2000

Statistical Mechanics
(do 2 out of 3 problems)

Please do **EACH** problem you attempt on a **SEPARATE** paper.
Put your name on each paper.

Put your name, section name and problem # on each sheet you turn in.

Do only two problems. Do not do all three problems.

Qualifying Exam Copy Disclaimer:

Solutions are submitted at an early stage in the Written Qualifying Exam preparation process. No effort is made to update solutions. Some questions may have been changed since the solution was written. Solutions may contain errors, inaccuracies and/or omissions. Use them cautiously.

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STATISTICAL MECHANICS - 1

1. Consider an intrinsic semiconductor with a filled valence band and an empty conduction band at $T = 0$. As T increases, some of the electrons will be thermally excited across the gap, $E_G = \epsilon_c - \epsilon_v$, where ϵ_c is the bottom of the conduction band and ϵ_v is the top of the valence band. Treat the valence band as a hole-band. Assume parabolic energy bands such that the density of states for electrons is

$$g_e(\epsilon) = C_e(\epsilon - \epsilon_c)^{1/2} \quad C_e = \frac{1}{2\pi^2}(\frac{2m_e}{\hbar^2})^{3/2}$$

$$g_h(\epsilon) = C_h(\epsilon_v - \epsilon)^{1/2} \quad C_h = \frac{1}{2\pi^2}(\frac{2m_h}{\hbar^2})^{3/2}$$

where m_e and m_h are the electron and hole effective masses.

a. Using Fermi-Dirac statistics, give equations for the number of electrons in the conduction band, n_o, and the number of holes, p_o, in the valence band. Leave as integrals, but write the integrals in terms of a dimensionless variable (Hint: remove the T-dependence).

b. Set $n_o = p_o$ to determine an equation for the chemical potential (Fermi energy ϵ_f) as a function of T.

c. In the non-degenerate case (ϵ_f is in the gap between bands),

$$f(\epsilon) \approx e^{\epsilon_f/kT}e^{-\epsilon/kT}.$$

Using this expression, show

$$n_o \approx N_c e^{\frac{\epsilon_f - \epsilon_c}{kT}}; p_o = N_v e^{-\frac{\epsilon_v - \epsilon_f}{kT}},$$

where

$$N_c = 2(\frac{m_e kT}{2\hbar^2\pi})^{3/2}; N_v = 2(\frac{m_h kT}{2\hbar^2\pi})^{3/2}.$$

(Note $\int_0^\infty y^{1/2}e^{-y}dy = \frac{1}{\sqrt{\pi}}$.)

d. Use equations in part (c) above to show

$$\epsilon_f = \frac{1}{2}(\epsilon_v + \epsilon_c) + \frac{3}{2}kT\ell n(m_h/m_e).$$

Statistical

SM#1

Detailed Balance in intrinsic semiconductors. Consider an intrinsic semiconductor with a filled valence band and an empty conduction band at $T=0$. As T increases, some of the electrons will be thermally excited across the gap $E_G = \mathcal{E}_c - \mathcal{E}_v$ where $\mathcal{E}_c$ is the bottom of the conduction band & $\mathcal{E}_v$ is the top of the valence band. Treat the valence band as a hole-band. Assume parabolic energy bands such that the density of states for electrons is

$$g_e(\mathcal{E}) = C_e\,(\mathcal{E}-\mathcal{E}_c)^{1/2} \qquad C_e = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}$$

$$g_h(\mathcal{E}) = C_h\,(\mathcal{E}_v-\mathcal{E})^{1/2}. \qquad C_h = \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar}\right)^{3/2}$$

where m_e & m_h are the electron & hole effective masses.

a) Using Fermi Dirac statistics, ~~write~~ give equations for the number of electrons in the conduction band n_0 & the number of holes p_0 in the valence band. Leave as integrals, but write integral in terms of a dimensionless ~~[illegible]~~ variable (Hint remove T dep.)

b) Set $n_0 = p_0$ to determine an equation for the chemical potential (Fermi energy $\mathcal{E}_f$) as a function of T.

c) In the non-degenerate case ($\mathcal{E}_f$ is in gap between bands) $f(\mathcal{E}) \approx e^{+\mathcal{E}_f/kT}\, e^{-\mathcal{E}/kT}$. Using this expression show

$$n_0 \cong N_c\, e^{\frac{(\mathcal{E}_f-\mathcal{E}_c)}{kT}} \;;\; p_0 = N_v\, e^{-\frac{(\mathcal{E}_v-\mathcal{E}_f)}{kT}}$$

②

SM #1

where $N_c = 2(m_e kT/2\hbar^2\pi)^{3/2}$; $N_v = 2(m_h kT/2\hbar^2\pi)^{3/2}$

[Note $\int_0^\infty y^{1/2} e^{-y}\, dy = 2/\sqrt{\pi}$] [but don't need it]

d) Solve equations in c) above to show

$$\varepsilon_F = 1/2(\varepsilon_v + \varepsilon_c) + 3/2 \ln(m_h/m_e)$$

SM#1

Solution

a) Number of carriers = $\int g(\varepsilon) f(\varepsilon)\, d\varepsilon$ in general

Conduction band

$$n_0 = \int_{\varepsilon_c}^{\infty} g_c\, f(\varepsilon)\, d\varepsilon = C_c \int (\varepsilon - \varepsilon_c)^{1/2} f(\varepsilon)\, d\varepsilon$$

$$= C_c (kT)^{3/2} \int_{\varepsilon_c/kT} \left(\frac{\varepsilon - \varepsilon_c}{kT}\right)^{1/2} \frac{1}{1 + e^{(\varepsilon - \varepsilon_F)/kT}} \frac{d\varepsilon}{kT}$$

$$= C_c (kT)^{3/2} \int_0^{\infty} y^{1/2} \frac{1}{1 + e^{y - \eta_0}}\, dy \qquad \eta_0 = \frac{\varepsilon_F - \varepsilon}{kT}$$

For valence band

$$p = \#\text{ of empty states} = \int_{-\infty}^{\varepsilon_v} \underset{\uparrow \text{ holes}}{g_v(\varepsilon)} \overbrace{\underset{\uparrow \text{ electrons}}{[1 - f(\varepsilon)]}}^{\text{holes}} d\varepsilon$$

If we rewrite in terms of holes, with ε measured from top of valence band, and note

$$1 - f(\varepsilon) = \frac{e^{+(\varepsilon - \varepsilon_F)/kT}}{1 + e^{+(\varepsilon - \varepsilon_F)/kT}} = \frac{1}{1 + e^{-(\varepsilon - \varepsilon_F)/kT}}$$

$$= \frac{1}{1 + e^{+(\varepsilon_F - \varepsilon)/kT}}$$

$$p_0 = C_h (kT)^{3/2} \int_0^{\infty} y^{1/2} \frac{1}{1 + e^{y - \eta_0'}}\, dy \qquad \eta_0' = \frac{\varepsilon_v - \varepsilon_F}{kT}$$

b) $n_0 = p_0 \Rightarrow$

$$C_c (kT)^{3/2} \int_0^{\infty} y^{1/2} \frac{1}{1 + e^{y - \eta_0}}\, dy = C_h (kT)^{3/2} \int y^{1/2} \frac{1}{1 + e^{y - \eta_0'}}\, d$$

Need to solve integrals in terms of η_0 + η_0' to get ε_F

SII#1

c) The non-degenerate case

$$\frac{1}{1+e^{y-y_0'}} \approx e^{-y} e^{y_0'}$$

Then equation (sub) becomes

$$C_e (kT)^{3/2} e^{+y_0} \int_0^\infty y^{1/2} e^{-y}\, dy = C_h (kT)^{3/2} e^{+y_0'} \int_0^\infty y^{1/2} e^{-y}\, dy$$

$$\Rightarrow \frac{C_e}{C_h} \cdot \left(\frac{m_e}{m_h}\right)^{3/2} = e^{-\frac{(\mathcal{E}_F - \mathcal{E}_c)}{kT}}\, e^{\frac{(\mathcal{E}_v - \mathcal{E}_c)}{kT}}$$

$$\cong e^{-\frac{2\mathcal{E}_F}{kT}}\, e^{\frac{\mathcal{E}_c + \mathcal{E}_v}{kT}}$$

Taking logs

$$\frac{2\mathcal{E}_F}{kT} = \frac{\mathcal{E}_c + \mathcal{E}_v}{kT} + 3/2 \ln\left(\frac{m_h}{m_e}\right)$$

$$\mathcal{E}_F = \frac{\mathcal{E}_c + \mathcal{E}_v}{2} + 3/2\, kT \ln\left(m_h/m_e\right)$$

STATISTICAL MECHANICS - 2

2. Two particles slide on a ring of radius R. The potential energy between them is

$$U = U_0 \log(\theta)$$

where U_0 is a constant and θ is the angle subtended by the first particle, the center of the ring and the second particle. The masses of the two particles are m_1 and m_2 respectively. Treat this system classically. The system is in contact with a heat bath of temperature T.

a. Write down the partition function for the system.
b. Calculate the free energy, F, as a function of temperature.
c. Calculate the energy, as a function of temperature.
d. At what temperature is there a singularity in F?

SM #2
Solution

STATISTICAL MECHANICS - 2

2. 1. Two particles slide on a ring of radius R. The potential energy between them is

$$U = U_0 \log(\theta)$$

where U_0 is a constant and θ is the angle subtended by the first particle, the center of the ring and the second particle. The masses of the two particles are m_1 and m_2 respectively.

Treat this system classically. The system is in contact with a heat bath of temperature T.

description

[(a)] Write down the partition function for the system.
Angular momentum L, and θ are canonically conjugate.

$$Z = \int_{-\infty}^{\infty} dL_1 \int_{-\infty}^{\infty} dL_2 \int_{-\pi}^{\pi} d\theta_1 \int_{-\pi}^{\pi} d\theta_2 e^{-H/k_BT}$$

where

$$H = \frac{1}{2}(\frac{L_1^2}{m_1R^2} + \frac{L_2^2}{m_2R^2}) + U_0 \log(\ min(|2\pi - |\theta_1 - \theta_2||, |\theta_1 - \theta_2|)$$

[(b)] Calculate the free energy, F, as a function of temperature.
Separate the kinetic and potential terms $Z \equiv Z_K Z_U$, we have

$$Z_K = \sqrt{2\pi T m_1 R^2}\sqrt{2\pi T m_2 R^2} = 2\pi T R^2 \sqrt{m_1 m_2}$$

Since the system has rotational invariance, we can fix particle 1 to $\theta_1 = 0$ and let θ_2 range from $-\pi$ to π. Then the integration over θ_1 gives just a factor of 2π.

$$Z_U = 2\pi \int_{-\pi}^{\pi} e^{-U_0 \log(|\theta|)/k_BT} = 4\pi \int_0^{\pi} \theta^{-U_0/k_BT} d\theta$$

integration is only defined for $U_0/k_BT \ < \ 1$

$$\frac{4\pi}{1 - U_0/k_BT} \pi^{1-U_0/k_BT}$$

The free energy $F = -k_BT \log Z$

[(c)] Calculate the energy, as a function of temperature.
The energy E is related to the partition function through

$$E \ = \ -\frac{\partial \log Z}{\partial \beta}$$

SM#2

with $\beta = 1/k_B T$.

From above, the energy is the sum of a kinetic and a potential part. The kinetic part by the equipartition theorem gives a contribution to the energy of $E_K = 2k_B T/2 = k_B T$. The potential part is

$$E_U = -\frac{\partial}{\partial\beta}(-\log(1 - U_0\beta)(1 - U_0\beta)\log\pi = U_0(\frac{1}{U_0\beta - 1} + \log\pi)$$

[(d)] At what temperature is there a singularity in F?

From (c) this happens when $U_0/k_B T = 1$ or

$$T = U_0/k_B.$$

STATISTICAL MECHANICS - 3

3. Consider the following Landau expansion for the free energy of a material undergoing a phase transition with order parameter m:

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

where c and d are assumed independent of the temperature, $c < 0$, $d > 0$, and

$$b(T) = \alpha(T - T^\star).$$

a. Explan why the transition is first order (i.e. m vanishes discontinuously). Also explain why the transition is not at $T^\star$. Sketch the free energy versus m for different temperatures, one of which (clearly marked) should be at the transition temperature T_c and another should be at $T^\star$.

b. Determine the value of m as T approaches T_c from below.

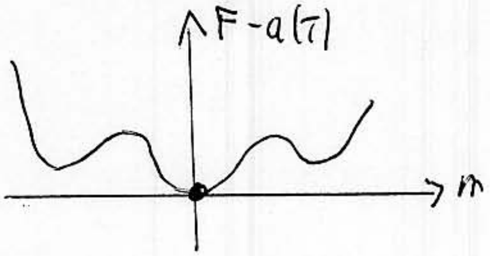
c. Determine the latent heat of transition. Note: You are given that the energy U is related to the free energy by $U = \partial(\beta F)/\partial\beta$, where $\beta = 1/(k_B T)$.

Statistical Mechanics (Solutions)

SM#3

1/ $F = a(T) + \frac{b(T)}{2} m^2 + \frac{c}{4} m^4 + \frac{d}{6} m^6$

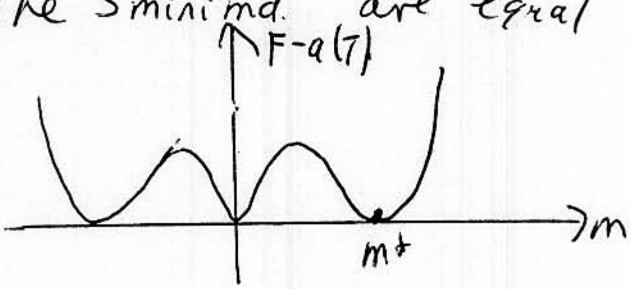
(a)/ $T > T_c$



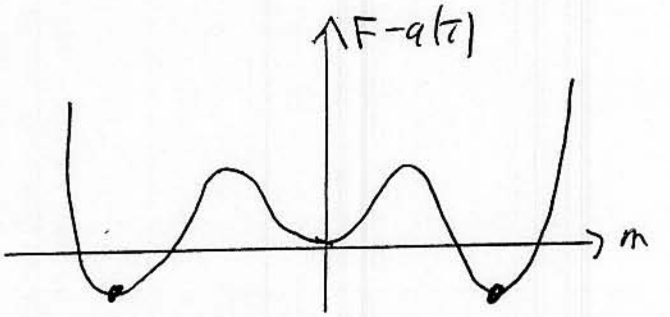
Need to find minimum of F

$\Rightarrow m = 0$

$T = T_c$ The 3 minima are eqal

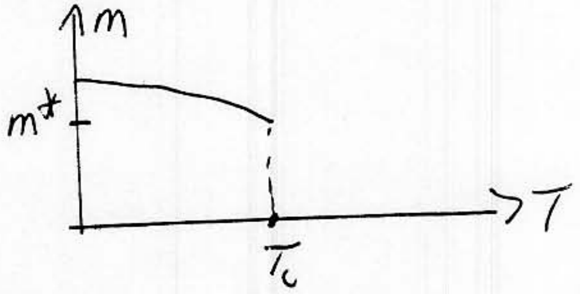


$T < T_c$

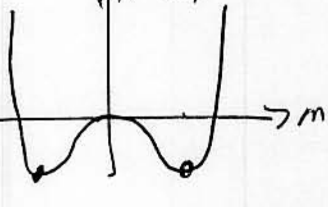


The sol^n with $m \neq 0$ are the equilibrium solution.

Hence



i.e Transition is discontinuous, (1st order).



Note at $T = T^*$ ~~we have~~ the coefficient of m^2 is zero so we have →

and the equilibrium value of m is non-~~x~~zero

i.e. $T_c > T^*$

(b) ~~A~~ The equilibrium magnetization is given by $\frac{\partial E}{\partial m}=0$, i.e. <u>either</u> $m=0$

<u>or</u> $b + cm^2 + dm^4 = 0$ ①

In addition, at T_c, $F-a(T)_{h}^{=0}$ at the ~~non zero~~ solutions with non-zero m, i.e

$$\frac{b}{2}m^2 + \frac{c}{4}m^4 + \frac{d}{6}m^6 = 0$$

which, for $m \neq 0$, can be written

$$b + \frac{c}{2}m^2 + \frac{d}{3}m^3 = 0 \qquad ②$$

m^* is the simultaneous solution of ① and ②, i.e subtracting

$$\frac{c}{2}m^{*2} + \frac{2d}{3}m^{*4} = 0$$

Remembering that $c<0$ this gives

$$\underline{\underline{m^* = \sqrt{\frac{-3c}{4d}}}}$$

(c) The latent heat is the change in energy, ΔU, at the transition,

Since $U = \frac{\partial}{\partial \beta}(\beta F) = F - \beta\frac{\partial F}{\partial \beta} = F + T\frac{\partial F}{\partial T}$

$$\Delta U = \underbrace{\Delta F}_{=0} + T\frac{\partial}{\partial T}\Delta F = \underline{T_c \frac{\partial}{\partial T}\Delta F\Big|_{T_c}}$$

Now $\Delta F = \frac{b(T)}{2}m^2 + \frac{c}{4}m^4 + \frac{d}{6}m^6$ (at $T=T_c$)

so $\frac{\partial}{\partial T}\Delta F = \frac{\alpha}{2}m^{*2} + \frac{\partial m}{\partial T}\Big|_{T_c}\Big(\underbrace{bm^* + cm^{*3} + dm^{*5}}_{=0 \text{ from } ①}\Big)$

Hence $\underline{\Delta U = \alpha T_c\left(\frac{-3c}{8d}\right)}$

Legendre Polynomials

1. Generating function:

$$g(t,x) = (1 - 2xt + t^2)^{-1/2} = \sum_{n=0}^{\infty} P_n(x) t^n$$

2. Recursion relations

$$(2n+1)xP_n(x) = (n+1)P_{n+1}(x) + nP_{n-1}(x)$$

$$(1-x)^2 P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0$$

3. Normalization

$$\int dx [P_n(x)]^2 = \frac{2}{2n+1}$$

Spherical Harmonics

1. $\ell = 0$:

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

2. $\ell = 1$:

$$Y_{1,\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin(\theta) e^{\pm i\phi} \qquad Y_{10} = \sqrt{\frac{3}{4\pi}} \cos(\theta)$$

2. Green's function:

$$\frac{1}{|\vec{x} - \vec{x}'|} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \frac{1}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_{lm}^*(\theta', \phi') Y_{lm}(\theta, \phi)$$

Bessel's Equation:

$$\frac{d^2R}{dx^2} + \frac{1}{x}\frac{dR}{dx} + (1 - \frac{\nu^2}{x^2})R = 0$$

Spherical Bessel Functions

$$j_\ell(kr) \rightarrow \frac{\sin(kr - \ell\pi/2)}{kr}$$

$$n_\ell(kr) \rightarrow -\frac{\cos(kr - \ell\pi/2)}{kr}$$

$$j_o(\rho) = \frac{\sin(\rho)}{\rho} \qquad n_o(\rho) = -\frac{\cos(\rho)}{\rho}$$

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos(\rho)}{\rho}$$

Gamma Function

1. Integral Representation:

$$\Gamma(z) = \int_0^\infty dt e^{-t} t^{z-1}$$

2. Functional relation:

$$\Gamma(z+1) = z\Gamma(z)$$

3. Special values:

$$\Gamma(1) = 1 \qquad \Gamma(1/2) = \sqrt{\pi}$$

Zeta Function

1. Integral representations:

$$\int_0^\infty \frac{x^{n-1}}{e^x - 1} = \Gamma(n)\zeta(n) \quad n > 1$$

$$\int_0^\infty \frac{x^{n-1}}{e^x + 1} = (1 - 2^{1-n}\Gamma(n))\zeta(n) \quad n > 1$$

2. Special values:

$$\zeta(0) = -\frac{1}{2} \qquad \zeta(3/2) = 2.612 \qquad \zeta(2) = \frac{\pi^2}{6}$$

$$\zeta(5/2) = 1.341 \qquad \zeta(4) = \frac{\pi^4}{90}$$

Classical Mechanics

1. Euler-Lagrange equations:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}$$

2. Force in a rotating frame:

$$\vec{F}_{eff} = \vec{F} - m\vec{a}_f - m\dot{\vec{\omega}} \times \vec{r} - m\vec{\omega} \times (\vec{\omega} \times \vec{r}) - 2m\vec{\omega} \times \vec{v}_r$$

where v_r is the velocity with respect to the rotating axes, a_f is the acceleration of the moving frame with respect to the fixed axes.

Quantum Mechanics

1. Harmonic Oscillator:

$$H = \hbar\omega(\frac{1}{2} + a^\dagger a)$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \qquad a|n\rangle = \sqrt{n}|n-1\rangle$$

2. Angular momentum:

$$J_\pm = J_1 \pm iJ_2 \qquad J_\pm|j\ m\rangle = \sqrt{j(j+1) - m(m\pm 1)}|j\ m-1\rangle$$

3. Spherically symmetric potentials:

$$\Psi_{Elm}(r,\theta,\phi) = R_{El}(r)Y_{lm}(\theta,\phi) = \frac{\rho_{El}(r)}{r}Y_{lm}$$

$$[-\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}(V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E)]\rho_{El}(r) = 0$$

3. Partial Wave Expansion:

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell}\sin(\delta_\ell)P_\ell(\cos(\theta))$$

$$\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$$

For resonance,

$$\cot(\delta_n) = -(E - E_r)\frac{2}{\Gamma}$$

4. Born Approximation

$$f(\Omega) = -\frac{m}{e2\pi\hbar^2}\int d^3\vec{r}' e^{-i\vec{q}\cdot\vec{r}'}V(\vec{r}')$$

Useful Integrals

1.

$$\int \frac{x^2 dx}{(x^2+b^2)^{1/2}} = \frac{x}{2}\sqrt{x^2+b^2} - \frac{b^2}{2}\ln(x + \sqrt{x^2+b^2})$$

Electromagnetism

1. Energy density:

$$u = \frac{1}{8\pi}(\vec{E}^2 + \vec{B}^2)$$

2. Poynting vector

$$\vec{S} = \frac{c}{4\pi}(\vec{E} \times \vec{B})$$

3. Maxwell stress tensor:

$$T_{ij} = \frac{1}{4\pi}(E_iE_j + B_iB_j - \frac{1}{2}(\vec{E}^2 + \vec{B}^2)\delta_{ij})$$

4. Dipole moment

$$\vec{p} = \int d^3x\vec{x}\rho(\vec{x})$$

5. Quadrupole moment:

$$Q_{ij} = \int d^3x(3x_ix_j - r^2\delta_{ij})\rho(\vec{x})$$

Vector Analysis

1. Cross product

$$(\vec{A} \times \vec{B})_i = \epsilon_{ijk}A_jB_k$$

2. ϵ tensor:

$$\epsilon_{123} = 1, \epsilon_{213} = -1, \epsilon_{112} = 0, \text{etc.}$$

$$\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$$

2001

Statistical Mechanics

(Turn in 2 out of 3 problems.)

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STATISTICAL MECHANICS - 1

1. A gas of molecules at temperature T has a density of n molecules per unit volume, which is low enough to treat the molecules as almost non-interacting. Each molecule has a dipole moment of magnitude p that can point in any direction. Calculate the dipole moment per unit volume as a function of p, the electric field E, and T. Treat the system classically.

Hint: The energy of a dipole in a field is $U = -\vec{p} \cdot \vec{E}$.

SM1 1/1

Problems

1. A gas of molecules at temperature T has a density of n molecules per unit volume, which is low enough to treat the molecules as almost non-interacting. Each molecule has a dipole moment of magnitude p that can point in any direction. Calculate the dipole moment per unit volume as a function of p, E, and T. Treat the system classically

Hint: The energy of a dipole in a field is $U = A - \mathbf{p} \cdot \mathbf{E}$.

Solution

$\mathbf{p}$ aligns with the field in the direction of the field. It's magnitude is $< U > /E$. Take E in the z direction.

$$< U >= \frac{\int d\phi \int d\cos(\theta) \exp(-\beta Ep\cos(\theta)) Ep\cos(\theta)}{\int d\phi \int d\cos(\theta) \exp(-\beta Ep\cos(\theta))}$$

Where $U = Ep\cos(\theta)$
So we calculate

$$Z \equiv \int d\cos(\theta) \exp(-\beta Ep\cos(\theta)) \ \propto \ \int_{-pE}^{pE} dU \exp(-\beta U)$$

and note that

$$< U >= \frac{\partial \ln Z}{\partial \beta}$$

Integrating we obtain

$$Z = \frac{1}{\beta} \sinh(\beta pE)$$

Therefore

$$< U >= pE\frac{\cosh(\beta pE)}{\sinh(\beta pE)} - \frac{1}{\beta} \ = \ pE\coth(\beta pE) - \frac{1}{\beta}$$

So that the dipole moment per unit volume is $n < U > /E >$ which is

$$N(p\coth(\beta pE) - \frac{1}{\beta E})$$

✓

STATISTICAL MECHANICS - 2

2. Consider a ferromagnet, which for long wavelengths has a continuous dispersion $\epsilon(\vec{k}) = \alpha k^2$, where $\vec{k}$ is the reciprocal wave vector for magnons.

a. Calculate the specific heat for a three dimensional ($d = 3$) system valid at low temperatures where the dispersion relation above holds.

b. Do the same for $d = 2$.

c. Show that for the same number of spins, the $d = 2$ system will have a larger specific heat than the $d = 3$ system as $T \to 0$, according to the answers obtained in parts a and b above.

d. Very briefly explain why does this not make sense and what is wrong with our assumptions that produce this result.

Problem #2 Solution

a) $D(k) = \frac{V}{(2\pi)^3} 4\pi k^2 dk = \frac{V}{2\pi^2} k^2 dk$

$$U_3 = \frac{V}{2\pi^2} \int_0^\infty \frac{k^2 \epsilon(k)}{e^{\beta\epsilon(k)}-1} dk = \frac{V\alpha}{2\pi^2} \int_0^\infty \frac{k^4\, dk}{e^{\alpha\beta k^2}-1}$$

let $z = (\alpha\beta)^{1/2} k \qquad dk = (\alpha\beta)^{-1/2} dz \qquad k^2 = (\alpha\beta)^{-1} z^2$

$$U_3 = \frac{V\alpha}{2\pi^2} (\alpha\beta)^{-5/2} \int_0^\infty \frac{z^4}{e^{z^2}-1} dz$$

$$U_3 = \frac{V(kT)^{5/2}}{2\pi^2 \alpha^{3/2}} \int_0^\infty \frac{z^4}{e^{z^2}-1} dz = D T^{5/2}$$

where $D =$ const

$$C_3 = 5/2\, D T^{3/2}$$

b) $D(k) = \frac{A}{(2\pi)^2} 2\pi k\, dk = \frac{A}{2\pi} k\, dk$

$$U_2 = \frac{A\alpha}{2\pi} \int_0^\infty \frac{k^3 dk}{e^{\alpha\beta k^2}-1} = \frac{A\alpha}{2\pi} (\alpha\beta)^{-2} \int_0^\infty \frac{z^3 dz}{e^{z^2}-1}$$

$$U_2 = \frac{A\,(kT)^2}{2\pi\alpha} \int_0^\infty \frac{z^3 dz}{e^{z^2}-1} = BT^2$$

where $B =$ const

$$C_2 = 2BT$$

c) $\frac{C_2}{C_3} = 4/5 \frac{B}{D} T^{-1/2} \to \infty$ as $T \to 0$, so C_2 dominates

d) at very low T, the densities of state are not continuous and the problem must be treated with discrete states. Treating them as continuous leads to the result that the ~~state~~ system with fewer degrees of freedom has a higher specific heat, ~~and~~ which is not correct.

3. Consider two spin-1 objects, $\vec{S}_1$ and $\vec{S}_2$, with Hamiltonian

$$\mathcal{H} = J\vec{S}_1 \cdot \vec{S}_2,$$

where $J > 0$. Use $\hbar = 1$.

a. Find the energy levels. Hint: Use $\left(\vec{S}_{tot}\right)^2 = \left(\vec{S}_1 + \vec{S}_2\right)^2$, where $\vec{S}_{tot}$ is the total spin, and note that the vector rule for the addition of angular momenta states that the allowed values of the total spin quantum number S_{tot} are 0, 1, and 2 (each value once).

b. Find the free energy, entropy and average energy as a function of temperature, T.

c. What are the limits of the entropy as (i) $T \rightarrow 0$ and (ii) $T \rightarrow \infty$? Explain how you could have obtained these values from elementary considerations without first determining the free energy.

Statistical Mechanics.

$\mathcal{H} = J\,\vec{S}_1 \cdot \vec{S}_2$ Spin-1.

(a) $\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left(\vec{S}_{tot}^{\,2} - \vec{S}_1^{\,2} - \vec{S}_2^{\,2}\right)$

$\vec{S}_{tot}^{\,2} = S_{tot}(S_{tot}+1)$, $S_1^2 = 1.2 = 2$

Hence Energy levels are $\frac{J}{2}\left[S_{tot}(S_{tot}+1) - 4\right]$

$= -2J$	$S_{tot} = 0$	degeneracy 1.
$-1J$	$S_{tot} = 1$	degeneracy 3
$1J$	$S_{tot} = 2$	degeneracy 5.

(b) Partition function, let $h = \beta J$

$$Z = e^{2h} + 3e^{h} + 5e^{-h}.$$

$$F = -k_B T \ln\left[e^{2h} + 3e^{h} + 5e^{-h}\right]$$

$$\frac{S}{k_B} = \frac{-\partial F}{k_B \partial T} = \ln\left[e^{2h} + 3e^{h} + 5e^{-h}\right] - \frac{TJ}{k_B T^2}\left[\frac{2e^{2h} + 3e^{h} - 5e^{-h}}{e^{2h} + 3e^{h} + 5e^{-h}}\right]$$

$$= -\frac{F}{T} + \frac{U}{T}$$

$F = U - TS$

$S = \frac{U}{T} - \frac{F}{T}$

$$U = -J\left[\frac{2e^{2h} + 3e^{h} - 5e^{-h}}{e^{2h} + 3e^{h} + 5e^{-h}}\right]$$

(c) $T \to 0$ $\frac{S}{k_B} = \ln e^{2h} - \frac{J}{k_B T} \times 2 = 0$

$T \to \infty$ $\frac{S}{k_B} = \ln 9$

$T \to \infty$ 9 states with equal occupation $\Rightarrow S = k_B \ln 9$.

$T \to 0$ g.s. is non degenerate $\therefore S = \ln$ degeneracy $= 0$

Legendre Polynomials

1. Generating function:

$$g(t,x) = (1-2xt+t^2)^{-1/2} = \sum_{n=0}^{\infty} P_n(x)t^n$$

2. Recursion relations

$$(2n+1)xP_n(x) = (n+1)P_{n+1}(x) + nP_{n-1}(x)$$

$$(1-x)^2P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0$$

3. Normalization

$$\int dx[P_n(x)]^2 = \frac{2}{2n+1}$$

Spherical Harmonics

1. $\ell = 0$:

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

2. $\ell = 1$:

$$Y_{11} = -\sqrt{\frac{3}{8\pi}}\sin(\theta)e^{i\phi} \qquad Y_{10} = \sqrt{\frac{3}{4\pi}}\cos(\theta)$$

3. Green's function:

$$\frac{1}{|\vec{x}-\vec{x}'|} = 4\pi \sum_{l=0}^{\infty}\sum_{m=-l}^{m=l} \frac{1}{2l+1}\frac{r_<^l}{r_>^{l+1}} Y_{lm}^*(\theta',\phi')Y_{lm}(\theta,\phi)$$

Bessel's Equation:

$$\frac{d^2R}{dx^2} + \frac{1}{x}\frac{dR}{dx} + (1-\frac{\nu^2}{x^2})R = 0$$

Spherical Bessel Functions

$$j_\ell(kr) \to \frac{\sin(kr-\ell\pi/2)}{kr}$$

$$n_\ell(kr) \to -\frac{\cos(kr-\ell\pi/2)}{kr}$$

$$j_o(\rho) = \frac{\sin(\rho)}{\rho} \qquad n_o(\rho) = -\frac{\cos(\rho)}{\rho}$$

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos(\rho)}{\rho}$$

Gamma Function

1. Integral Representation:

$$\Gamma(z) = \int_0^{\infty} dte^{-t}t^{z-1}$$

2. Functional relation:

$$\Gamma(z+1) = z\Gamma(z)$$

3. Special values:

$$\Gamma(1) = 1 \qquad \Gamma(1/2) = \sqrt{\pi}$$

Fourier Transform

1. Discrete Fourier transform:

$$f(x) = \sum_{m=-\infty}^{\infty} c_m e^{\frac{2\pi i m x}{L}} \qquad c_m = \frac{1}{L}\int_o^L dx\ f(x) e^{-\frac{2\pi i m x}{L}}$$

2. Continuous Fourier Transform:

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{d}k\ f(k) e^{ikx} \qquad \tilde{f}(k) = \int_{-\infty}^{\infty} dx\ e^{-ikx} f(x)$$

Zeta Function

1. Integral representations:

$$\int_0^\infty \frac{x^{n-1}}{e^x - 1} = \Gamma(n)\zeta(n) \quad n > 1$$

$$\int_0^\infty \frac{x^{n-1}}{e^x + 1} = (1 - 2^{1-n}\Gamma(n))\zeta(n) \quad n > 1$$

2. Special values:

$$\zeta(0) = -\frac{1}{2} \qquad \zeta(3/2) = 2.612 \qquad \zeta(2) = \frac{\pi^2}{6}$$

$$\zeta(5/2) = 1.341 \qquad \zeta(4) = \frac{\pi^4}{90}$$

Classical Mechanics

1. Euler-Lagrange equations:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}$$

2. Force in a rotating frame:

$$\vec{F}_{eff} = \vec{F} - m\vec{a}_f - m\dot{\vec{\omega}} \times \vec{r} - m\vec{\omega} \times (\vec{\omega} \times \vec{r}) - 2m\vec{\omega} \times \vec{v}_r$$

where v_r is the velocity with respect to the rotating axes, a_f is the acceleration of the moving frame with respect to the fixed axes.

Quantum Mechanics

1. Harmonic Oscillator:

$$H = \hbar\omega(\frac{1}{2} + a^\dagger a)$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \qquad a|n\rangle = \sqrt{n}|n-1\rangle$$

2. Angular momentum:

$$J_\pm = J_1 \pm iJ_2 \qquad J_\pm|j\ m\rangle = \sqrt{j(j+1) - m(m\pm 1)}|j\ m\pm 1\rangle$$

3. Spherically symmetric potentials:

$$\Psi_{Elm}(r,\theta,\phi) = R_{El}(r)Y_{lm}(\theta,\phi) = \frac{\rho_{El}(r)}{r}Y_{lm}$$

$$[-\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}(V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E)]\rho_{El}(r) = 0$$

4. Partial Wave Expansion:

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell}\sin(\delta_\ell)P_\ell(\cos(\theta))$$

$$\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$$

For resonance,

$$\cot(\delta_n) = -(E-E_r)\frac{2}{\Gamma}$$

5. Born Approximation

$$f(\Omega) = -\frac{m}{e2\pi\hbar^2}\int d^3\vec{r}'\,e^{-i\vec{q}\cdot\vec{r}'}V(\vec{r}')$$

Useful Integrals

1.

$$\int\frac{x^2dx}{(x^2+b^2)^{1/2}} = \frac{x}{2}\sqrt{x^2+b^2} - \frac{b^2}{2}\ln(x+\sqrt{x^2+b^2})$$

2.

$$\int_{-\infty}^{\infty}dx\frac{\sin^2(x)}{x^2} = \pi$$

Electromagnetism

1. Energy density:

$$u = \frac{1}{8\pi}(\vec{E}^2+\vec{B}^2)$$

2. Poynting vector

$$\vec{S} = \frac{c}{4\pi}(\vec{E}\times\vec{B})$$

3. Maxwell stress tensor:

$$T_{ij} = \frac{1}{4\pi}(E_iE_j + B_iB_j - \frac{1}{2}(\vec{E}^2+\vec{B}^2)\delta_{ij})$$

4. Dipole moment

$$\vec{p} = \int d^3x\vec{x}\rho(\vec{x})$$

5. Quadrupole moment:

$$Q_{ij} = \int d^3x(3x_ix_j - r^2\delta_{ij})\rho(\vec{x})$$

Vector Analysis

1. Cross product

$$(\vec{A}\times\vec{B})_i = \epsilon_{ijk}A_jB_k$$

2. ϵ tensor:

$$\epsilon_{123}=1, \epsilon_{213}=-1, \epsilon_{112}=0, \text{etc.}$$

$$\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$$

Complex Analysis

1. Principal Part or Principal Value, an example:

$$\text{PP}\frac{1}{x-x_o} = \frac{1}{2\pi i}(\frac{1}{x-x_o-i\epsilon} - \frac{1}{x-x_o+i\epsilon})$$

Equivalently, one can do integrals over a small circle in the complex plane about x_o, weighted with $\frac{1}{2\pi i}$.

PHYSICAL CONSTANTS

Revised 1989 by B.N. Taylor. Based mainly on the "1986 Adjustment of the Fundamental Physical Constants" by E.R. Cohen and B.N. Taylor, Rev. Mod. Phys. 59, 1121 (1987). The figures in parentheses after the values give the 1-standard-deviation uncertainties in the last digits; the uncertainties in parts per million (ppm) are given in the last column. The uncertainties of the values from a least-squares adjustment are in general correlated, and the laws of error propagation must be used in calculating additional quantities; the full variance matrix is given in the cited paper. The set of constants resulting from the 1986 adjustment has been recommended for international use by CODATA (Committee on Data for Science and Technology), and is the most up-to-date, generally accepted set available.

Quantity	Symbol, equation	Value	Uncert. (ppm)
speed of light	c	299 792 458 m s^{-1}	(exact)*
Planck constant	h	6.626 075 5(40)$\times10^{-34}$ J s	0.60
Planck constant, reduced	$\hbar \equiv h/2\pi$	1.054 572 66(63)$\times10^{-34}$ J s	0.60
		= 6.582 122 0(20)$\times10^{-22}$ MeV s	0.30
electron charge magnitude	e	1.602 177 33(49)$\times10^{-19}$ C = 4.803 206 8(15)$\times10^{-10}$ esu	0.30, 0.03
conversion constant	$\hbar c$	197.327 053(59) MeV fm	0.30
conversion constant	$(\hbar c)^2$	0.389 379 66(23) GeV^2 mbarn	0.59
electron mass	m_e	0.510 999 06(15) MeV/c^2 = 9.109 389 7(54)$\times10^{-31}$ kg	0.30, 0.59
proton mass	m_p	938.272 31(28) MeV/c^2 = 1.672 623 1(10)$\times10^{-27}$ kg	0.30, 0.59
		= 1.007 276 470(12) u = 1836.152 701(37) m_e	0.012, 0.020
deuteron mass	m_d	1875.613 39(57) MeV/c^2	0.30
unified atomic mass unit (u)	(mass C^{12} atom)/12 = (1 g)/N_A	931.494 32(28) MeV/c^2 = 1.660 540 2(10)$\times10^{-27}$ kg	0.30, 0.59
permittivity of free space	ϵ_0 $\epsilon_0\mu_0 = 1/c^2$	8.854 187 817 ... $\times10^{-12}$ F m^{-1}	(exact)
permeability of free space	μ_0	$4\pi\times10^{-7}$ N A^{-2} = 12.566 370 614 ... $\times10^{-7}$ N A^{-2}	(exact)
fine structure constant	$\alpha = e^2/4\pi\epsilon_0\hbar c$	1/137.035 989 5(61)†	0.045
classical electron radius	$r_e = e^2/4\pi\epsilon_0 m_e c^2$	2.817 940 92(38)$\times10^{-15}$ m	0.13
electron Compton wavelength	$\lambda\!\!\!^{-}_e = \hbar/m_e c = r_e\alpha^{-1}$	3.861 593 23(35)$\times10^{-13}$ m	0.089
Bohr radius ($m_{\rm nucleus} = \infty$)	$a_\infty = 4\pi\epsilon_0\hbar^2/m_e e^2 = r_e\alpha^{-2}$	0.529 177 249(24)$\times10^{-10}$ m	0.045
wavelength of 1 eV/c particle	hc/e	1.239 842 44(37)$\times10^{-6}$ m	0.30
Rydberg energy	$hcR_\infty = m_e e^4/2(4\pi\epsilon_0)^2\hbar^2 = m_e c^2\alpha^2/2$	13.605 698 1(40) eV§	0.30
Thomson cross section	$\sigma_T = 8\pi r_e^2/3$	0.665 246 16(18) barn	0.27
Bohr magneton	$\mu_B = e\hbar/2m_e$	5.788 382 63(52)$\times10^{-11}$ MeV T^{-1}	0.089
nuclear magneton	$\mu_N = e\hbar/2m_p$	3.152 451 66(28)$\times10^{-14}$ MeV T^{-1}	0.089
electron cyclotron freq./field	$\omega^e_{\rm cycl}/B = e/m_e$	1.758 819 62(53)$\times10^{11}$ rad s^{-1} T^{-1}	0.30
proton cyclotron freq./field	$\omega^p_{\rm cycl}/B = e/m_p$	9.578 830 9(29)$\times10^{7}$ rad s^{-1} T^{-1}	0.30
gravitational constant	G_N	6.672 59(85)$\times10^{-11}$ m^3 kg^{-1} s^{-2}	128
		= 6.707 11(86)$\times10^{-39}$ $\hbar c$ (GeV/c^2)$^{-2}$	128
standard grav. accel., sea level	g	9.806 65 m s^{-2}	(exact)
Avogadro number	N_A	6.022 136 7(36)$\times10^{23}$ mol^{-1}	0.59
Boltzmann constant	k	1.380 658(12)$\times10^{-23}$ J K$^{-1\S}$	8.5
		= 8.617 385(73)$\times10^{-5}$ eV K$^{-1\S}$	8.4
Wien displacement law constant	$b = \lambda_{\rm max}T$	2.897 756(24)$\times10^{-3}$ m K§	8.4
molar volume, ideal gas at STP	$N_A k$(273.15 K)/(1 atmosphere)	22.414 10(19)$\times10^{-3}$ m^3 mol$^{-1\S}$	8.4
Stefan-Boltzmann constant	$\sigma = \pi^2k^4/60\hbar^3c^2$	5.670 51(19)$\times10^{-8}$ W m^{-2} K$^{-4\S}$	34
Fermi coupling constant	$G_F/(\hbar c)^3$	1.166 37(2)$\times10^{-5}$ GeV^{-2}	17
weak mixing angle	$\sin^2\theta_W$	0.2259±0.0046	
$W^\pm$ boson mass	m_W	80.6±0.4 GeV/c^2	
Z^0 boson mass	m_Z	91.161±0.031 GeV/c^2	

[redacted]

2002

STATISTICAL MECHANICS

(Do only 2 out of 3 problems)

Please do **EACH** problem you attempt on a **SEPARATE** paper.
Put your name on each paper.

STATISTICAL MECHANICS - 1

1. Consider a large system of N non-interacting particles in a magnetic field $\vec{B}$, each fixed in position and carrying a magnetic moment $\vec{\mu}$ that can point either in the same direction as $\vec{B}$ or in the opposite direction.

a. Find the entropy for the system in terms of the number, n, of spins pointing against the field.

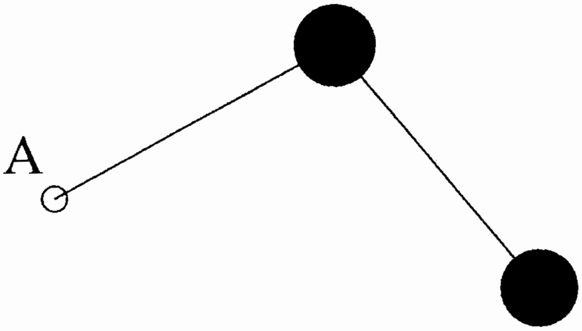
b. Find the maximum of the entropy in terms of n.

c. Find the conditions under which the temperature of the system is negative.

d. How can the system be prepared such that it has a negative temperature?

e. If the system has a negative temperature and is put into contact with a system with a positive temperature, which way will heat flow?

2. Consider a classical double pendulum in the absence of gravity as shown below.



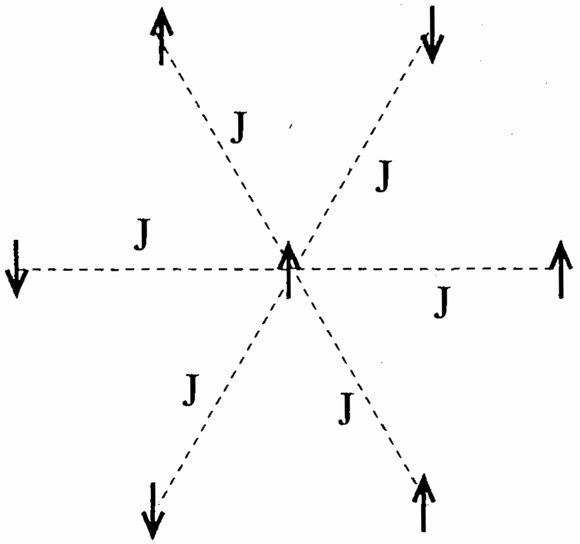
It consists of two rigid rods tethered at point A, with all joints freely hinged. The system is in contact with a heat bath at temperature T. The masses of the two rods and their moments of inertia are the same. The masses of the two black spheres are the same. For simplicity, consider the problem in two dimensions.

a. Calculate the probability distribution for the end to end vector between the point A and the end sphere.

b. Calculate the energy as a function of temperature.

STATISTICAL MECHANICS - 3

3. N Ising spins $S_i = \pm 1$, where $i = 1, 2, 3, ...N$ are all connected to a central spin s_0, but not each other, through a ferromagnetic coupling J as shown below.



They are all in a uniform magnetic field. The Hamiltonian for the system is

$$H = -J \sum_{i=0}^{N} S_0 S_i - h \sum_{i=0}^{N} S_i \quad .$$

a. Calculate the partition function for arbitrary N.

b. For very large N, calculate $< S_1 >$ as a function of β and h.

c. In the large N limit, state if there is a discontinuity in $< S_1 >$ as a function of h and for what temperature(s) it appears. Calculate the size of the discontinuity.

Qualifier #1 [redacted]

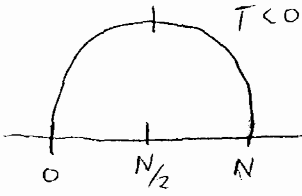
STAT MEC
2002

9)
$$\Omega = \frac{N!}{n!(N-n)!}$$

$$S = k_B \ln \Omega \simeq k_B\{N \ln N - n \ln n - (N-n)\ln(N-n)\}$$

$$\frac{\partial S}{\partial n} = 0 \quad \text{for maximum entropy}$$

$$\frac{\partial S}{\partial n} = -k_B\{\ln n - \ln(N-n)\} = 0$$



$$n = N - n \qquad n = \frac{N}{2}$$

$$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_V \qquad S_{max} = k_B[N \ln N - 2N \ln \tfrac{1}{2}N]$$
$$= k_B N \ln 2$$

$$U = n\mu B + (N-n)(-\mu B) = 2n\mu B - N\mu B$$

$$dU = 2\mu B\, dn$$

$$T = \frac{2\mu B}{(\partial S/\partial n)}$$

for $\frac{\partial S}{\partial n} < 0$ we have $T < 0$

this can be achieved by a field reversal done quickly

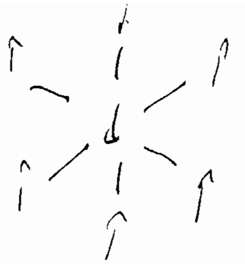
$$\frac{dS}{dt} = \frac{dU_A}{dt}\left(\frac{\partial S_A}{\partial U_A}\right)_V + \frac{dU_B}{dt}\left(\frac{\partial S_B}{\partial U_B}\right)_V$$

$$= \frac{dU_A}{dt}\left[\left(\frac{\partial S_A}{\partial U_A}\right)_V - \left(\frac{\partial S_B}{\partial U_B}\right)_V\right]$$

$$= \frac{dU_A}{dt}\left[\frac{1}{T_A} - \frac{1}{T_B}\right] > 0 \qquad \text{2nd Law}$$

if $T_A < 0$ & $T_B > 0$, then

$\frac{dU_A}{dt} < 0$, so heat flows from A to B



STAT MECH III

$$H_1 = -(h + J S_0) \sum_{i=1}^{N} s_i$$

$$Z = Z(S_0 = -1) + Z(S_0 = +1)$$

$$= \left(e^{-\beta(h-J)} + e^{\beta(h-J)}\right)^N$$

$$+ \left(e^{-\beta(h+J)} + e^{\beta(h+J)}\right)^N$$

$$= 2^N\left[\cosh^N(\beta(h-J)) + \cosh^N(\beta(h+J))\right]$$

$$\langle S_1 \rangle = \frac{1}{N} \left\langle \sum_{i=1}^{N} s_i \right\rangle = +\frac{T}{N} \frac{\partial \ln Z}{\partial h}$$

for $h > 0$ $\lim_{N \to \infty} \ln Z = N \ln 2 + N \ln \cosh(\beta(h+J))$

$h < 0$ " " = " $+ N \ln \cosh(\beta(h-J))$

$$\therefore \langle S_1 \rangle = +\frac{T}{N} N \tanh(\beta(h+J)) \cdot \beta = + \tanh(\beta(h+J)) \quad h$$

$$= \tanh(\beta(h-J)) \quad h <$$

discontinuity @ $h = 0$ of $2 \tanh(\beta J)$

Statistical Mechanics

2003

[redacted]

1. *Specific heat due to interaction with the walls.*
   The partition function for a classical system of particles is given by

$$Z = \frac{1}{N!\,(2\pi\hbar)^{3N}} \int \prod_{i=1}^{N} \left(d^3p_i d^3r_i\right) \exp\left(-\mathcal{H}[\vec{p},\vec{r}]/k_BT\right)$$

   where $\mathcal{H}[\vec{p},\vec{r}]$ is the Hamiltonian, which depends on the coordinates $\{\vec{r}_i\}$ and momenta $\{\vec{p}_i\}$ of the N particles.

   (a) A classical non-interacting gas is repelled by the walls of its container. The force can be represented by a step in the potential energy which is W a short distance ℓ from the wall and zero further away.

   Find an expression for the additional energy produced by this effect in terms of $k_B, T, W, \ell, N,$ the volume of the gas V, and the wall area A.

   (b) Assuming that $V \gg A\ell$, show that the corresponding extra specific heat, ΔC, tends to zero when k_BT is very large or very small compared with W, but that

$$\Delta C \sim Nk_B\frac{\ell A}{V}$$

   when k_BT is of order W.

(2003)

Statmech Solutions [redacted]

1. $$Z = \frac{1}{N!(2\pi\hbar)^{3N}} \int \prod \left(d^3p_i\, d^3q_i\right) e^{-\beta \mathcal{H}}$$

where $$\mathcal{H} = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_i U(\cancel{q}\vec{r}_i)$$ where

$$U(\vec{r}_i) = \begin{cases} W & \text{if } \vec{r}_i \text{ is within a distance } l \text{ of the walls} \\ 0 & \text{otherwise.} \end{cases}$$

(a) $$Z = Z_{KE}\, Z_{PE}$$ where

$$Z_{KE} = (\;) \int \prod_i d^3p_i\; e^{-\sum_i \beta p_i^2/2m}$$

$$Z_{PE} = \int \prod d^3r_i\; e^{-\sum \beta U(\vec{r}_i)}$$

$$= z_{PE}^{N} \quad \text{where } z_{PE} = \int d^3r\, e^{-\beta U(\vec{r})} = \underline{V - Al + Al e^{-\beta}}$$

Hence $F = F_{KE} + F_{PE}$ and $U = U_{KE} + U_{PE}$

We are interested in U_{PE} where

$$U_{PE} = N\frac{\partial}{\partial \beta}\left(-\cancel{\beta}\ln \cancel{Z}z_{PE}\right) = \frac{NAl\,We^{-\beta W}}{V + Al(e^{-\beta W} - 1)} \simeq \underline{\underline{\frac{Al}{V} We^{-\beta W}}}$$

(b) Specific Heat

$$C_{PE} = \frac{\partial U_{PE}}{\partial T}$$

$$\Rightarrow \underline{\frac{C_{PE}}{Nk_B} = \left(\frac{W}{k_BT}\right)^2 e^{-\beta W}\, \frac{Al}{V}}$$

$T \to \infty \quad \Rightarrow \quad \left(\frac{W}{T}\right)^2 \to 0$

$T \to 0 \quad \Rightarrow \quad e^{-W/T} \to 0$

For $k_BT = W$, $$\underline{C_{PE} \sim Nk_B \frac{Al}{V}}$$

2. *Elasticity due to entropy*
Consider a simple model of a polymer constrained to lie in one-dimension. The polymer consists of N segments ($N \gg 1$), of unit length, which can either point to the right or to the left along a line.

   (a) Calculate the free energy, F, of the system at a temperature T as a function of the end to end distance, x.
   Note: There is no energy in this problem, only entropy, so you need to think about the *number* of configurations with a given value of x.

   (b) Show that
   $$F(x) = F(0) + \frac{1}{2}Kx^2$$
   (*i.e.* one has Hooke's law: Force $= -Kx$) as long as x is small compared with the fully stretched length of the polymer.

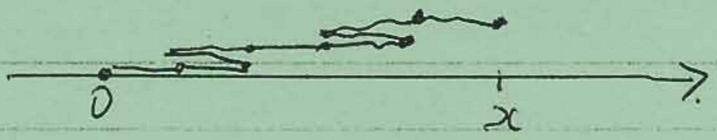
   (c) Show that the elastic constant, K, is proportional to temperature.

Note: This is believed to be the why rubber, which consists of cross-linked polymers, has an elastic constant which *increases* with T, whereas most substances get softer as they heat up so their elastic constant *decreases*.

(2003)

Stat Mech Solutions, [redacted]

2)



(a) Let there be N_r segments which go to right
N_L - - - - - - - - left

Clearly $N_r + N_L = N$ so $N_r = \frac{1}{2}(N+x)$

$N_r - N_L = x$. $N_\ell = \frac{1}{2}(N-x)$

How many ways are there of choosing N_r segment to right

Ans. Binomial coefficient $g(N,x) = \frac{N!}{N_L!\, N_r!} = \underline{\frac{N!}{\left[\frac{N}{2}(1+x)\right]!\, \left[\frac{N}{2}(1-x)\right]!}}$

Free energy

$$\underline{\underline{F = -k_B T \ln g(N,x).}}$$

(b) From Stirlings approximation

$$\ln g(N,x) = \ln N! - \ln\left[\left(\tfrac{N}{2}(1+x)\right)!\right] - \ln\left[\left(\tfrac{N}{2}(1-x)\right)!\right]$$

$$\hat{=} N\ln N - N - \left\{ \tfrac{N}{2}(1+x)\ln\left[\tfrac{N}{2}(1+x)\right] - \tfrac{N}{2}(1+x) \right\}$$
$$- \left\{ \tfrac{N}{2}(1-x)\ln\left[\tfrac{N}{2}(1-x)\right] - \tfrac{N}{2}(1-x) \right\}$$

$$= \cancel{N\ln N} - \tfrac{N}{2}(1+x)\ln\left[\cancel{N}(1+x)\right] - \tfrac{N}{2}(1-x)\ln\left[\cancel{N}(1-x)\right] + N\ln 2.$$

For $x \ll N$, expand to lowest non vanishing order in x

$$\ln\left[g(N,x)\right] = N\left[\ln 2 - \frac{x^2}{2}\right]$$

Hence $\underline{\underline{F = F_0 + k_B T\, N \frac{x^2}{2}}}$

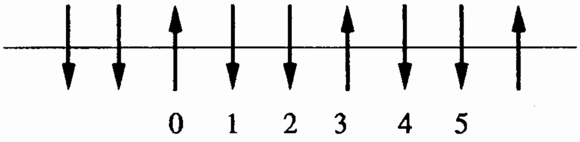
~~Tie~~.

(c) Force constant k is given by $\underline{\underline{K = N k_B T}}$ (i.e. $\propto T$)

[redacted]

STATISTICAL MECHANICS - 1

2. Consider a long linear chain of N Ising spins, where the spin value is $S_i = \pm 1$ and the interaction between spins is $-J$, where $J > 0$.



1) Write the Hamiltonian for this system.
2) Write the partition function for this system.
3) Rewrite the partition function for this system having summed over the odd numbered spins.
4) Rewrite the partition function again, but in the same form as the original Hamiltonian, but with the sum over the even spins only, multiplied by a function only of the temperature, and at different effective temperature, T'. This could be written in the form

$$Z(N,T) = f(T)^{N/2} Z(N/2, T') \tag{1}$$

Show the equation for T' in terms of T and the equation for $f(T)$. Is the new temperature higher or lower than the original one?
5) Explain why this exercise demonstrates that the system never has a phase transition or long-range order.

Solution

1) $$\mathcal{H} = -J \sum_{i=-\infty}^{\infty} S_i S_{i+1}$$

2) $$Z = \sum e^{J\beta(\cdots + S_0S_1 + S_1S_2 + S_2S_3 + S_3S_4 + \cdots)}$$

3) $$Z = \sum \cdots e^{J\beta(S_0S_1 + S_1S_2)} \, e^{J\beta(S_2S_3 + S_3S_4)} \cdots$$

$$Z = \sum \cdots \left[e^{J\beta(S_0+S_2)} + e^{-J\beta(S_0+S_2)}\right]\left[e^{J\beta(S_2+S_4)} + e^{-J\beta(S_2+S_4)}\right] \cdots$$

4) $$e^{J\beta(S_0+S_2)} + e^{-J\beta(S_0+S_2)} = f(T)\, e^{+J\beta' S_0 S_2}$$

for $S_0 = S_2 = 1, -1$

$$e^{2J\beta} + e^{-2J\beta} = f(T)\, e^{J\beta'}$$

for $S_0 = -S_2 = 1, -1$

$$2 = f(T)\, e^{-J\beta'}$$

divide to get $\cosh 2J\beta = e^{2J\beta'}$

$$2J\beta' = \ln(\cosh 2J\beta)$$

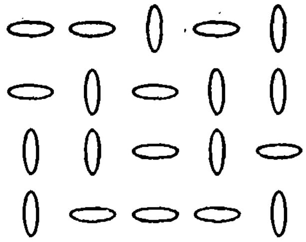
$$T' = \frac{2J}{k \ln(\cosh 2J/kT)} \qquad T' > T$$

$$f(T) = 2e^{J\beta'} = 2\cosh^{1/2}(2J\beta)$$

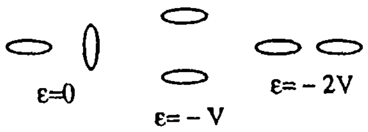
$$f(T) = 2\cosh^{1/2}\left(\frac{2J}{kT}\right)$$

5) there are no singular points where a transition takes place. Since the system is disordered at high T, it must always be disordered and no long-range order can take place

3 [illegible]. Cigar shaped molecules are arranged on a square lattice, as illustrated in the sketch below:



Each molecule may be oriented only along the x or y axes. The molecules interact only if they are nearest neighbors, and the energy of this interaction may be 0, -V or -2V (V > 0) depending on the relative orientation of the molecules.



This system will undergo a phase transition to an ordered state at low temperature. Within a mean field approximation use the *effective field on each molecule* to calculate, self consistently,the transition temperature. Then determine (again in mean field) either the value (if continuous) or the discontinuity (if discontinuous) of the system at the transition temperature. *for:*

(a) the energy

(b) the entropy

The self consistency condition is that the normalized weight associated with the ⬯ orientation should be p, i.e.

$$p = \frac{\exp[6pV\beta]}{\exp[6pV\beta] + \exp[6(1-p)V\beta]}$$

Writing $p = \frac{1}{2}(1+f)$, we obtain

$$f = \tanh[3V\beta f].$$

This always has a solution $f=0$. At low temperatures, however, the $f=0$ solution loses stability to a pair of solutions at $f = \pm f_0$. As for magnets, the critical temperature is found by expanding the RHS in powers of f, which yields

$$3V\beta_c = 1.$$

For $\beta \gtrsim \beta_c$, $f \approx 0$. For $3V\beta = 1+\epsilon$, expanding in powers of f we have

$$f = (1+\epsilon)f - \frac{[(1+\epsilon)f]^3}{3} + \dots$$

i.e., $-\epsilon f \approx -\frac{f^3}{3}$, so that $f = \pm\sqrt{3\epsilon} + O(\epsilon^{3/2})$

This is a second order transition, so that the energy and entropy are continuous, but the specific heat is not.

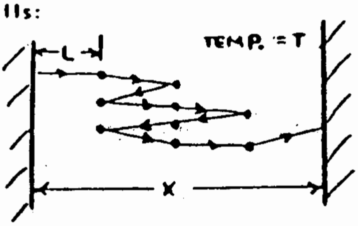
a) The energy per molecule at T_c is given by $-\frac{\partial}{\partial\beta}\ln Z$

$$= p\cdot(-6pV) + (1-p)(-6(1-p)V)$$

$$= (\text{since } f_c = 0) \quad -3V$$

b) The entropy per molecule at T_c is found by using $S = -k\sum p_i \ln p_i$. Since both the ⬯ and the ⬭ orientation have probability $= \frac{1}{2}$ at T_c, $S = k\ln 2$.

5. There is a chain consisting of $n \gg 1$ links at temperature T, between two walls:



Let the length of each link be L and let the distance between the endpoints be x. The joints between the links are frictionless and turn freely. No external forces, other than the connections to the walls at the two endpoints, act on the chain. Consider this as a one-dimensional problem, i.e., each link can assume only one of the two orientations: •→• OR •←•

a) Find the entropy of this chain as a function of x.

b) Determine the relation between the temperature of the chain and the force (tension) which is necessary to maintain the distance x.

5. a) If there are n_+ links pointing forward and n_- pointing backwards,

$$n_+ - n_- = x/L$$
$$n_+ + n_- = n$$

So that

$$n_+ = \tfrac{1}{2}(n + x/L)$$
$$n_- = \tfrac{1}{2}(n - x/L)$$

The number of configurations we can construct is ${}^{n}C_{n_+}$. Therefore the entropy is

$$S = k_B \ln \Omega = k_B \left\{ n\ln n - n - n_+ \ln n_+ + n_+ - n_- \ln n_- + n_- \right\}$$

Expanding this expression in powers of x,

$$S = k_B \left\{ n\ln n - \left[\frac{n}{2} \ln n/2 + \frac{1}{2}\frac{x}{L}\cdot\frac{x}{nL}\right] \times 2 \right\}$$

$$= k_B \left\{ n \ln 2 - x^2/nL^2 + O(x^3) \right\}$$

b) $dF = -S\,dT + f\,dx$, $F = U - TS = -TS$.

$$f = \partial F/\partial x \Big|_T = 2k_B T x / nL^2$$

Bonus: If we stretch a rubberband, $dU = dQ + f\,dx = C$

We see that the energy spent in stretching the band flows out to the environment as heat. (In real rubber, although $U \neq 0$, $-TS$ dominates the free energy, so assuming $U = 0$ is not a bad approximation).

(One can also derive, from this expression, that i) stretched rubber left to itself will spontaneously contract in an irreversible process ii) when we heat rubber it will contract.)

[redacted]
Statistical/04

2004
STATISTICAL MECHANICS
(Turn in 2 0ut of 3 Problems)

INSTRUCTIONS:
DO EACH PROBLEM ON SEPARATE PAPER.

WRITE YOUR NAME, SECTION, PROBLEM# ON EACH SHEET YOU TURN IN.

TURN IN ONLY TWO PROBLEMS. A THIRD PROBLEM WILL NOT BE GRADED.

Statistical Mechanics #1

1. Consider a one-dimensional Ising model with ferromagnetic coupling $J > 0$ on a chain with N sites, with randomly placed impurity atoms. The impurity atoms are located between lattice sites, and destroy the ferromagnetic coupling. Thus the energy of a spin configuration is given by

$$E = -J \sum_{i=1}^{N-1} n_i S_i S_{i+1}$$

where $S_i = \pm 1$ is the Ising spin on the i'th site, and $n_i = 0$ if there is an impurity atom on the i'th bond while $n_i = 1$ otherwise. Assume that N is extremely large. You should take free boundary conditions rather than periodic boundary conditions.

   (a) For the pure system, i.e. all the n's are equal to 1, calculate the free energy and energy per site.

   (b) Calculate the free energy per site if the impurity atoms are free to drift in and out of the chain, i.e. the impurity variables $\{n_i\}$ are in equilibrium with the spin variables.

   (c) In part b, what is $1 - \langle n_i \rangle$, the average density of impurity atoms?

Statistical Mechanics #2

2. Consider non interacting fermions with spin 1/2 at finite temperature. The specific heat at finite temperature, as measured in the lab, is given by

$$C = \left(\frac{\partial U}{\partial T}\right)_N = -k_B\beta^2\left(\frac{\partial U}{\partial \beta}\right)_N$$

where U is the internal energy and $\beta = 1/(k_BT)$.

   (a) Write down expressions for the energy and mean number of particles N in the grand canonical ensemble in terms of the Fermi function

$$f(\epsilon) = \frac{1}{\exp(\beta(\epsilon-\mu)+1}$$

   (where μ is the chemical potential), and the density of states $g(\epsilon)$.

   (b) In order to keep the number of particles constant show that μ must vary with β as

$$\left(\frac{\partial \mu}{\partial \beta}\right)_N = -\left(\frac{\partial N}{\partial \beta}\right)_\mu / \left(\frac{\partial N}{\partial \mu}\right)_\beta .$$

   (c) Hence find an expression for the specific heat involving partial derivatives of U and N, assumed to be functions of μ and β.

   (d) Write the partial derivatives in part 2c in terms of integrals over $f'(\epsilon)$.

   (e) By using the Sommerfield expansion

$$\int A(\epsilon)f'(\epsilon)\,d\epsilon = -\left[A(\mu) + \frac{\pi^2}{6}k_B^2T^2A''(\mu) + \cdots\right],$$

   (which you are **not** required to prove), valid at low-T, where $A(\epsilon)$ is an arbitrary function, evaluate each of the partial derivatives in part 2e to lowest order in T, and hence determine the specific heat at low temperature to leading order. *Note:* You should find the specific heat to be linear in T.

Statistical Mechanics #3

3. Consider electromagnetic radiation inside a cubic box of volume V at temperature T.

   (a) Calculate the allowed wave-vectors for the photons. To make this simpler, you can consider periodic boundary conditions for an $L \times L \times L$ box.

   (b) Calculate the density of states of the photons, that is, the number of states in frequency range ω to $\omega + d\omega$.

   (c) State what is the average number of photons that occupy a single state at frequency ω if the temperature is T?

   (d) Calculate the energy density per unit frequency range inside the box.

   (e) Show that the answer to part d has a maximum at $\omega = \omega_c$ where

   $$\hbar\omega_c = C\, k_B T$$

   where C is a numerical constant. You should explain how C is obtained but you do not need to determine its numerical value.

Qualifying Examination, 2004

Statistical Mechanics

Solutions

1. (a) If all the n_i are equal to 1 we just have the regular one-dimensional Ising model with energy

$$E = -J \sum_{i=1}^{N-1} S_i S_{i+1} .$$

With free boundary conditions, the simplest way to determine the partition function is to trace out an end spin, $i = N$ say, since this is independent of spin S_{N-1}. The sum gives

$$\sum_{S_N=\pm 1} e^{\beta J S_{N-1} S_N} = e^{\beta J} + e^{-\beta J} = 2\cosh \beta J .$$

The process can be repeated for spins $N-1, N-2, \cdots, 3, 2$. This just leaves spin S_1 which then has no coupling and summing over it gives a factor of 2. Hence the partition function is given by

$$Z = 2(2\cosh \beta J)^{N-1} .$$

The free energy per site is given by $f = -N^{-1} k_B T \ln Z$, i.e.

$$\boxed{f = -k_B T \ln(2\cosh \beta J) ,}$$

in which the difference between $N-1$ and N has been neglected (valid for large N).

The energy per site, u, is given by

$$u = \frac{\partial}{\partial \beta}(\beta f) = \boxed{-J \tanh \beta J .}$$

Note: These results can also be obtained by transfer matrices.

(b) We now repeat the procedure in the first part but including the n_i. We start by tracing out the end spin S_N and the end bond n_{N-1}:

$$\sum_{n_{N-1}=0,1} \sum_{S_N=\pm 1} e^{\beta J n_{N-1} S_{N-1} S_N} = 2 + e^{\beta J} + e^{-\beta J} = 2(1 + \cosh \beta J) . \qquad (1)$$

Repeating for spins $N-1, N-2, \cdots, 3, 2$ we get

$$Z = 2^N (1 + \cosh \beta J)^{N-1} .$$

The free energy per site is therefore

$$\boxed{f = -k_B T \ln(2 + 2\cosh \beta J) ,}$$

Note: Again, these results can also be obtained by transfer matrices.

(c) Now $1 - \langle n_i \rangle$ is the ratio of the statistical sum with n_i fixed to be zero divided by the total statistical sum. This is given by the ratio of the terms in Eq. (1) with $n_i = 0$ to the total in Eq. (1), i.e.

$$1 - \langle n_i \rangle = \frac{2}{2(1 + \cosh \beta J)} = \boxed{\frac{1}{1 + \cosh \beta J}} .$$

2. (a) The expressions for the energy, U, and mean number of particles, N, are

$$\boxed{U = 2\int_0^\infty \epsilon f(\epsilon) g(\epsilon)\, d\epsilon\,,}$$

$$\boxed{N = 2\int_0^\infty f(\epsilon) g(\epsilon)\, d\epsilon\,,}$$

(the factor of 2 comes from the spin degeneracy).

(b) We need $dN = 0$, i.e.

$$0 = dN = \left(\frac{\partial N}{\partial \mu}\right)_\beta d\mu + \left(\frac{\partial N}{\partial \beta}\right)_\mu d\beta$$

and so

$$\boxed{\left(\frac{\partial \mu}{\partial \beta}\right)_N = -\left(\frac{\partial N}{\partial \beta}\right)_\mu \Big/ \left(\frac{\partial N}{\partial \mu}\right)_\beta .}$$

(c) The specific heat is given by

$$\begin{aligned} C &= -k_B\beta^2\left(\frac{\partial U(\beta,\mu)}{\partial \beta}\right)_N = -k_B\beta^2\left[\left(\frac{\partial U}{\partial \beta}\right)_\mu + \left(\frac{\partial U}{\partial \mu}\right)_\beta \left(\frac{\partial \mu}{\partial \beta}\right)_N\right] \\ &= \boxed{-k_B\beta^2\left[\left(\frac{\partial U}{\partial \beta}\right)_\mu - \left(\frac{\partial U}{\partial \mu}\right)_\beta \left(\frac{\partial N}{\partial \beta}\right)_\mu \Big/ \left(\frac{\partial N}{\partial \mu}\right)_\beta\right]} . \end{aligned}$$

(d) The partial derivatives in the last section can easily be obtained from the results in part. 2a:

$$\begin{aligned} \left(\frac{\partial U}{\partial \beta}\right)_\mu &= \boxed{\frac{2}{\beta}\int_0^\infty \epsilon(\epsilon-\mu) f'(\epsilon) g(\epsilon)\, d\epsilon} \\ \left(\frac{\partial U}{\partial \mu}\right)_\beta &= \boxed{-2\int_0^\infty \epsilon f'(\epsilon) g(\epsilon)\, d\epsilon\,,} \\ \left(\frac{\partial N}{\partial \beta}\right)_\mu &= \boxed{\frac{2}{\beta}\int_0^\infty (\epsilon-\mu) f'(\epsilon) g(\epsilon)\, d\epsilon\,,} \\ \left(\frac{\partial N}{\partial \mu}\right)_\beta &= \boxed{-2\int_0^\infty f'(\epsilon) g(\epsilon)\, d\epsilon\,,} \end{aligned}$$

(e) Using the Sommerfield expansion, the expressions in the last part can be written, to leading order in T,

$$\begin{aligned} \left(\frac{\partial U}{\partial \beta}\right)_\mu &= -\frac{4}{\beta}\frac{\pi^2}{6} k_B^2 T^2 (\mu g'(\mu) + g(\mu))\,, \\ \left(\frac{\partial U}{\partial \mu}\right)_\beta &= 2\mu g(\mu)\,, \\ \left(\frac{\partial N}{\partial \beta}\right)_\mu &= -\frac{4}{\beta}\frac{\pi^2}{6} k_B^2 T^2 g'(\mu)\,, \\ \left(\frac{\partial N}{\partial \mu}\right)_\beta &= 2g(\mu) \end{aligned}$$

Combining we get

$$C = k_B \beta^2 \frac{4}{\beta} g(\mu) \frac{\pi^2}{6} k_B^2 T^2 = \boxed{\frac{2}{3}\pi^2 k_B^2 T g(\mu)\,,}$$

which is linear in T.

3. (a) Calculate the allowed wave-vectors for the photons. To make this simpler, you can consider periodic boundary conditions for an $L \times L \times L$ box.

With plane waves, continuity implies

$$\boxed{\mathbf{k} = (2\pi/L)(n_x\hat{i} + n_y\hat{j} + n_z\hat{k})\,,}$$

where the n's take on all integral values. There are 2 distinct polarization states at every allowed value of k.

(b) Calculate the density of states of the photons, that is, the number of states in frequency range ω to $\omega + d\omega$.

The number of k-values per unit volume of k-space is $(L/2\pi)^3$ and so

$$\tilde{g}(k)dk = 2\left(\frac{L}{2\pi}\right)^3 4\pi k^2 dk\,,$$

where $\tilde{g}(k)dk$ is the number of states for which $|\mathbf{k}|$ lies between k and $k + dk$. Now $\omega = ck$, and so, in terms of ω rather than k, we have

$$g(\omega)d\omega = \tilde{g}(k)dk = 2\left(\frac{L}{2\pi}\right)^3 4\pi k^2 dk = 2\left(\frac{L}{2\pi}\right)^3 4\pi\left(\frac{\omega}{c}\right)^2 \frac{1}{c}d\omega\,.$$

Equating the first and last expressions in the previous equation gives

$$\boxed{g(\omega) = \frac{L^3}{c^3\pi^2}\,\omega^2\,.}$$

(c) At a temperature T, what is the average number of photons that occupy a single state at frequency ω?

Photons are bosons, and have no constraint on total number. Hence they obey the Planck distribution. Since the energy of a photon is $E = \hbar\omega$ we have

$$\boxed{\langle n\rangle = \frac{1}{e^{\beta\hbar\omega} - 1}\,.}$$

(d) Calculate the energy density per unit frequency range inside the box.

The energy in the frequency range ω to $\omega + \omega$ is $\langle n\rangle\hbar\omega g(\omega)d\omega$. Dividing by L^3 to get the energy per unit volume, and denoting the result by $e(\omega)d\omega$ we have

$$\boxed{e(\omega) = \frac{\hbar\omega^3}{c^3\pi^2}\frac{1}{e^{\beta\hbar\omega} - 1}\,.}$$

(e) Show that the answer to part 3d has a maximum when $\hbar\omega = C\,k_B T$.

We need to find the maximum of

$$\omega^3 \frac{1}{e^{\beta\hbar\omega} - 1}$$

with respect to ω. This is at $\omega = \omega_c$ where

$$3\omega_c^2 \frac{1}{e^{\beta\hbar\omega_c} - 1} = \omega_c^3 \beta\hbar \frac{e^{\beta\hbar\omega_c}}{(e^{\beta\hbar\omega_c} - 1)^2}$$

or

$$3k_BT = \hbar\omega_c \frac{1}{1 - e^{-\beta\hbar\omega}}.$$

Letting $\boxed{\hbar\omega_c = Ck_BT}$ we have

$$\boxed{C = 3(1 - e^{-C})\,.}$$

(You are not required to determine the value of C. The actual value is about 2.82.)