occupation probabilities f and g for the upper and lower energy levels respectively.

$$Z_1 = \prod_i^2 Z_i \quad , \quad Z_i = \sum_n^{0,1} e^{-\beta N_n (E_i - \mu)}$$

$$= 1 + e^{-\beta(E_i - \mu)}$$

$$Z_1 = (1 + e^{\beta\mu})(1 + e^{\beta\mu - \beta\Delta})$$

There are N copies, so $N = \prod^N Z_1 = (1+e^{\beta\mu})^N (1+e^{\beta\mu-\beta\Delta})^N$

Then $\langle N \rangle = \frac{1}{\beta}\frac{d}{d\mu}\ln(Z) = \frac{1}{\beta}\cdot N \cdot \left[\frac{(1+e^{\beta\mu})(\beta e^{\beta\mu-\beta\Delta}) + (1+e^{\beta\mu-\beta\Delta})(\beta e^{\beta\mu})}{(1+e^{\beta\mu})(1+e^{\beta\mu-\beta\Delta})} \right.$

$$= \frac{N \cdot e^{\beta\mu-\beta\Delta}}{1+e^{\beta\mu-\beta\Delta}} + \frac{N e^{\beta\mu}}{1+e^{\beta\mu}}$$

$$= \frac{N}{e^{-\beta\mu+\beta\Delta}+1} + \frac{N}{e^{-\beta\mu}+1}$$

$$\therefore \boxed{\langle N \rangle = \frac{N}{e^{-\mu\beta}+1} + \frac{N}{e^{(\Delta-\mu)\beta}+1}}$$

if $\langle N \rangle = N \rightarrow \therefore \; e^{(\Delta - 2\mu)\beta} = 1$ s.t. $\Delta/2 = \mu \rightarrow$ and this simply determines $f + g$ inside $\frac{\langle N \rangle}{N}$

b Now, describe the system using the canonical ensemble. Write down the partition function and find the occupation probabilities f and g in the thermodynamic limit of $N \to \infty$ $(n! = (n/e)^n)$

—

Because the total energy is $n \cdot \Delta = E_n$ the partition function can also be written in terms of n, the number of particles in the higher energy states. The combinatoric factor for taking n states from the N lower to N upper is

$$P(n) = \left(\frac{N!}{n!(N-n)!}\right)^2 \quad \& \quad Z = \sum_{n=0}^{N} \left(\frac{N!}{n!(N-n)!}\right)^2 e^{-\beta E_n} \qquad E_n = n\Delta$$

Then, as $N \to \infty$ we see that the largest term dominates the sum

$$\frac{d}{dn}\left[\left(\frac{N!}{n!(N-n)!}\right)^2 e^{-\Delta n \beta}\right] = \frac{d}{dn}\left[\frac{N^N e^{-N} e^{-\Delta n \beta}}{n^n e^{-n} (N-n)^{N-n} e^{-N+n}}\right]$$

$$\ldots \text{ max for } n = \frac{N}{e^{\Delta\beta/2}+1} \quad \& \quad f = \frac{n}{N}, \quad g = \frac{N-n}{N}$$ ✓

2. Magnetic system in a fixed magnetic field

Consider an equilibrium magnetic system in a fixed magnetic field $B=0$. The free energy $G(m,T)$ of the system as a function of magnetization m can be written as:

$$G(m,T) = a + \frac{b}{2} m^2 + \frac{c}{4} m^4 + \frac{d}{6} m^6$$

In some relevant range of temperatures T, the coefficients b and d can be taken to be positive constants, $b, d > 0$, while c goes through 0 at some temperature T^* in this range:

$$c(T) = C_0 \cdot (T - T^*), \quad C_0 > 0$$

a) The free energy G describes a phase transition, in which the system goes from the state with no magnetization, $m=0$, to the magnetized state $m = m_0 \neq 0$ at some temperature T_0. Find T_0.

—

for $b, c, d > 0$ the minimum occurs for $m = 0$, but if we let $c < 0$ then another minimum appears (at $T = T_0$)

Then $G(0, T_0) = G(m_0, T_0)$

$$a = a + \frac{b}{2} m_0^2 + \frac{c}{4} m_0^4 + \frac{d}{6} m_0^6 \rightarrow \frac{d}{3} m_0^4 + \frac{c}{2} m_0^2 + b = 0$$

then $m_0^2 = -\frac{3c}{4d} \pm \left[\left(\frac{3c}{4d}\right)^2 - \frac{3b}{d} \right]^{1/2}$ which exists and is minimum for $[\;] = 0$

$$\therefore \frac{3c}{4d} = \pm \sqrt{\frac{3b}{d}} \rightarrow c = +4\sqrt{\frac{bd}{3}}$$

$$\therefore \underbrace{4\sqrt{\frac{bd}{3}}}_{= C(T_0)} = C_0 \cdot (T_0 - T^*) \rightarrow \boxed{T_0 = T^* - \frac{4}{C_0}\sqrt{\frac{bd}{3}}}$$

b) Find the magnitude of the magnetization m_0 appearing at the transition temperature T_0. What is the type of this phase transition?

When m_0 gets a second, real solution $(\sqrt{0})$ the solution to the quadratic equation in part a) is simply

$$m_0^2 = -\frac{3c}{4d} \qquad \text{and using } \quad c(T_0) = 4\sqrt{\frac{bd}{3}}$$

yields

$$m_0^2 = \sqrt{\frac{3b}{d}}$$

Here we see $m = 0 \to m_0 \neq 0$. Thus we have a first order phase transition in the value of m and of G (discontinuous functions).

c) Calculate the latent heat L of the transition. State qualitatively, for what direction of the temperature change, this heat is absorbed/released by the system.

latent heat in a 1st order phase transition is given by

$$L = T_0 \, \Delta S$$

where

$$S = -\left(\frac{\partial G}{\partial T}\right)\bigg|_B$$

s.t.

$$\Delta S = \frac{dG}{dT}\bigg|_{m=m_0} - \cancel{\frac{dG}{dT}}\bigg|_{m=0}$$

0 since $m = 0$ + a ca[illegible]

$$= \left(\frac{\partial G}{\partial m}\bigg|_{m=m_0} \cdot \frac{dm}{dT}\bigg|_{m=m_0}\right) + \frac{\partial G}{\partial T}\bigg|_{m=m_0}$$

0 since we are at minimum

$$\frac{m_0^4}{4}\frac{dc}{dT}$$

$$\& \quad \frac{dc}{dT} = C_0$$

$$\Delta S = \frac{m_0^4}{4} C_0$$

& L is > 0, ∴ heat is released when cooled down → exothermic.

$$L = \left(T^* - \frac{4}{[illegible]}\sqrt{\frac{bd}{[illegible]}}\right)\left(\frac{3b}{[illegible]} \cdot \frac{C_0}{4}\right)$$

3. Ising chain in zero magnetic field.

Consider the hamiltonian for the ising model on a one-dimensional lattice without external magnetic field, which may be writen as

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

where the classical ising spin variable $\sigma_i = \pm 1$ on each site i, and $\langle ij \rangle$ denotes nearest-neighbor pairs of sites. Consider this model in thermal equilibrium at temperature T in the thermodynamic limit. Take the ferromagnetic case $J > 0$. Derive exact expressions for

a) The specific heat per spin, C

take $\frac{1}{k_B T} = \beta$ + $\beta J = K$. The total number of sites is N.

The partition function is then

$$e^{\Sigma i} = \Pi e^{i}$$

$$Z = \sum_{\sigma_n} e^{-\beta H} = \sum_{\sigma_n} \prod_{ij} e^{K \sigma_i \sigma_j}$$

and the free energy per site is

$$F/N = \lim_{N \to \infty} -k_B T \cdot \frac{\ln Z}{N}$$

since $e^{K\sigma_i\sigma_j} = \cosh(K)(1 + \sigma_i\sigma_j \tanh(k))$

then $Z = \cosh^N(k) \sum_{\sigma_n} \prod_{ij} (1 + \sigma_i\sigma_j \tanh(k))$

using graph expansions only the full chain contributes s.t.

$$Z = \cosh^N(k)\,(1 + \tanh^N(k)) = \cosh^N(k) + \sinh^N(k)$$

Or we can use the transfer matrix s.t.

$$\tau = \begin{pmatrix} e^{k} & e^{-k} \\ e^{-k} & e^{k} \end{pmatrix}$$

eigen values of τ.

$$Z = \mathrm{Tr}(\tau^N) = \lambda_1^N + \lambda_2^N, \quad \lambda_1 = \cosh k, \quad \lambda_2 = \sinh k$$

for $N \to \infty$ $\tanh^N(k) \to 0$ and so we get

$$F/N = -k_B T \lim_{N \to \infty} \frac{1}{\cancel{N}} \ln(\cosh^{\cancel{N}}(k))$$

$$\boxed{F/N = -k_B T \ln(\cosh(k))}$$

where $k = \beta J$

and then $\dfrac{\langle U \rangle}{N} = \dfrac{1}{\beta} \dfrac{\partial}{\partial \beta}(\beta \cdot F/N) = -J \tanh(k)$

and $C/N = \dfrac{d}{dT} \dfrac{\langle U \rangle}{N} = -k_B \beta^2 \dfrac{dU}{d\beta} = \dfrac{k_B k^2}{\cosh^2(k)}$

$k = \beta J$

b) The spin-spin correlation function $\langle\sigma_0\sigma_r\rangle$, where r denotes lattice site.

$$\langle\sigma_0\sigma_r\rangle = \frac{1}{Z}\sum_{\sigma_n}\sigma_0\sigma_r e^{-\beta H} = \frac{\sum_{\sigma_n}\sigma_0\sigma_r\prod_{ij}(1+\sigma_i\sigma_j\tanh(k))}{\sum_{\sigma_n}\prod_{ij}(1+\sigma_i\sigma_j\tanh(k))}$$

$$= \tanh^r(k) + \tanh^{N-r}(k)$$

& for $N\to\infty$ $\tanh^{N-r}(k) \to 0$

$$= \tanh^r(k)$$

c) the zero field magnetic susceptibility per spin, χ

a) $H \to H - B\sum_i\sigma_i \to B=0$ & resolve part a)

$$T = \begin{pmatrix} e^{k+\beta B} & e^{-k} \\ e^{-k} & e^{k-\beta B}\end{pmatrix} \quad \& \quad \lambda_{1,2} = e^k\left[\cosh(\beta B) \pm\sqrt{\sinh^2(\beta B)+e^{-4k}}\right]$$

$$Z = \mathrm{Tr}\,[T]^N \quad \& \quad M = -\frac{1}{\beta}\frac{\partial F/N}{\partial B} = \frac{\sinh(B\beta)}{\left[\sinh^2(B\beta)+e^{-4k}\right]^{1/2}}$$

$$\left(M = \frac{1}{N}\frac{1}{\beta}\frac{\partial}{\partial\beta}\ln(Z)\right) \qquad \& \; \chi = \frac{\partial M}{\partial B} \text{ as } B\to 0.$$

$$\chi = \beta e^{2k}$$

Or b) $$\chi = \beta\sum_r\langle\sigma_0\sigma_r\rangle = 1 + 2\sum_{r=1}^{\infty}\tanh^r(k)$$

$$= -1 + 2\sum_{r=0}^{\infty}\tanh^r(k)$$

$$= -1 + \frac{2}{1-\tanh(k)} = \boxed{e^{2k} = \chi}$$

1

Spring 2015 comp Stat Mech (2 + 3 important)

1. Heat capacity and heat conductance in a ballistic (free) system.

Consider a one-dimensional system of free, massless bosons with one polarization, and the dispersion relation $E_k = \hbar v|k|$, where v is the particle velocity, $|k|$ is wave vector, E_k the energy. The particles are non-interacting either among themselves or with external scattering potentials. If the system is in equilibrium at temperature T,

a) Calculate the specific heat capacity C.

$$Z = \prod_k^{\infty} \sum_n^{\infty} e^{-\beta n E_n(k)} \qquad \text{Where } E_n(k) = \hbar v|k|, \quad dE(k) = \hbar v\, d|k|$$

$$= \prod_k^{\infty} \frac{1}{1 - e^{-\beta\hbar v|k|}}$$

$$\text{then } \ln Z = -\sum_k^{\infty} \ln(1 - e^{-\beta\hbar v|k|}) \simeq \frac{-L}{2\pi}\int_{-\infty}^{\infty} dk \ln(1 - e^{-\beta\hbar v|k|})$$

since $E \sim |k|$ just take $+k$ region twice.

$$\simeq \underbrace{2}_{\text{1D angle}} \cdot \frac{-L}{2\pi}\int_0^{\infty} \underbrace{dk}_{\frac{dE}{\hbar v}} \ln(1 - e^{-\beta\hbar v|k|})$$

$$\ln Z = \frac{-L}{\hbar\pi v}\int_0^{\infty} dE \ln(1 - e^{-\beta E})$$

$$E = -\frac{\partial}{\partial\beta}\ln(Z) = \frac{-L}{\hbar\pi v} \cdot \int_0^{\infty} \frac{E e^{-\beta E}}{1 - e^{-\beta E}} dE$$

$$\therefore E_{tot} = \frac{-L}{\pi\hbar v\beta^2}\int_0^{\infty} \frac{x e^{-x}}{1 - e^{-x}} dx$$

and we see that $\int_0^\infty \frac{x\,dx}{e^x - 1} = \sum_{k=1}^{\infty} \int_0^\infty x e^{-kx}\,dx = \sum_{k=1}^{\infty} \frac{1}{k^2}$

$= \frac{\pi^2}{6}$

$\therefore \frac{E_{tot}}{L} = \frac{\pi (k_B T)^2}{6 \hbar v}$

$\& \boxed{C = \frac{dT}{dL} = \frac{\pi k_B^2 T}{3\hbar v}}$

---

b) Calculate the heat conductance G_{th}

To find heat conductance assum right movers and left movers have δT difference in temperature.
Then total energy flux carried by the system is given as

$$J = v \cdot \left(\frac{1}{2} E(T+\delta T) - \frac{1}{2} E(T) \right) = \frac{1}{2} v \frac{dE}{dT} \cdot dT$$

$$\& \; G_{Th} = \frac{J}{\delta T} = \frac{v}{2} \frac{dE}{dT} = \frac{v}{2} C_v = \boxed{\frac{\pi k_B^2 T}{6\hbar} = G_{Th}}$$

Which is independent of velocity etc.

---

c) repeat for massive fermions with $E_k = \hbar^2 k^2 / 2m$ with chemical potential μ far above the bottom of the energy spectrum $\mu \gg k_B T$.

Now we get $v \cdot \hbar \equiv \frac{dE}{dk} = \frac{\hbar^2 k}{m} \rightarrow v = \frac{\hbar k}{m}$

$= \ldots$

hard integrals involving fermi energy level,

Just replace $n_{BE} \rightarrow n_{FD}$ and $v \rightarrow v_{fermi}$ and it works out

2. Ising model in an external magnetic field

Consider the ising model of N spins $\sigma_i = \pm 1$ in an external magnetic field h. Within the mean field approximation, its Hamiltonian can be written as

$$H_{MF} - \frac{1}{2} N J m^2 - (Jm + h) \sum_i \sigma_i$$

Where the co-ordination number of the lattice has been absorbed into the coupling constant J, and m is the magnetization.

The magnetization, specific heat and magnetic susceptibility are defined as

$$m = \frac{\partial F/N}{\partial h} = \frac{\partial f}{\partial h}, \quad C = \frac{\partial \langle E \rangle}{\partial T}, \quad \chi = \frac{\partial M}{\partial h}$$

a) Derive the (mean field) partition function following from H_{MF} and hence calculate the free energy of the system

$$Z = \sum_{\sigma_i} e^{-\beta H_{MF}} = \sum_{\sigma_i} \exp\left[-\beta \frac{1}{2} N J m^2 + \beta(Jm+h) \sum_i \sigma_i \right]$$

$$e^{\sum_i x_i} = \prod_i e^{x_i}$$

$$= e^{-\frac{\beta}{2} N J m^2} \prod_i^N \sum_{\sigma_i = \pm 1} e^{\beta(Jm+h)\sigma_i}$$

$$= e^{-\frac{\beta}{2} N J m^2} \cdot \left(2 \cosh(\beta(Jm+h)) \right)^N$$

$$Z = \left[e^{-\frac{\beta}{2} J m^2} \cdot 2 \cdot \cosh(\beta(Jm+h)) \right]^N$$

Then $$F = -\frac{1}{\beta} \ln(Z_{MF}) = -\frac{N}{\beta} \ln\left[e^{-\frac{\beta}{2} J m^2} \cdot 2 \cosh(\beta(Jm+h)) \right]$$

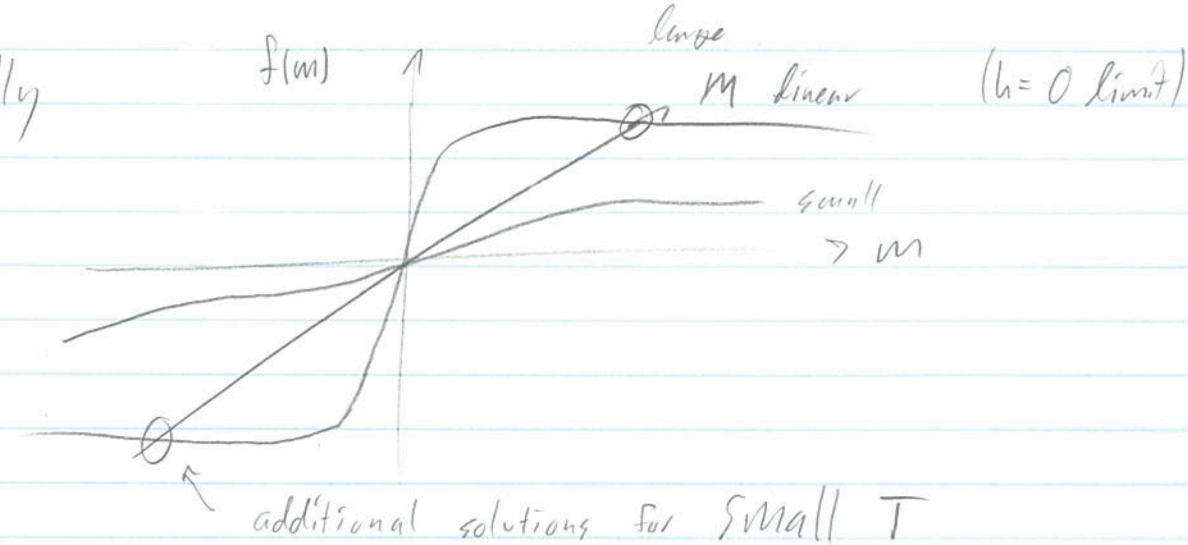
$$= \frac{N}{2} J m^2 - \frac{N}{\beta} \ln\left(2 \cosh(\beta(Jm+h)) \right)$$

4 b) Derive the magnetization, and graphically solve it for $h = 0$. Discuss the physical nature of the various solutions as a function of temperature T. Identify a critical temperature T_c in terms of the system parameters & discuss meaning.

Then $$m = \frac{1}{N} \cdot \frac{d}{dh} F = -\frac{1}{\beta} \frac{[-2\sinh(\beta(Jm+h))] \cdot \beta}{2\cosh[\beta(Jm+h)]}$$

$$\boxed{m = \tanh[\beta(Jm+h)]}$$

Graphically



if $\left.\frac{d\tanh(\beta J m)}{dm}\right|_{m=0}$ is larger than $\left.\frac{dm}{dm}\right|_{m=0} = 1$ then

small T solution matters.

→ occurs at $\beta J = 1$ $\therefore$ $T = T_c = \frac{J}{k_B}$

So for $T < T_c$ we have 2 nonzero magnetizations for zero h → phase transition.

9

c) Derive the expression for the dependence of the magnetization, the specific heat, and the magnetic susceptibility on the quantity

$$t = \frac{T-T_c}{T_c}$$

Where T_c is the critical temperature, and thereby determine the mean field critical exponents $\alpha_c, \beta_c, \gamma_c$ which are defined through the relations

$$m \sim |T-T_c|^{\beta_c}, \quad C \sim |T_c - T|^{-\alpha_c}, \quad \chi = \left.\frac{dm}{dh}\right|_{h=0} \sim |T_c - T|^{-\gamma_c}$$

for the calculation of the specific heat, note that, within the mean field approximation near the critical point, the internal energy is $U \propto Jm^2$

We can expand the result from a) as

$$m = \tanh(x) \simeq \frac{e^x - e^{-x}}{e^x + e^{-x}} \simeq \frac{2}{2}\frac{(x + x^3/6 + ..)}{(1 + x^2/2 + ..)} \simeq x - \frac{x^3}{3}$$

$$\therefore m \simeq \beta(Jm + h)\left[1 - \frac{\beta(Jm+h)^3}{3}\right]$$

$$\downarrow h=0$$

$$1 \simeq \beta J - \frac{\beta^3 J^3 m^2}{3} \rightarrow m = \pm \sqrt{\frac{-3(\underbrace{1-\beta J}_{(1-\beta J)^{1/2} \to (T-T_c)})}{(\beta J)^3}}$$

$$\simeq \left(\frac{T_c - T}{T}\right)^{1/2} \cdot \text{Stuff}$$

$$\beta_c = 1/2$$

$$E = -\frac{\partial}{\partial \beta}\ln(Z) = \left(\frac{-N \cdot \frac{Jm^2}{2} \cdot e^{-\frac{\beta}{2}Jm^2} \cdot 2\cosh(\beta J m)}{e^{-\frac{\beta}{2}Jm^2} \cdot 2\cosh(\beta J m)} - \frac{N e^{-\frac{\beta}{2}Jm^2}}{e^{-\frac{\beta}{2}Jm^2}} \cdot \frac{2}{2} \cdot \underbrace{\tanh(\beta J m)}_{\simeq \beta J m} \cdot Jm \right)$$

$$E \simeq -\frac{NJm^2}{2} - N\beta J^2 m^2$$

$$m^2 \propto (T - T_c)$$

$$\propto \frac{T-T_c}{T}$$

then $E = -N\left(\frac{Jm^2}{2} + \beta J^2 m^2\right)$

$$C = \frac{dE}{dT} \cong -\frac{NJ}{2^2} + O(1/T^2)$$

$\therefore\ \alpha_c = 0$ no dependence

& $\frac{\partial m}{\partial h} = \frac{\partial}{\partial h}\left[\beta(Jm + h)\left(1 - \frac{(\beta(Jm+h))^3}{3}\right)\right]$

$$= \beta\left(1 + J\frac{\partial m}{\partial h}\right)\left[1 - (\beta(H + Jm))^2\right]$$

$\to 0$

set $h = 0$, $T = T_c$, m small, $\therefore$

$$\therefore\ \frac{\partial m}{\partial h}(1 - \beta J) = \beta$$

$$\left.\frac{\partial m}{\partial h}\right|_{h=0} = \frac{\beta}{1-\beta J} \simeq \frac{1}{T - T_c} \qquad \therefore\ \gamma_c = 1$$

$$\frac{1}{T-T_c} = (T - T_c)^{-1}$$

7

3. Vapor Pressure

a) Write down the condition for thermodynamic equilibrium between the liquid and gas phase along a liquid-gas coexistence curve

The condition for thermal equilibrium is equivalent gibbs free energies

$$G_l(T,P) = G_g(T,P) \quad + \quad dG = -SdT + VdP + \mu dN$$

$$\therefore \; -S_1 dT + V_1 dP = -S_2 dT + V_2 dP \qquad T + P = \text{ in equilibrium.}$$

$$(S_2 - S_1)dT = (V_2 - V_1)dP$$

$$\boxed{\frac{dP}{dT} = \frac{\Delta S}{\Delta V}}$$ is our condition

b) Using your solution to part a) and taking into account the entropy change at a liquid-gas phase transition, derive the relation for vapor pressure along a liquid-gas coexistence curve.

$$\Delta S = L/T \quad \therefore \quad dP = \frac{dT}{T} \cdot \frac{L}{V_g - \underbrace{\cancel{V_l}}_{\text{small}}} \qquad + \; PV = NkT$$

$$\frac{dP}{P} = \frac{dT}{T^2} \cdot \frac{L}{Nk_B}$$

$$\ln\left(\frac{P}{P_{atm}}\right) = \left(\frac{L}{Nk_B}\right) \cdot -\left(\frac{1}{T_{boiling}} - \frac{1}{T}\right)$$

$$\boxed{P = P_{atm}\, e^{-\frac{L}{Nk_B}\left(\frac{1}{T_b} - \frac{1}{T}\right)}}$$

373.15 K

c) What about $T = 27°C$? $= 300\,K$ $\quad k_B = \sim \quad l = \sim \quad \rightarrow \quad P = 4.14 \times 10^{-2}$ atm

Fall 2015 comprehensive exam Stat Mech

1. Skip

2. 2D non-relativistic bose gas

A two dimensional, ideal, spinless and nonrelativistic Bose gas is maintained in an area A with finite temperature T and chemical potential μ, with $z = e^{\mu\beta} = e^{\mu/k_B T}$

a) Calculate the grand partition function $\mathcal{Z}(z, A, T)$. Separate the zero momentum part.

$$\mathcal{Z} = \prod_p^{\infty} \sum_n^{\infty} e^{-\beta n(E_p - \mu)} = \prod_p^{\infty} \frac{1}{1 - e^{-\beta(E_p - \mu)}}$$

$$\& \quad E_p = \frac{p^2}{2m}$$

Then, $$\ln \mathcal{Z} = -\sum_p^{\infty} \ln\left(1 - e^{-\beta\left(\frac{p^2}{2m} - \mu\right)}\right)$$

$$= \frac{-A}{(2\pi)^2} \int d^2\vec{p} \, \ln\left(1 - z e^{-\frac{\beta p^2}{2m}}\right)$$

$$2\pi \int_0^{\infty} dp \cdot p$$ which $= 0$ for $k = 0$

$\therefore$ we can pull off the $p = 0$ term of the sum in advance

$$\boxed{\ln \mathcal{Z} = -\ln(1 - z) - \frac{A}{2\pi} \int_0^{\infty} p \, dp \, \ln\left(1 - z e^{-\frac{\beta p^2}{2m}}\right)}$$

$e^{\beta\mu}$

$x = p^2 \cdot \beta/2m$
$dx = 2p\,dp \cdot \beta/2m$

b) Calculate the average density of bosons $n(z, A, T)$. Show that $z = e^{\beta\mu}$ must be less than 1 for any density.

$$n = \frac{N}{A} = \frac{1}{A} \cdot \frac{1}{\beta} \frac{1}{d\mu} \ln(Z)$$

$$= \frac{1}{\beta A} \cdot \left[-\frac{(-\beta)}{1-z} \cdot z - \frac{A}{2\pi} \int_0^\infty p\,dp \left(\frac{-\beta z e^{-\frac{\beta p^2}{2m}}}{1 - z e^{-\frac{\beta p^2}{2m}}} \right) \right]$$

$$\boxed{n = \frac{1}{A}\left(\frac{z}{1-z}\right) + \frac{z}{2\pi} \int_0^\infty \frac{p\,dp}{z e^{-\frac{\beta p^2}{2m}} - 1}}$$

$p \to x^{1/2}$ via
$p\,dp = \frac{1}{2} dx \frac{2m}{\beta}$

$z < 1$ else $p = 0$ diverges or is negative

c) Can the 2D bose gas condense? Explain.

$g_1(1) = \zeta(1) = \infty$

$x^{1-1} \to g_1(z)$

$N_0 \to$ because the integral $\frac{m}{2\pi\beta} \int_0^\infty \frac{z\,dx}{z e^{-x} - 1}$

at $z = 1$ yields the Reimann ζ function.

$$= \zeta(1) = \infty$$

and so there is an obvious problem

$$\frac{1}{A}\left(\frac{z}{1-z}\right) = n_{\text{condensate}} = n_{\text{total}} - c\,\zeta(1)$$

both infinite, and so $n_{\text{condensate}}$ is trivially small comparitively (since it cannot be negative)!

d) What changes in these arguments for $d = 3$ & why?

Because the integral has measure $k^2 dk$ we get $g(z) \to \zeta(2) = $ finite!

$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

3. Mean-field theory of an Ising-type model in a transverse field.

Consider the system of spins-½ on a lattice with q nearest-neighbors for each site, characterized by the hamiltonian

$$H = -J\left[\sum_{\langle i,j\rangle} \sigma_z^i \sigma_z^j + g\sum_i \sigma_x^i\right]$$

in equilibrium at temperature T. Here σ_z^i + σ_x^i are the pauli matrices of the ith spin, and the sum in the first term is taken over the pairs of the nearest neighbor spins. As usual, the dimensionality of the lattice does not affect the results in the mean-field approximation.

a) Adopting the standard mean-field approach, introduce the effective single-spin Hamiltonian H_0 and calculate the thermal averages

$$m_z = \langle \sigma_z^i \rangle, \quad m_x = \langle \sigma_x^i \rangle$$

As usual, the mean-field approximation requires us to make an effective single-spin Hamiltonian by replacing the interacting spins with their average values

$$\text{i.e. } H_0 = -J\left[q m_z \sigma_z + g\sigma_x\right]$$

Then $\underset{\substack{\uparrow \\ 0 = \text{mean-field}}}{Z_0} = \sum_{\substack{\text{diagonals} \\ \text{(spins)}}} e^{-\beta H_0} = \mathrm{Tr}\{e^{-\beta H_0}\} = \mathrm{Tr}\{e^{\vec{r}\cdot\vec{\sigma}}\}$

with $\vec{r} = \beta J(g, 0, q m_z)$

+ $\mathrm{Tr}[A] = \sum_i \lambda_i$ sum over eigenvalues or just take the trace.

$$e^{\vec{r}\cdot\vec{\sigma}} = \mathbb{1}\cdot\cosh(|\vec{r}|) + \hat{r}\cdot\vec{\sigma}\sinh(|\vec{r}|)$$

$$\therefore \quad e^{\vec{r}\cdot\vec{\sigma}} = \mathbb{1}\cdot \cosh\left(\beta J\sqrt{g^2+q^2m_z^2}\right) + \left(\frac{g\sigma_x + qm_z\sigma_z}{\sqrt{g^2+q^2m_z^2}}\right)\sinh\left(\beta J\sqrt{g^2+q^2m_z^2}\right)$$

$\therefore$ Our trace is just the diagonals, which are the Cosh's and the σ_z cancels out

$$\boxed{Z = 2\cosh\left(\beta J\sqrt{g^2+q^2m_z^2}\right)}$$

or we could have done the Eigenvalue problem, but that would be a disaster.

Then we get $\langle m_z \rangle = +\dfrac{1}{q\beta J}\dfrac{\partial}{\partial m_z}\ln(Z) = \dfrac{\frac{1}{2}\cdot 2q^2m_z}{\sqrt{q^2m_z^2+g^2}}\tanh\left(\beta J\sqrt{g^2+q^2m_z^2}\right)$

$\langle m_x \rangle = +\dfrac{1}{\beta J}\dfrac{\partial}{\partial g}\ln(Z) = \dfrac{\frac{1}{2}\cdot 2\cdot g}{\sqrt{g^2+q^2m_z^2}}\tanh\left(\beta J\sqrt{g^2+q^2m_z^2}\right)$

$$\boxed{\begin{aligned}\langle m_z\rangle &= \frac{qm_z}{\sqrt{q^2m_z^2+g^2}}\tanh\left(\beta J\sqrt{g^2+q^2m_z^2}\right)\\ \langle m_x\rangle &= \frac{g}{\sqrt{q^2m_z^2+g^2}}\tanh\left(\beta J\sqrt{g^2+q^2m_z^2}\right)\end{aligned}}$$

b) Imposing the relevant self-consistency condition, find the transition temperature T_c of the temperature driven phase transition from the paramagnetic (vanishing m_z) to ferromagnetic (non-vanishing m_z) state, and determine the range of the parameter g, when such a phase transition exists. What is the expression for T_c as $q \to 0$?

$$m_z = \frac{q m_z}{\sqrt{g^2+q^2m_z^2}} \tanh\left(\beta J \sqrt{g^2+q^2m_z^2}\right)$$ from a) is our consistency equation.

$$\therefore \; \underbrace{\left((g/q)^2+m_z^2\right)^{1/2}}_{\text{circle}} = \underbrace{\tanh\left(\beta J \left(g^2+q^2m_z^2\right)^{1/2}\right)}_{\tanh}$$ is our graphical problem

For $T > T_c$ the condition requires $m_z = 0 \rightarrow$

$$\boxed{g/q = \tanh(\beta J g)}$$ $\rightarrow$ constrained to $[-1, 1]$ domain

$$\therefore \; \beta_c = \frac{1}{Jg} \operatorname{arctanh}\left[\, g/q \,\right]$$ $\therefore g < q$ required

Since $\tanh(x) \simeq x - \frac{x^3}{3}$ we get

$$g/q \simeq \beta J g \left(1 - \frac{(\beta J g)^2}{3}\right)$$

as $q \to 0$ then $\frac{1}{\beta_c} = q \cdot J + \ldots$

$$\boxed{T_c = \frac{qJ}{k_B}}$$

6

c) In the situation with vanishing temperature, $T=0$, analyze m_z as a function of g from the same self consistency condition. Determine the point g_c of a "quantum phase transition" into a ferromagnetic state, and find m_z and m_x as functions of the small difference $\delta g = g_c - g$

→ For $\beta \to \infty$ $\tanh \to 1$ and we get

$$m_z = \frac{q m_z}{\left[(q m_z)^2 + g^2\right]^{1/2}} \qquad \text{s.t. } m_z = \sqrt{1 - g^2/q^2}$$

which is real for $g < g_c = q$ and is $= 0$ for $g > q$

for $\delta g = g_c - g \ll g_c$ $(g \sim q)$ we get

$$m_z \simeq \begin{cases} \left(\dfrac{2(\overset{g_c}{q} - g)}{\underset{g_c}{q}}\right)^{1/2} & g < g_c = q \\ 0 & g > g_c = q \end{cases}$$

$\beta = 1/2$ critical exponent.

m_x comes from $T=0$ limit

$$m_x^2 + m_z^2 = 1 \rightarrow m_x = \begin{cases} \sqrt{1 - \dfrac{2(q-g)}{q}} & g < g_c = q \\ 1 & g > g_c = q \end{cases}$$

Spring 2016 Comp Stat Mech

I. Ultra-relativistic electron gas

Consider an ideal 3D gas of N ultra-relativistic electrons with energies $\varepsilon = pc$ where $\vec{p}$ is the electron's momentum, and c is the speed of light), confined to volume V.

a) For the gas in equilibrium at zero temperature, calculate its chemical potential μ (i.e. the fermi energy $\varepsilon_F = \mu$) and the total energy E_0, and express E_0 in terms of N and ε_F.

The density of states comes from

$$\sum_n \vec{n} = \underset{\nearrow}{g} \cdot \frac{V}{(2\pi\hbar)^3} \int d^3p \qquad \text{with} \quad E = pc, \quad dE = dp\, c$$

2 fold spin degeneracy

$$= \frac{4\pi \cdot 2 \cdot V}{(2\pi\hbar)^3} \int_0^\infty \underbrace{p^2 dp}_{\frac{E^2 dE}{c^3}} = \frac{V}{\pi^2(\hbar c)^3} \int_0^\infty E^2 dE$$

$$\therefore \boxed{g(E) = \frac{V}{\pi^2(\hbar c)^3} E^2}$$

At zero temperature all fermions fall into $\varepsilon < \varepsilon_f$ energy states in the n_{FD} distribution s.t.

$$N = \int_0^{\varepsilon_f} g(\varepsilon) \cdot d\varepsilon = \boxed{\frac{\varepsilon_f^3}{3} \cdot \frac{V}{\pi^2(\hbar c)^3} = N}$$

$$\therefore \boxed{\varepsilon_f = \left(\frac{3\pi^2 N}{V}\right)^{1/3} \cdot \hbar c}$$

$$E = \int_0^{\varepsilon_f} \varepsilon g(\varepsilon) \cdot d\varepsilon = \frac{\varepsilon_f^4}{4} \cdot \frac{V}{\pi^2(\hbar c)^3} = \boxed{\frac{3}{4} \cdot N \varepsilon_f = E_{tot}}$$

b) Now consider the gas in equilibrium at a low temperature $T << \varepsilon_f / k_B$. In the first non-vanishing approximation in T, calculate the chemical potential, and express your result in terms of ε_f and T,

follow reason on the given Somerfeld expansion, for some reason

$$\frac{\varepsilon_f^3 - \mu^3}{3} \simeq \varepsilon_f^2 (\varepsilon_f - \mu)$$

for $\varepsilon_f \sim \mu$
and let $\mu = \varepsilon_f$ elsewhere
to solve for $\mu(\varepsilon_f)$.

Just
taylor expand!
in $(\varepsilon_f^3 - \mu^3)$

2. Magnetic Refrigeration

An external magnetic field $\vec{B}$ is applied to a set of N non-interacting spin $1/2$ particles with gyromagnetic ratio γ, and fixed spatial positions. For the thermal equilibrium at temperature T, calculate:

a) The average energy and heat capacity.

$$H = -\vec{M}\cdot\vec{B} = -\gamma\vec{S}\cdot\vec{B} = -\frac{\hbar\gamma}{2}\vec{B}\cdot\vec{\sigma}$$ pick $\hat{z}$

$$E_\pm = \mp\frac{\hbar\gamma B}{2}$$

$$\text{Then } Z = \prod_{n}^{\infty}\sum_{E_\pm} e^{\pm\beta\frac{\hbar\gamma B}{2}} = \prod_{n}^{\infty} \mathrm{Tr}\, e^{-\beta\hat{H}}$$

$$= \left(2\cosh\left(\beta\frac{\hbar\gamma B}{2}\right)\right)^N$$

$$\& \ \frac{E}{N} = -\frac{\partial}{\partial\beta}\ln(Z) = -\frac{N}{N}\cdot\frac{\hbar\gamma B}{2}\tanh\left(\beta\frac{\hbar\gamma B}{2}\right)$$

$$= -\frac{\hbar\gamma B}{2}\tanh\left(\beta\frac{\hbar\gamma B}{2}\right)$$

$$\boxed{\frac{C}{N} = \frac{dE/N}{dT} = -\frac{\hbar\gamma B}{2}\cdot -\frac{\beta^2}{k_B}\left(1-\tanh^2\left(\frac{\beta\hbar\gamma B}{2}\right)\right)}$$

$$\boxed{\frac{\partial}{\partial x}\tanh(x) = 1-\tanh^2(x)}$$

4

b) The average magnetic moment of the system and the variance of its fluctuations.

$$\langle M \rangle = +\frac{1}{B}\frac{\partial}{\partial \beta} \ln(Z) = N \cdot \frac{\hbar\gamma}{2} \tanh\left(\beta \frac{\hbar\gamma B}{2}\right)$$

$$\langle m \rangle = \frac{1}{N} \cdot \langle M \rangle$$

$$\langle M^2 \rangle = -\frac{1}{B^2} \cdot \frac{\partial^2}{\partial \beta^2} \ln(Z) = N\left(\frac{\hbar\gamma}{2}\right)^2 \left(1 - \tanh^2\left(\frac{\hbar\gamma B}{2}\beta\right)\right)$$

$$\therefore \sigma m = \langle m \rangle^2 - \langle m^2 \rangle = -\frac{\hbar^2\gamma^2}{4}\left(1 - 2\tanh^2\left(\frac{\hbar\gamma B}{2}\beta\right)\right)$$

?

c) entropy per spin: Some derivative.

d) Sketch ...

e) refrigerator.

3. Skip.

1

Fall 2016 Comp Stat Mech

I. Blackbody Radiation and its Fluctuations

This problem addresses properties of the spontaneous electromagnetic radiation at thermal equilibrium

a) Calculate the probability for a one-dimensional quantum harmonic oscillator of eigen frequency ω to be on its n^{th} energy level, in thermal equilibrium at temperature T.

The gibbs distribution is $e^{-\beta H} = e^{-\beta\hbar\omega(n+1/2)}$ ← shift g.s. away

$$Z = \sum_n e^{-\beta\hbar\omega n} = \frac{1}{1-e^{-\beta\hbar\omega}}$$

Then $\boxed{P(n) = \frac{e^{-\beta\hbar\omega n}}{1-e^{-\beta\hbar\omega}}}$

b) Calculate the average energy, the free energy, and the entropy of the oscillator, and discuss their dependences on temperature.

$$E = -\frac{\partial}{\partial\beta}\ln(Z) = \frac{\partial}{\partial\beta}\ln\left(1-e^{-\beta\hbar\omega}\right) = \frac{-(-\hbar\omega)e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}$$

$$\boxed{E = \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}}$$

$$F = -\frac{1}{\beta}\ln(Z) = \frac{1}{\beta}\ln\left(1-e^{-\hbar\omega\beta}\right)$$

$$S = -\frac{\partial}{\partial T}F = \frac{\langle E\rangle - F}{T} = \frac{\hbar\omega/T}{e^{\hbar\omega/k_BT}-1} + k_BT\ln\left(1-e^{-\hbar\omega/k_BT}\right)$$

$S \to + k_BT(1-\ln(\hbar\omega$

limits as $T\to 0$ $\langle E\rangle$, F, + $S \to 0$. $T\to\infty$ $\langle E\rangle \to k_BT$, $F\to +k_BT\ln(\hbar\omega\beta)$

c) Calculate the variance (dispersion) of fluctuations of the oscillator's energy, and express it via the average energy and $\hbar\omega$.

$$\sigma_E^2 = \langle E^2\rangle - \langle E\rangle^2 = -\frac{\partial}{\partial\beta}\langle E\rangle$$

$$= \frac{-\hbar\omega \cdot -1}{(e^{\beta\hbar\omega}-1)^2} \cdot \hbar\omega e^{\beta\hbar\omega} = \langle E\rangle^2 e^{\beta\hbar\omega}$$

$$\sigma_E^2 = \langle E\rangle^2 e^{\beta\hbar\omega}$$ Which is always larger than $\langle E\rangle^2$

$= \infty$ at $T = 0$

$= 0$ at $T = \infty$ mistake in solutions ???

d) Calculate the number of electromagnetic standing waves in a large, closed free-space volume V, with frequencies within a narrow interval $[\omega, \omega + d\omega]$, where $d\omega$ is much smaller than ω, but still large enough to contain many modes. Briefly explain why each mode may be treated as a one-dimensional quantum SHO.

What is $g(\omega)\, d\omega$? $\sum_n \vec{n} = \int d^3\vec{n} = \frac{gV}{(2\pi)^3}\int d^3k$

Where $g = 2$ for 2 polarizations + $k = \omega/c$

$$\therefore \sum_n \vec{n} = \frac{2V}{(2\pi)^3}\cdot 4\pi \cdot \frac{1}{c^3}\int \omega^2 d\omega = \int g(\omega)\, d\omega$$

$$\therefore g(\omega) = \frac{V}{\pi^2 c^3}\omega^2$$

Each mode can be treated as a 1-d SHO because Maxwell's equations devolve to SHO's also in the free limit.

e) Calculate the average total energy of the electromagnetic field in volume V (including all essential modes), and the variance of its fluctuations. Express the variance via the average energy and temperature, and find the dependence of the relative r.m.s. fluctuation of the energy on temperature T and volume V.

$$\langle E \rangle = \int_0^\infty E\, g(E)\, dE = \int_0^\infty \frac{\hbar\omega}{e^{\hbar\omega\beta}-1} \cdot V \frac{\omega^2}{\pi^2 c^3} d\omega = \frac{V}{\hbar^3 \pi^2 c^3} \frac{1}{\beta^4} \underbrace{\int_0^\infty \frac{x^3 dx}{e^x - 1}}_{\frac{\pi^4}{15}}$$

$$\delta \langle E^2 \rangle = -\frac{\partial}{\partial\beta} \langle E \rangle = \frac{4 \langle E \rangle}{\beta}$$

$$\therefore \frac{\delta \langle E \rangle}{\langle E \rangle} = 2 \Big/ \sqrt{\beta \langle E \rangle} \propto \frac{1}{T^{3/2} V^{1/2}}$$

f) How large should the volume V be for your results to be qualitatively valid? Evaluate the condition for room temperature.

$$\text{from } g(\omega)\, d\omega \propto \frac{V \omega^2 d\omega}{c^3} \rightarrow \boxed{\frac{V}{(c/\omega)^3} \gg 1}$$

then the important frequencies are $\hbar\omega \sim k_B T$

$$\therefore V \gg \left(\frac{c}{k_B T/\hbar}\right)^3 \sim \left(\frac{c\hbar}{k_B T}\right)^3 \sim (10\,\mu m)^3 ✓$$

2. Ising model on a triangle

The ising Model on a triangle is described by the energy:

$$E = -J(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1) - h(\sigma_1 + \sigma_2 + \sigma_3)$$

Here J and h are known parameters: exchange energy and external magnetic field, respectively. The ising spins $\sigma_{1,2,3}$ are the only degrees of freedom in the problem and they are taking values ± 1. Assume that the temperature of the system is T.

a) Compute the partition function of the model.

$$Z = \sum_{\sigma} e^{-\beta E_\sigma} \quad \text{with } \beta = \frac{1}{k_B T}$$

There are 2 states per spin + & −, ∴ $2^3 = 8$ states

$\uparrow\uparrow\uparrow$, $\uparrow\uparrow\downarrow$ $\uparrow\downarrow\uparrow$ $\downarrow\uparrow\uparrow$, $\uparrow\downarrow\downarrow$ $\downarrow\uparrow\downarrow$ $\downarrow\downarrow\uparrow$, $\downarrow\downarrow\downarrow$ $= 8$

$E(\uparrow\uparrow\uparrow) = -J(3) - h(3) = -3(J+h)$

$E(\uparrow\uparrow\downarrow) = -J(1-2) - h(2-1) = J-h$ = others

$E(\uparrow\downarrow\downarrow) = -J(1-2) - h(1-2) = J+h$ = others

$E(\downarrow\downarrow\downarrow) = -J(3) - h(-3) = -3(J-h)$

$$\therefore Z = e^{3\beta(J+h)} + 3e^{-\beta(J-h)} + 3e^{-\beta(J+h)} + e^{3\beta(J-h)}$$

$$\boxed{Z = e^{3\beta J} \cdot 2\cosh(3\beta h) + 3 \cdot e^{-\beta J} \cdot 2\cosh(\beta h)}$$

b) Compute the free energy of the model + entropy

$$F = -\frac{1}{\beta}\ln(Z) = -k_B T \ln\left(2e^{3J\beta}\cosh(3h\beta) + 6e^{-J\beta}\cosh(h\beta)\right)$$

$$S = -\frac{\partial F}{\partial T} = k_B \ln\left(2e^{3J\beta}\cos(3h\beta) + 6e^{-J\beta}\cosh(h\beta)\right)$$
$$- J\beta k_B\left(\frac{3e^{3J\beta} - 3e^{-J\beta}}{e^{3J\beta} + 3e^{-J\beta}}\right)$$

c) find $C(h=0)$ + plot (use $E = F + TS$)

. . .

d) $M = \langle\sigma\rangle = \langle\sigma_1 + \sigma_2 + \sigma_3\rangle = -\frac{\partial F}{\partial h} \simeq 3\tanh\left(\frac{3h}{T}\right)$

$$\chi = \left.\frac{\partial M}{\partial h}\right|_{h\to 0} \simeq \frac{9}{T} \quad \text{curies law}$$

e) $\langle\langle\sigma^2\rangle\rangle = -T\frac{\partial^2 F}{\partial h^2} = T\frac{\partial M}{\partial h} = \frac{9}{\cosh^2(3h/T)}$

$$1 - \tanh^2 = \frac{1}{\cosh^2}$$

since $\cosh^2 - \sinh^2 = 1$

3. BEC

This problem addresses the Bose-Einstein condensation (BEC) of the gas $N \gg 1$ indistinguishable, non interacting bosons of mass m, in various confining potentials.

a) Calculate the critical temperature T_c of the condensation in a rectangular, hard-wall box of volume $V = a \times b \times c$, with all linear sizes of the same order. What is the exact value of the chemical potential μ at $T < T_c$?

$$E_{\vec{n}} = \frac{\pi^2 \hbar^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

basically the same problem as earlier