

TFY4245/FY8917 Solid State Physics, Advanced Course

NTNU

Problemset 6



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SUGGESTED SOLUTION

Problem 1, part I

(a) Taking the left edge of the shell as the origin $x = 0$, we have an ion with charge -1 at position $a/4$ and an ion with charge $+1$ at position $3a/4$. So the polarization, or dipole moment per unit length, is:

$$\begin{aligned}
 p &= \frac{1}{a} \sum_i q_i x_i \\
 &= \frac{1}{a} (-1 \times 1/4 + 1 \times 3a/4) \\
 &= \frac{1}{2}.
 \end{aligned} \tag{1}$$

(b) Again taking the left edge of the unit cell as the origin, this time there is a positively charged ion at position $a/4$, and a negatively charged ion at $3a/4$. So

$$\begin{aligned}
 p &= \frac{1}{a} (+1 \times 1/4 - 1 \times 3a/4) \\
 &= -\frac{1}{2}.
 \end{aligned} \tag{2}$$

Again a non-zero value, and this time different from the value we obtained using the other, equally valid unit cell, by an amount a .

Problem 1, part II

(a) For the left unit cell (with the edge at $x = 0$), we get

$$\begin{aligned}
 p &= \frac{1}{a} \sum_i q_i x_i \\
 &= \frac{1}{a} [-1 \times a/4 + 1 \times (3a/4 + d)] \\
 &= \frac{1}{2} + \frac{d}{a}.
 \end{aligned} \tag{3}$$

For the right, following the same procedure

$$\begin{aligned}
 p &= \frac{1}{a} [+1 \times (a/4 + d) - 1 \times 3a/4] \\
 &= -\frac{1}{2} + \frac{d}{a}.
 \end{aligned} \tag{4}$$

They differ by exactly one polarization quantum.

(b) Again the two answers are different in (a), but this time that does not worry us, because we recognize that they differ by exactly one polarization quantum. Next comes the key point. Let us

calculate the change in polarization δp between the polar and non-polar chains using each unit cell as our basis. First for the cell on the left,

$$\delta p = \left(\frac{1}{2} + \frac{d}{a}\right) - \frac{1}{2} = \frac{d}{a}. \quad (5)$$

For the cell on the right,

$$\delta p = -\left(-\frac{1}{2} + \frac{d}{a}\right) - \left(-\frac{1}{2}\right) = \frac{d}{a}. \quad (6)$$

In both cases the change in polarization between polar and non-polar chains is the same.

Problem 2

(a) The coefficient in front of the largest term kept in the expansion must always be positive (in this case, sixth order) to ensure that the free energy is bounded from below. So we know that $g_6 > 0$.

If we had kept only terms up to and including fourth order, we know that the phase transition is of second order if $g_4 > 0$, given that g_2 can become negative at some temperature. Adding a $g_6 > 0$ term to this expansion does not change anything qualitatively: the transition remains second order. Therefore, $g_4 < 0$ is a requirement to get a first order phase transition.

(b) The equilibrium condition for P is found by $\partial F / \partial P = 0$. This gives (at $E = 0$):

$$\gamma(T - T_0) - |g_4|P^2 + g_6P^4 = 0. \quad (7)$$

This also holds at $T = T_c$ for $P = P(T_c)$.

(c) At the critical temperature, the free energy of the state with polarization is equal to the free energy of the state without polarization. Hence:

$$F[P(T_c), T_c] = F(0, T_c). \quad (8)$$

(d) Let $P_s = P(T_c)$. Then we have

$$\begin{aligned} \gamma(T_c - T_0) - |g_4|P_s^2 + g_6P_s^4 &= 0, \\ \frac{1}{2}\gamma(T_c - T_0)P_s^2 - \frac{1}{4}|g_4|P_s^4 + \frac{1}{6}g_6P_s^6 &= 0. \end{aligned} \quad (9)$$

Eliminating $\gamma(T_c - T_0)$ from the equations gives

$$-|g_4|P_s^2 + g_6P_s^4 = -\frac{1}{2}|g_4|P_s^2 + \frac{1}{3}g_6P_s^4 \quad (10)$$

which is solved by

$$P_s = P(T_c) = \sqrt{\frac{3|g_4|}{4g_6}}. \quad (11)$$