Ex 5958: Mean field approximation for the Model of ferroelectricity

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The problem:

Model of ferroelectricity: Consider electric dipoles $\mathbf{p}$ on sites of a simple cubic lattice which point along one of the crystal axes, $\pm\langle 100\rangle$. The interaction between dipoles is

$$U = \frac{\mathbf{p}_1 \cdot \mathbf{p}_2 - 3(\mathbf{p}_1 \cdot \mathbf{r})(\mathbf{p}_2 \cdot \mathbf{r})/r^2}{4\pi\epsilon_0 r^3}$$

where $\mathbf{r}$ is the distance between the dipoles, $r = |\mathbf{r}|$ and ϵ_0 is the dielectric constant.

(a) Assume nearest neighbour interactions and find the ground state configuration. Consider either ferroelectric (parallel dipoles) or anti-ferroelectric alignment (anti-parallel) between neighbours in various directions.

(b) Develop a mean field theory for the ordering in (a) for the average polarization P at a given site at temperature T: Write a mean field equation for $P(T)$ and find the critical temperature T_c.

(c) Find the susceptibility $\chi = \left(\frac{\partial P}{\partial E}\right)_{E=0}$ at $T > T_c$ for an electric field $E||\langle 100\rangle$, using the mean field theory.

The solution:

(a)

$$U = \frac{p_i \cdot p_j - 3(p_i \cdot r_{ij})(p_j \cdot r_{ij})/r_{ij}^2}{4\pi\epsilon_0 r^3} \tag{1}$$

For $r_{ij}||p_i, p_j$ which mean's that $r_{ij}||\hat{x}$ we get:

$$U_{ij} = \frac{-2p_i \cdot p_j}{4\pi\epsilon_0 r^3} \tag{2}$$

The lowest enrgy is when $p_i = p_j$ so that $U_{ij} = -2U_0$ where $U_0 = \frac{p^2}{4\pi\epsilon_0 r^3}$

For $r_{ij} \perp p_i, p_j$ which mean's that $r_{ij} \perp \hat{x}$ we get:

$$U_{ij} = \frac{+p_i \cdot p_j}{4\pi\epsilon_0 r^3} \tag{3}$$

So $p_i = -p_j$ (in opposite direction),which mean's that $U_{ij} = -U_0$

The ground state:

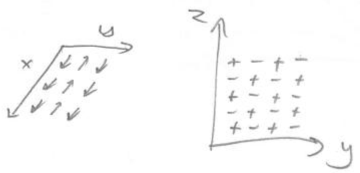

FIG.1 **We have a chain in $\hat{x}$ direction as each chain four different neighboring chains with opposite polarity.**

(b) Lets define two sublattice:
A=positive moment +, which means that y+z=even.
B=negative moment -, which means that y+z=odd.
we get the Hamiltonian:

$$
\begin{aligned}
H &= -2U_o \sum_{i\in A, j\in A}^{r_{ij}||\hat{x}} \frac{p_i \cdot p_j}{p^2} + U_o \sum_{i\in A, j\in B}^{r_{ij}||\hat{y}} \frac{p_i \cdot p_j}{p^2} + U_o \sum_{i\in A, j\in B}^{r_{ij}||\hat{z}} \frac{p_i \cdot p_j}{p^2} - E_{elctric} \sum_{i\in A, i\in B} p_i \\
&= -2U_o \sum_{i\in B, j\in B}^{r_{ij}||\hat{x}} \frac{p_i \cdot p_j}{p^2} + 2U_o \sum_{i\in B, j\in A}^{r_{ij}||\hat{y},\hat{z}} \frac{p_i \cdot p_j}{p^2} - E_{el} \sum_{i\in A} p_i - E_{el} \sum_{i\in B} p_i \qquad (4)
\end{aligned}
$$

we make a mean field approximation (not curfully) to get:

$$
H_A = -2U_o P_A \sum_{i\in A} \frac{p_i}{p^2} + 2U_o P_B \sum_{i\in A} \frac{p_i}{p^2} - E_{el} \sum_{i\in A} p_i \qquad (5)
$$

$$
H_B = -2U_o P_B \sum_{i\in B} \frac{p_i}{p^2} + 2U_o P_A \sum_{i\in B} \frac{p_i}{p^2} - E_{el} \sum_{i\in B} p_i \qquad (6)
$$

$H = H_A + H_B$ to find the enrgy for one site .we took $p_A = -p_B$ (in opossite direction)

$$
E = \frac{1}{2}\left(-2U_0 \frac{P^2}{P^2} + 2U_0 \frac{P_B(P_A)}{P^2} - E_{el} P_A - 2U_0 \frac{P^2}{P^2} + 2U_0 \frac{P_A(P_B)}{P^2} - E_{el} P_B\right)
$$
$$
\Rightarrow \quad E = -4U_o \qquad (7)
$$

In zero filed we look at average filed P_{av}

$$
H^{MF}_{E=0} = -4U_0 P_{av} \frac{p_i}{p^2} \qquad (8)
$$

$$
P_{av} = \frac{+pe^{\beta 4U_0 \frac{P_{av}}{p}} - pe^{-\beta 4U_0 \frac{P_{av}}{p}}}{e^{\beta 4U_0 \frac{P_{av}}{p}} + e^{-\beta 4U_0 \frac{P_{av}}{p}}} = p \tanh\left(\beta 4U_0 \frac{P_{av}}{p}\right) \qquad (9)
$$

To find T_c we take the first order in $\tanh\left(\beta 4U_0 \frac{P_{av}}{p}\right)$

$$
\frac{P_{av}}{p} = Tanh(\beta 4U_0 \frac{P_{av}}{p}) \quad \rightarrow \quad \frac{P_{av}}{p} = \beta 4U_0 \frac{P_{av}}{p} \quad \Rightarrow T_c = 4U_0 \qquad (10)
$$

To see the behaviour near the critical temperature:

$$\beta 4U_0 \frac{P_{av}}{p} = Tanh^{-1}(\frac{P_{av}}{p}) \cong \frac{P_{av}}{p} + \frac{(\frac{P_{av}}{p})^3}{3} \rightarrow \quad 3(\frac{T_c}{T} - 1) = (\frac{P_{av}}{p})^2 \tag{11}$$

(c) To Find the susceptibility $\chi = \left(\frac{\partial P}{\partial E}\right)_{E=0}$ at $T > T_c$. we take first order in Taylor Series for $tanh^{-1}(x)$

$$\begin{aligned} P_A &= p \tanh\left(\beta 2U_0 \frac{P_A}{p} - \beta 2U_0 \frac{P_B}{p} + \beta E p\right) \\ P_B &= p \tanh\left(\beta 2U_0 \frac{P_B}{p} - \beta 2U_0 \frac{P_A}{p} + \beta E p\right) \end{aligned} \tag{12}$$

$$\begin{aligned} \tanh^{-1}\left(\frac{P_A}{p}\right) &= \beta 2U_0 \frac{P_A}{p} - \beta 2U_0 \frac{P_B}{p} + \beta E p \\ \tanh^{-1}\left(\frac{P_B}{p}\right) &= \beta 2U_0 \frac{P_B}{p} - \beta 2U_0 \frac{P_A}{p} + \beta E p \\ \rightarrow \frac{P_A}{p} &= \beta 2U_0 \frac{P_A}{p} - \beta 2U_0 \frac{P_B}{p} + \beta E p \\ \rightarrow \frac{P_B}{p} &= \beta 2U_0 \frac{P_B}{p} - \beta 2U_0 \frac{P_A}{p} + \beta E p \end{aligned} \tag{13}$$

$$P = \frac{N}{2}(P_A + P_B) \quad \Rightarrow \qquad P = N\beta E p^2 \tag{14}$$

$$\chi = \frac{\partial P}{\partial E}|_{E=0} = N\beta p^2 \tag{15}$$