Physics 552: Midterm 2

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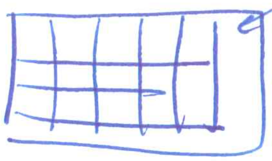
Problem 1: Ensemble theory

Consider a very large system (total system) with fixed energy, volume, and number of particles. Assume that this system is subdivided into M smaller systems which can exchange energy as well as volume with each other. Work out the ensemble theory corresponding to such a system, by deriving an expression for the probability of one of the M systems being in a state with a particular value of the energy and volume, as well as one for the partition function and the free energy. Identify all relevant thermodynamics variables such as the Lagrange multipliers. (Hint: it may help to discretize the energy and the volume.)

total system: fixed N, E, V

subsystems (M)



$$E = \sum_{i=1}^{M} E_i \rightarrow \text{fixed}$$

$$V = \sum_{i=1}^{M} V_i \rightarrow \text{fixed}$$

let M_i - number of subsystems in state "i"

$$E = \sum_i M_i E_i \qquad V = \sum_i M_i V_i$$

multiplicity: $\dfrac{M!}{M_1! M_2! \dots}$

total entropy: $S_t = k_B \ln \dfrac{M!}{M_1! M_2! \dots} = k_B \left[M \ln M - \sum_i M_i \ln M_i \right]$

$$= k_B \left[\sum_i M_i \ln M - \sum_i M_i \ln M_i \right]$$

$$= -k_B \sum_i M_i \ln \frac{M_i}{M}$$

entropy per subsystem

$$S = -k_B \sum_i P_i \ln P_i$$

average energy and volume

$$\bar{V} = \sum_i P_i V_i \qquad \bar{E} = \sum_i P_i E_i \Rightarrow \text{constrained}$$

(continue on worksheet!)

Problem 2: Phase space distributions

Consider a harmonic oscillator with Hamiltonian $\frac{p^2}{2m} + k\frac{x^2}{2}$. Determine whether the following distributions are equilibrium distributions:

1. $\rho(p, x) = \text{constant}$.
2. $\rho(p, x) = \exp\left[-\beta\left(\frac{p^2}{2m} + k\frac{x^2}{2}\right)\right]$
3. $\rho(p, x) = \exp\left[-\beta\left(\frac{p^2}{2m} + k\frac{x^5}{2}\right)\right]$

equilibrium → stationary solution of Liouville equation

1.) $\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial p}\frac{\partial p}{\partial t} + \frac{\partial \rho}{\partial x}\frac{\partial x}{\partial t} = 0$ ⇒ could be equilibrium

2.) $\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial p} F(x) + \frac{\partial \rho}{\partial x} v = -\beta \rho(p,x)\left[-\frac{p}{m} F(x) + kxv\right]$

$= -\frac{\partial \rho}{\partial p}\frac{\partial H}{\partial x} + \frac{\partial \rho}{\partial x}\frac{\partial H}{\partial p} = \beta \rho(p,x)\left[-\frac{p}{m} F(x) + kxv\right] = 0$

⇒ equilibrium

3.) $\frac{\partial \rho}{\partial t} = -\exp\left(-\frac{\beta p^2}{2m} - \frac{\beta k x^5}{2}\right)\left(-\frac{\beta p}{m}\right) kx$

$+ \exp\left(-\frac{\beta p^2}{2m} - \frac{\beta k x^5}{2}\right)\left(-\frac{5\beta k x^4}{2}\right)\frac{p}{m} \neq 0$

not stationary solution of

Liouville ⇒ not equilibrium

Problem 3: Cluster mean-field theory

Consider the Ising model on the triangular lattice, with nearest neighbor interaction K, and magnetic field B. Assume that K is ferromagnetic. Consider clusters of three sites (as done on page 199 of Reichl). To the bonds connecting these clusters, apply mean-field theory, in other words, substitute the expression for the $\sigma_i = \bar{\sigma} + \delta\sigma_i$, express the Hamiltonian, and neglect terms which are second order in the fluctuations $\delta\sigma_i$. Then derive the equation for $\bar{\sigma}$.

$$H = -K \sum_I \sum_{i\in I} \sum_{j\in I} \sigma_i \sigma_j - K \sum_I \sum_J \sum_{i\in I} \sum_{j\in J} \sigma_i \sigma_j - B \sum_i \sigma_i$$

mean-field approximation: for second term (for now no B-field!)

$$H_{mf} = -K \sum_I \sum_{i\in I} \sum_{j\in I} \sigma_i \sigma_j - K \sum_I \sum_J \sum_{i\in I} \sum_{j\in J} (\delta\sigma_i + \bar{\sigma})(\delta\sigma_j + \bar{\sigma})$$

$$= -K \sum_I \sum_{i\in I} \sum_{j\in I} \sigma_i \sigma_j - K \sum_I \sum_J \sum_{i\in I} \sum_{j\in J} [\underbrace{\delta\sigma_i \delta\sigma_j}_{0} + \delta\sigma_i \bar{\sigma} + \delta\sigma_j \bar{\sigma} + \bar{\sigma}^2]$$

$$= -K \sum_I \sum_{i\in I} \sum_{j\in I} \sigma_i \sigma_j - K \sum_I \sum_J \sum_{i\in I} \sum_{j\in J} (\sigma_i \bar{\sigma} + \sigma_j \bar{\sigma} - \bar{\sigma}^2)$$

$$\boxed{H_{mf} = -K \sum_I \sum_{i\in I} \sum_{j\in I} \sigma_i \sigma_j - 4K\bar{\sigma} \sum_{i\in I} \sigma_i + 2K\bar{\sigma}^2 N \cancel{- B \sum_{i\in I} \sigma_i}}$$

mean-field Hamiltonian (without field)

solve by: $$Q = \sum_{\sigma_1} \cdots \sum_{\sigma_N} \prod \left[e^{K \sum_{ij} \sigma_i \sigma_j + 4K\bar{\sigma} \sum_i \sigma_i} \right]^{N/3} e^{-2\beta K\bar{\sigma}^2 N}$$

$$Q = \Big[\underbrace{\sum_{\sigma_1} \sum_{\sigma_2} \sum_{\sigma_3} e^{K \sum_{\langle i,j\rangle} \sigma_i \sigma_2 + 4K\bar{\sigma} \sum_i \sigma_i}}_{\tilde{Q}_3} \Big]^{N/3} e^{-2\beta K\bar{\sigma}^2 N}$$

sum over configurations:

σ_1	σ_2	σ_3
1	1	1
+1	+1	-1
1	-1	1
-1	1	1

σ_1	σ_2	σ_3
-1	-1	-1
-1	-1	1
-1	1	-1
1	-1	-1

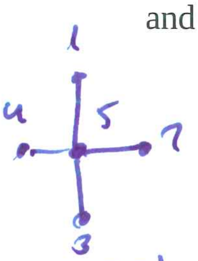
$$\Rightarrow \tilde{Q}_3 = e^{3K + 12K\bar{\sigma}} + 3e^{-K + 4K\bar{\sigma}} + 3e^{-K - 4K\bar{\sigma}} + e^{3K - 12K\bar{\sigma}}$$

(con't on worksheet)

Solution of this problem proceeds as Δ lattice in Reichl, see pp. 158 – 161

Problem 4: Renormalization

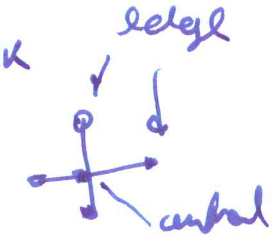
Consider the two-dimensional Ising model on a square lattice with nearest neighbor interaction K and under a magnetic field B. Derive the renormalization transformation for this system using the same blocking as Problem 5.15 in Reichl, but instead of majority rule, assign the central spin of the cross shape of the block to be the block-spin. Do not worry about critical exponents, derive only the relation between the parameters of the block Hamiltonian to those of the original Hamiltonian (the analog of Eqs. (5.204) and (5.205)), using the same cumulant expansion Reichl uses for the triangular lattice.



	σ_1	σ_2	σ_3	σ_4	σ_5	weight	degeneracy	$\langle\sigma\rangle$
$S=1$	1	1	1	1	1	e^{4K}	1	
	-1	1	1	1	1	e^{2K}	4	
	-1	-1	1	1	1	1	6	
	-1	-1	-1	1	1	e^{-2K}	4	
	-1	-1	-1	-1	1	e^{-4K}	1	
$S=1$	-1	-1	-1	-1	-1	e^{4K}	1	
	+1	-1	-1	-1	-1	e^{2K}	4	
	+1	+1	-1	-1	-1	1	6	
	+1	+1	+1	-1	-1	e^{-2K}	4	
	+1	+1	+1	+1	-1	e^{-4K}	1	

$$H = \underbrace{-K\sum_I \sum_{i\in I}\sum_{j\in I}\sigma_i\sigma_j}_{H_0} \underbrace{- K\sum_I\sum_J\sum_{i\in I}\sum_{j\in J}\sigma_i\sigma_j - B\sum_i\sigma_i}_{V}$$

$$Z_0 = \sum_{\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5} e^{-H_0} = e^{4K} + 4e^{2K} + 6 + 4e^{-2K} + e^{-4K}$$



need also $\langle\sigma\rangle \to$ different for edge spins from central spins

$$\langle\sigma\rangle_{central} = S \qquad \langle\sigma\rangle_{edge} = \frac{e^{4K} + 2e^{2K} - 2e^{-2K} - e^{-4K}}{Z_0} S$$

(cont. on 3)

(Problem 1 - continued!)

Worksheet 1:

maximize entropy with constraints $\bar{E} = \sum_i P_i E_i$ $\bar{V} = \sum_i P_i V_i$ $\sum_i P_i = 1$

$$\tilde{S} = -k_B \sum_i P_i \ln P_i + \bar{\alpha}\left(\sum_i P_i - 1\right) + \bar{\beta}\left(\sum_i P_i E_i - \bar{E}\right) + \bar{\gamma}\left(\sum_i P_i V_i - \bar{V}\right)$$

$$\frac{\partial \tilde{S}}{\partial P_i} = -k_B - k_B \ln P_i + \bar{\alpha} + \bar{\beta} E_i + \bar{\gamma} V_i = 0$$

$$\Rightarrow P_i = e^{\frac{\bar{\alpha}}{k_B} - 1} e^{\frac{\bar{\beta}}{k_B} E_i} e^{\frac{\bar{\gamma}}{k_B} V_i}$$

$$\sum_i P_i = 1 \Rightarrow \underbrace{\sum_i e^{\frac{\bar{\beta}}{k_B} E_i} e^{\frac{\bar{\gamma}}{k_B} V_i}}_{Q \text{ - partition function}} = e^{1 - \bar{\alpha}/k_B}$$

free energy $\tilde{G} = -k_B T \ln Q = -k_B T\left(1 - \frac{\bar{\alpha}}{k_B}\right) = \bar{\alpha} T - k_B T$
$= (\bar{\alpha} - k_B) T$

$$\sum_i P_i \frac{\partial \tilde{S}}{\partial P_i} = 0 \quad \text{since} \quad \frac{\partial \tilde{S}}{\partial P_i} = 0$$

$$\Rightarrow \quad TS + T\bar{\beta}\bar{E} + T\bar{\gamma}\bar{V} + T(\bar{\alpha} - k_B) = 0$$

$$TS + T\bar{\beta}\bar{E} + T\bar{\gamma}\bar{V} + \tilde{G} = 0$$

$$\tilde{G} = U - TS + PV$$

$$\tilde{G} = \bar{E} - TS + PV$$

(identify $\tilde{G}$ with Gibbs free energy)

$$T\bar{\beta} = -1 \qquad \bar{\beta} = -1/T$$

$$T\bar{\gamma} = -P \qquad \bar{\gamma} = -P/T$$

(Problem 2 continued)

Worksheet 2:

$$Q = \left(2\left[e^{3K}\cosh(12\beta K\bar{\sigma}) + 3e^{-K}\cosh(4\beta K\bar{\sigma})\right]\right)^{N/3} e^{-2\beta K\bar{\sigma}^2 N}$$

free energy: $F = -\frac{1}{\beta}\ln Q$

mean-field equations $\frac{\partial F}{\partial\bar{\sigma}} = 0$

with B-field

$$\cancel{Q = \left[2\left(e^{3K}\cosh(12K\bar{\sigma}+B\bar{\sigma}) + 3e^{-K}\cosh(8K\bar{\sigma}+B\bar{\sigma})\right)\right]^{N/3} e^{-2\beta K\bar{\sigma}^2 N}}$$

$$Q = \left[2\left(e^{3K}\cosh[\beta(12K\bar{\sigma}+3B\bar{\sigma})] + 3e^{-K}\cosh[\beta(4K\bar{\sigma}+B\bar{\sigma})]\right)\right]^{N/3} e^{-2\beta K\bar{\sigma}^2 N}$$

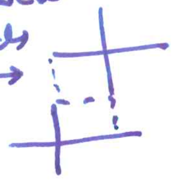
mean. field equations

$$-\frac{1}{\beta}\frac{1}{Q}\frac{\partial Q}{\partial\bar{\sigma}} = -\frac{1}{\beta}\frac{N}{3Q}\Big[2e^{3K}\sinh[\beta\bar{\sigma}(12K+3B)]\,\beta(12K+3B)$$
$$+ 3e^{-K}\sinh[\beta\bar{\sigma}(4K+B)]\,\beta(4K+B)\Big]^{1}$$
$$+ 4K\bar{\sigma}N = 0$$

$$\Rightarrow \cancel{\frac{2}{3}\frac{e^{3K}\sinh[\beta\bar{\sigma}(12K+3B)](12K+3B) + 3e^{-K}\sinh[\beta\bar{\sigma}(4K+B)]}{e^{3K}\cosh[\beta\bar{\sigma}(12K+B)] + 3e^{-K}\cosh[\beta\bar{\sigma}(8K+}}$$

$$2e^{3K}\sinh[\beta\bar{\sigma}(12K+3B)](12K+3B) +$$

3 interblock bonds



$M_L = M/5$

Worksheet 3:

$$H(K_L, B_L, \{S_L\}) = -M \ln Z_0 - 3K \sum_{IJ} \left(\frac{e^{4K} + 2e^{2K} - 2e^{-2K} - e^{-4K}}{e^{4K} + 4e^{2K} + 6 + 4e^{-2K} + e^{-4K}} \right)^2 S_I S_J$$

$$- B \sum \left[4 \left(\frac{e^{4K} + 2e^{2K} - 2e^{-2K} - e^{-4K}}{e^{4K} + 4e^{2K} + 6 + 4e^{-2K} + e^{-4K}} \right) S_I + S_J \right]$$

renormalization equations:

$$\boxed{\begin{aligned} K_L &= 3K \left(\frac{e^{4K} + 2e^{2K} - 2e^{-2K} - e^{-4K}}{e^{4K} + 4e^{2K} + 6 + 4e^{-2K} + e^{-4K}} \right)^2 \cancel{+4} \\ B_L &= 4B \left(\frac{e^{4K} + 2e^{2K} - 2e^{-2K} - e^{-4K}}{e^{4K} + 4e^{2K} + 6 + 4e^{-2K} + e^{-4K}} \right) + 1 \end{aligned}}$$

Worksheet 4: