PHYSICS 210A : STATISTICAL PHYSICS
HW ASSIGNMENT #3 SOLUTIONS

(1) Consider a system of noninteracting spin trimers, each of which is described by the Hamiltonian

$$\hat{H} = -J\big(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1\big) - \mu_0 \mathsf{H}\big(\sigma_1 + \sigma_2 + \sigma_3\big) \ .$$

The individual spin polarizations σ_i are two-state Ising variables, with $\sigma_i = \pm 1$.

(a) Find the single trimer partition function ζ.

(b) Find the magnetization per trimer $m = \mu_0 \, \langle \sigma_1 + \sigma_2 + \sigma_3 \rangle$.

(c) Suppose there are $N_\triangle$ trimers in a volume V. The magnetization density is $M = N_\triangle m/V$. Find the zero field susceptibility $\chi(T) = (\partial M/\partial \mathsf{H})_{\mathsf{H}=0}$.

(d) Find the entropy $S(T, \mathsf{H}, N_\triangle)$.

(e) Interpret your results for parts (b), (c), and (d) physically for the limits $J \to +\infty$, $J \to 0$, and $J \to -\infty$.

Solution : The eight trimer configurations and their corresponding energies are listed in the table below.

$\vert\,\sigma_1\sigma_2\sigma_3\,\rangle$	E	$\vert\,\sigma_1\sigma_2\sigma_3\,\rangle$	E
$\vert\uparrow\uparrow\uparrow\rangle$	$-3J - 3\mu_0\mathsf{H}$	$\vert\downarrow\downarrow\downarrow\rangle$	$-3J + 3\mu_0\mathsf{H}$
$\vert\uparrow\uparrow\downarrow\rangle$	$+J - \mu_0\mathsf{H}$	$\vert\downarrow\downarrow\uparrow\rangle$	$+J + \mu_0\mathsf{H}$
$\vert\uparrow\downarrow\uparrow\rangle$	$+J - \mu_0\mathsf{H}$	$\vert\downarrow\uparrow\downarrow\rangle$	$+J + \mu_0\mathsf{H}$
$\vert\downarrow\uparrow\uparrow\rangle$	$+J - \mu_0\mathsf{H}$	$\vert\uparrow\downarrow\downarrow\rangle$	$+J + \mu_0\mathsf{H}$

Table 1: Spin configurations and their corresponding energies.

(a) The single trimer partition function is then

$$\zeta = \sum_\alpha e^{-\beta E_\alpha} = 2\, e^{3\beta J} \cosh(3\beta\mu_0\mathsf{H}) + 6\, e^{-\beta J} \cosh(\beta\mu_0\mathsf{H}) \ .$$

(b) The magnetization is

$$m = \frac{1}{\beta\zeta}\frac{\partial\zeta}{\partial\mathsf{H}} = 3\mu_0 \cdot \left(\frac{e^{3\beta J}\sinh(3\beta\mu_0\mathsf{H}) + e^{-\beta J}\sinh(\beta\mu_0\mathsf{H})}{e^{3\beta J}\cosh(3\beta\mu_0 J) + 3\, e^{-\beta J}\cosh(\beta\mu_0\mathsf{H})} \right)$$

(c) Expanding $m(T, \mathsf{H})$ to lowest order in H, we have

$$m = 3\beta\mu_0^2\,\mathsf{H} \cdot \left(\frac{3\, e^{3\beta J} + e^{-\beta J}}{e^{3\beta J} + 3\, e^{-\beta J}} \right) + \mathcal{O}(\mathsf{H}^3) \ .$$

Thus,

$$\chi(T) = \frac{N_\triangle}{V} \cdot \frac{3\mu_0^2}{k_B T} \cdot \left(\frac{3\, e^{3J/k_B T} + e^{-J/k_B T}}{e^{3J/k_B T} + 3\, e^{-J/k_B T}} \right) .$$

(d) Note that

$$F = \frac{1}{\beta} \ln Z \quad , \quad E = \frac{\partial \ln Z}{\partial \beta} .$$

Thus,

$$S = \frac{E - F}{T} = k_B \left(\ln Z - \beta\, \frac{\partial \ln Z}{\partial \beta} \right) = N_\triangle k_B \left(\ln \zeta - \beta\, \frac{\partial \ln \zeta}{\partial \beta} \right) .$$

So the entropy is

$$\begin{aligned} S(T, \mathsf{H}, N_\triangle) &= N_\triangle k_B \ln \Big(2\, e^{3\beta J} \cosh(3\beta\mu_0 \mathsf{H}) + 6\, e^{-\beta J} \cosh(\beta\mu_0 \mathsf{H}) \Big) \\ &\qquad - 6 N_\triangle \beta J k_B \cdot \left(\frac{e^{3\beta J} \cosh(3\beta\mu_0 \mathsf{H}) - e^{-\beta J} \cosh(\beta\mu_0 \mathsf{H})}{2\, e^{3\beta J} \cosh(3\beta\mu_0 \mathsf{H}) + 6\, e^{-\beta J} \cosh(\beta\mu_0 \mathsf{H})} \right) \\ &\qquad\quad - 6 N_\triangle \beta \mu_0 \mathsf{H} k_B \cdot \left(\frac{e^{3\beta J} \sinh(3\beta\mu_0 \mathsf{H}) + e^{-\beta J} \sinh(\beta\mu_0 \mathsf{H})}{2\, e^{3\beta J} \cosh(3\beta\mu_0 \mathsf{H}) + 6\, e^{-\beta J} \cosh(\beta\mu_0 \mathsf{H})} \right) . \end{aligned}$$

Setting $\mathsf{H} = 0$ we have

$$\begin{aligned} S(T, \mathsf{H} = 0, N_\triangle) &= N_\triangle k_B \ln 2 + N_\triangle k_B \ln \big(1 + 3\, e^{-4J/k_B T} \big) + \frac{N_\triangle J}{T} \cdot \left(\frac{12\, e^{-4J/k_B T}}{1 + 3\, e^{-4J/k_B T}} \right) \\ &= N_\triangle k_B \ln 6 + N_\triangle k_B \ln \big(1 + \tfrac{1}{3}\, e^{4J/k_B T} \big) - \frac{N_\triangle J}{T} \cdot \left(\frac{4\, e^{4J/k_B T}}{3 + e^{4J/k_B T}} \right) . \end{aligned}$$

(e) Note that for $J = 0$ we have $m = 3\mu_0^2 \mathsf{H}/k_B T$, corresponding to three independent Ising spins. The $\mathsf{H} = 0$ entropy is then $N_\triangle k_B \ln 8 = 3 N_\triangle k_B \ln 2$, as expected. As $J \to +\infty$ we have $m = 9\mu_0^2\, \mathsf{H}/k_B T = (3\mu_0)^2 \mathsf{H}/k_B T$, and each trimer acts as a single $\mathbb{Z}_2$ Ising spin, but with moment $3\mu_0$. The zero field entropy in this limit tends to $N_\triangle k_B \ln 2$, again corresponding to a single $\mathbb{Z}_2$ Ising degree of freedom per trimer. For $J \to -\infty$, we have $m = \mu_0^2\, \mathsf{H}/k_B T$ and $S = N_\triangle k_B \ln 6$. This is because the only allowed (*i.e.* finite energy) states of each trimer are the three states with magnetization $+\mu_0$ and the three states with magnetization $-\mu_0$, all of which are degenerate at $\mathsf{H} = 0$.

(2) The potential energy density for an isotropic elastic solid is given by

$$\begin{aligned} \mathcal{U}(\boldsymbol{x}) &= \mu\, \mathsf{Tr}\, \varepsilon^2 + \tfrac{1}{2}\lambda\, (\mathsf{Tr}\, \varepsilon)^2 \\ &= \mu \sum_{\alpha,\beta} \varepsilon_{\alpha\beta}^2(\boldsymbol{x}) + \tfrac{1}{2}\lambda \Big(\sum_\alpha \varepsilon_{\alpha\alpha}(\boldsymbol{x}) \Big)^2 , \end{aligned}$$

where μ and λ are the Lamé parameters and

$$\varepsilon_{\alpha\beta} = \frac{1}{2} \left(\frac{\partial u^\alpha}{\partial x^\beta} + \frac{\partial u^\beta}{\partial x^\alpha} \right) ,$$

with $\boldsymbol{u}(\boldsymbol{x})$ the local displacement field, is the *strain tensor*. The Cartesian indices α and β run over x, y, z. The kinetic energy density is

$$\mathcal{T}(\boldsymbol{x}) = \tfrac{1}{2}\rho\,\dot{\boldsymbol{u}}^2(\boldsymbol{x}) \ .$$

(a) Assume periodic boundary conditions, and Fourier transform to wavevector space,

$$\begin{aligned} u^\alpha(\boldsymbol{x},t) &= \tfrac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} \hat{u}^\alpha_{\boldsymbol{k}}(t)\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \\ \hat{u}^\alpha_{\boldsymbol{k}}(t) &= \tfrac{1}{\sqrt{V}} \int\! d^3\!x\, u^\alpha(\boldsymbol{x},t)\, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \ . \end{aligned}$$

Write the Lagrangian $L = \int\! d^3\!x\, \big(\mathcal{T} - \mathcal{U}\big)$ in terms of the generalized coordinates $\hat{u}^\alpha_{\boldsymbol{k}}(t)$ and generalized velocities $\dot{\hat{u}}^\alpha_{\boldsymbol{k}}(t)$.

(b) Find the Hamiltonian H in terms of the generalized coordinates $\hat{u}^\alpha_{\boldsymbol{k}}(t)$ and generalized momenta $\hat{\pi}^\alpha_{\boldsymbol{k}}(t)$.

(c) Find the thermodynamic average $\langle \boldsymbol{u}(0)\cdot\boldsymbol{u}(\boldsymbol{x})\rangle$.

(d) Suppose we add in a nonlocal interaction of the strain field of the form

$$\Delta U = \tfrac{1}{2}\int\! d^3\!x \int\! d^3\!x'\ \mathsf{Tr}\,\varepsilon(\boldsymbol{x})\ \mathsf{Tr}\,\varepsilon(\boldsymbol{x}')\ v(\boldsymbol{x}-\boldsymbol{x}') \ .$$

Repeat parts (b) and (c).

Solution : To do the mode counting we are placing the system in a box of dimensions $L_x \times L_y \times L_z$ and imposing periodic boundary conditions. The allowed wavevectors $\boldsymbol{k}$ are of the form

$$\boldsymbol{k} = \bigg(\frac{2\pi n_x}{L_x} \, , \, \frac{2\pi n_y}{L_y} \, , \, \frac{2\pi n_z}{L_z} \bigg) \ .$$

We shall repeatedly invoke the orthogonality of the plane waves:

$$\int\limits_0^{L_x}\!\! dx \int\limits_0^{L_y}\!\! dy \int\limits_0^{L_z}\!\! dz\ e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{x}} = V\,\delta_{\boldsymbol{k},\boldsymbol{k}'} \ ,$$

where $V = L_x L_y L_z$ is the volume. When we Fourier decompose the displacement field, we must take care to note that $\hat{u}^\alpha_{\boldsymbol{k}}$ is complex, and furthermore that $\hat{u}^\alpha_{-\boldsymbol{k}} = \big(\hat{u}^\alpha_{\boldsymbol{k}}\big)^*$, since $u^\alpha(\boldsymbol{x})$ is a real function.

(a) We then have

$$T = \int\limits_{-\infty}^{\infty}\!\! dx\ \tfrac{1}{2}\rho\,\dot{\boldsymbol{u}}^2(\boldsymbol{x},t) = \tfrac{1}{2}\rho \sum_{\boldsymbol{k}} \big|\dot{\hat{u}}^\alpha_{\boldsymbol{k}}(t)\big|^2$$

and

$$U = \int_{-\infty}^{\infty} \!dx \left[\tfrac{1}{2}\mu \, \frac{\partial u^\alpha}{\partial x^\beta} \, \frac{\partial u^\alpha}{\partial x^\beta} + \tfrac{1}{2}(\lambda+\mu) \, (\boldsymbol{\nabla}\!\cdot\!\boldsymbol{u})^2 \right]$$

$$= \tfrac{1}{2} \sum_{\boldsymbol{k}} \Big(\mu \, \delta^{\alpha\beta} + (\lambda+\mu) \, \hat{k}^\alpha \, \hat{k}^\beta \Big) \, \boldsymbol{k}^2 \, \hat{u}^\alpha_{\boldsymbol{k}}(t) \, \hat{u}^\beta_{-\boldsymbol{k}}(t) \ .$$

The Lagrangian is of course $L = T - U$.

(b) The momentum $\hat{\pi}^\alpha_{\boldsymbol{k}}$ conjugate to the generalized coordinate $\hat{u}^\alpha_{\boldsymbol{k}}$ is

$$\hat{\pi}^\alpha_{\boldsymbol{k}} = \frac{\partial L}{\partial \dot{\hat{u}}^\alpha_{\boldsymbol{k}}} = \rho \, \dot{\hat{u}}^\alpha_{-\boldsymbol{k}} \ ,$$

and the Hamiltonian is

$$H = \sum_{\boldsymbol{k}} \hat{\pi}^\alpha_{\boldsymbol{k}} \, \dot{\hat{u}}^\alpha_{\boldsymbol{k}} - L$$

$$= \sum_{\boldsymbol{k}} \left\{ \frac{\big|\hat{\pi}^\alpha_{\boldsymbol{k}}\big|^2}{2\rho} + \tfrac{1}{2} \Big[\mu \, \big(\delta^{\alpha\beta} - \hat{k}^\alpha \, \hat{k}^\beta \big) + (\lambda + 2\mu) \, \hat{k}^\alpha \, \hat{k}^\beta \Big] \boldsymbol{k}^2 \, \hat{u}^\alpha_{\boldsymbol{k}} \, \hat{u}^\beta_{-\boldsymbol{k}} \right\} .$$

Note that we have added and subtracted a term $\mu \, \hat{k}^\alpha \, \hat{k}^\beta$ within the expression for the potential energy. This is because $\mathbb{P}_{\alpha\beta} = \hat{k}^\alpha \, \hat{k}^\beta$ and $\mathbb{Q}_{\alpha\beta} = \delta^{\alpha\beta} - \hat{k}^\alpha \, \hat{k}^\beta$ are *projection operators* satisfying $\mathbb{P}^2 = \mathbb{P}$ and $\mathbb{Q}^2 = \mathbb{Q}$, with $\mathbb{P} + \mathbb{Q} = \mathbb{I}$, the identity. $\mathbb{P}$ projects any vector onto the direction $\hat{\boldsymbol{k}}$, and $\mathbb{Q}$ is the projector onto the (two-dimensional) subspace orthogonal to $\hat{\boldsymbol{k}}$.

(c) We can decompose $\hat{\boldsymbol{u}}_{\boldsymbol{k}}$ into a *longitudinal* component parallel to $\hat{\boldsymbol{k}}$ and a *transverse* component perpendicular to $\hat{\boldsymbol{k}}$, writing

$$\hat{\boldsymbol{u}}_{\boldsymbol{k}} = i\hat{\boldsymbol{k}} \, \hat{u}^{\parallel}_{\boldsymbol{k}} + i\hat{\boldsymbol{e}}_{\boldsymbol{k},1} \, \hat{u}^{\perp,1}_{\boldsymbol{k}} + i\hat{\boldsymbol{e}}_{\boldsymbol{k},2} \, \hat{u}^{\perp,2}_{\boldsymbol{k}} \ ,$$

where $\{\hat{\boldsymbol{e}}_{\boldsymbol{k},1} \, , \, \hat{\boldsymbol{e}}_{\boldsymbol{k},2} \, , \, \hat{\boldsymbol{k}}\}$ is a right-handed orthonormal triad for each direction $\hat{\boldsymbol{k}}$. A factor of i is included so that $\hat{u}^{\parallel}_{-\boldsymbol{k}} = \big(\hat{u}^{\parallel}_{\boldsymbol{k}}\big)^*$, *etc.* With this decomposition, the potential energy takes the form

$$U = \tfrac{1}{2} \sum_{\boldsymbol{k}} \Big[\mu \, \boldsymbol{k}^2 \, \Big(\big|\hat{u}^{\perp,1}_{\boldsymbol{k}}\big|^2 + \big|\hat{u}^{\perp,2}_{\boldsymbol{k}}\big|^2 \Big) + (\lambda + 2\mu) \, \boldsymbol{k}^2 \, \big|\hat{u}^{\parallel}_{\boldsymbol{k}}\big|^2 \Big] \ .$$

Equipartition then means each independent degree of freedom which is quadratic in the potential contributes an average of $\frac{1}{2}k_{\rm B}T$ to the total energy. Recalling that $u^{\parallel}_{\boldsymbol{k}}$ and $u^{\perp,j}_{\boldsymbol{k}}$ ($j = 1, 2$) are complex functions, and that they are each the Fourier transform of a real function (so that $\boldsymbol{k}$ and $-\boldsymbol{k}$ terms in the sum for U are equal), we have

$$\Big\langle \mu \, \boldsymbol{k}^2 \, \big|\hat{u}^{\perp,1}_{\boldsymbol{k}}\big|^2 \Big\rangle = \Big\langle \mu \, \boldsymbol{k}^2 \, \big|\hat{u}^{\perp,2}_{\boldsymbol{k}}\big|^2 \Big\rangle = 2 \times \tfrac{1}{2} k_{\rm B} T$$

$$\Big\langle (\lambda + 2\mu) \, \boldsymbol{k}^2 \, \big|\hat{u}^{\parallel}_{\boldsymbol{k}}\big|^2 \Big\rangle = 2 \times \tfrac{1}{2} k_{\rm B} T \ .$$

Thus,

$$\begin{aligned}\big\langle |\hat{\boldsymbol{u}}_{\boldsymbol{k}}|^2\big\rangle &= 4\times\tfrac{1}{2}k_{\rm B}T\times\frac{1}{\mu\boldsymbol{k}^2}+2\times\tfrac{1}{2}k_{\rm B}T\times\frac{1}{(\lambda+2\mu)\,\boldsymbol{k}^2}\\ &=\bigg(\frac{2}{\mu}+\frac{1}{\lambda+2\mu}\bigg)\frac{k_{\rm B}T}{\boldsymbol{k}^2}\ .\end{aligned}$$

Then

$$\begin{aligned}\big\langle \boldsymbol{u}(0)\cdot\boldsymbol{u}(\boldsymbol{x})\big\rangle &= \frac{1}{V}\sum_{\boldsymbol{k}}\big\langle |\hat{\boldsymbol{u}}_{\boldsymbol{k}}|^2\big\rangle\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\\ &=\int\!\frac{d^3\!k}{(2\pi)^3}\,\bigg(\frac{2}{\mu}+\frac{1}{\lambda+2\mu}\bigg)\frac{k_{\rm B}T}{\boldsymbol{k}^2}\,e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\\ &=\bigg(\frac{2}{\mu}+\frac{1}{\lambda+2\mu}\bigg)\frac{k_{\rm B}T}{4\pi|\boldsymbol{x}|}\ .\end{aligned}$$

Recall that in three space dimensions the Fourier transform of $4\pi/\boldsymbol{k}^2$ is $1/|\boldsymbol{x}|$.

(d) The $\boldsymbol{k}$-space representation of ΔU is

$$\Delta U=\tfrac{1}{2}\sum_{\boldsymbol{k}}\boldsymbol{k}^2\,\hat{v}(\boldsymbol{k})\,\hat{k}^\alpha\,\hat{k}^\beta\,\hat{u}^\alpha_{\boldsymbol{k}}\,\hat{u}^\beta_{-\boldsymbol{k}}\ ,$$

where $\hat{v}(\boldsymbol{k})$ is the Fourier transform of the interaction $v(\boldsymbol{x}-\boldsymbol{x}')$:

$$\hat{v}(\boldsymbol{k})=\!\int\!\!d^3\!r\;v(\boldsymbol{r})\,e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\ .$$

We see then that the effect of ΔU is to replace the Lamé parameter λ with the $\boldsymbol{k}$-dependent quantity,

$$\lambda\to\lambda(\boldsymbol{k})\equiv\lambda+\hat{v}(\boldsymbol{k})\ .$$

With this simple replacement, the results of parts (b) and (c) retain their original forms, *mutatis mutandis*.