Physics 212 – Problem Set # 4

(due Friday, October 28)

1. This problem analyzes a simple model of a crystal with structural phase transitions. Here is the situation: A crystal with atoms on a cubic lattice can have an instability toward lengthening the $\hat{x}$ or the $\hat{y}$ crystal axis. (I omit $\hat{z}$ for simplicity.) Let d_x and d_y represent the extensions of the lattice in the $\hat{x}$ and $\hat{y}$ directions. These are the order parameters. Assume that the symmetry of the original crystal is D_4, the group of rotations about the $\hat{z}$ axis by $\pi/2$ plus reflections in the $\hat{x}$ or $\hat{y}$ axis.

   (a) To construct the Landau theory, we first construct the quadratic terms. Show that the most general set of quadratic terms in the Landau theory consistent with the symmetry is

   $$G = \int d^3x \left\{ \frac{1}{2}((\vec{\nabla} d_x)^2 + (\vec{\nabla} d_y)^2) + \frac{1}{2}A(T)(d_x^2 + d_y^2) \right\} \tag{1}$$

   (b) At quartic order, there are two possible terms. I will write them

   $$G = (\text{above}) + \int d^3x \left\{ \frac{1}{4}B(d_x^2 + d_y^2)^2 + \frac{1}{2}C(d_x^2 d_y^2) \right\} \tag{2}$$

   Show that there are no other quartic terms allowed by the symmetry.

   (c) Show that G is stable at large values of (d_x, d_y) only if $B \geq 0$. Show that C can be negative consistent with stability. Find a lower bound on C assuming $B > 0$. Assume, from here on, that $B > 0$ and C is strictly greater than this lower bound.

   (d) Find the minima of this potential in the cases $A > 0$ and $A < 0$, in each case, for $C = 0$, $C > 0$, and $C < 0$.

   (e) Let

   $$A(T) = a(T - T_c) \tag{3}$$

   Show that T_c is a critical point below which expectation values of the order parameters d_x and d_y turn on.

   Assume, from here on, that $T < T_c$, so $A < 0$.

   (f) Consider first the case $C = 0$. Show that, for $T < T_c$, there are multiple degenerate possible thermodynamic states, of which

   $$\langle d_x \rangle > 0 \qquad \langle d_y \rangle = 0 \tag{4}$$

   is one possibility. For this choice, use Landau theory to compute $\langle d_x \rangle$ and to compute the correlation functions

   $$\langle d_x(x) d_x(y) \rangle \;, \qquad \langle d_x(x) d_y(y) \rangle \;, \qquad \langle d_y(x) d_y(y) \rangle \tag{5}$$

(g) For $C > 0$, show that only discrete states are allowed. Find these states. There is one such state satisfying eq. (4). For this state, compute $\langle d_x \rangle$ and the correlation functions in eq. (5).

(h) For $C < 0$, show that only discrete states are allowed. Find these states. There is one such state satisfying

$$\langle d_x \rangle > 0 \qquad \langle d_y \rangle > 0 \ , \tag{6}$$

For this state, compute $\langle d_x \rangle$ and $\langle d_y \rangle$ and the correlation functions in eq. (f).

(i) Let C in eq. (2) have the form

$$C(T) = c(T - T_*) \tag{7}$$

where $T_* < T_c$. Show that there is a second critical point at $T = T_*$ and describe its physics. Describe the behavior of the correlation functions in eq. (5) as one passes through this phase transition. In particular, how do the correlation lengths vary as T passes through T_*?

The type of structural phase transition described in part (i) can also occur as a result of adjusting other control parameters, such as the external pressure or the concentration of component elements.