Tutorial 5

1. Charge Density Waves

a) Describe in your own words: What is a Peierls instability and what are the ingredients?

b) In the lecture, we introduced the Lindhard response function

$$\chi(q) = \int \frac{d\boldsymbol{k}}{(2\pi)^d} \frac{f(\boldsymbol{k}) - f(\boldsymbol{k}+\boldsymbol{q})}{\varepsilon(\boldsymbol{k}) - \varepsilon(\boldsymbol{k}+\boldsymbol{q})}$$

Calculate $\chi(\boldsymbol{q})$ for 1 and 3 dimensions for a simple dispersion $\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{N_0\pi}{2L}\right)^2 = \frac{\hbar^2 k_F^2}{2m_e}$. Compare your result with the graph shown in the lecture. Assume low temperatures. Plot for both cases $\chi(q)/\chi(0)$. [Hint I: remember that the Fermi functions act like a cutoff function at the Fermi level. Hint II: rescale the boundaries of the integral and look up the expression].

c) In the lecture we introduced the reduced frequency of phonon modes

$$\omega_{ren,2k_F}^2 = \omega_{2k_F}^2 - \frac{g^2 n(\varepsilon_F)\omega_{2k_F}}{\hbar} \cdot ln\left(\frac{1.14\epsilon_0}{k_B T}\right)$$

The critical exponent for $\omega_{ren,2k_F}(T)$ approaching T_{CDW} is resulting from this is (Gruener, p. 36)

$$\omega_{\text{ren},2k_F} = \omega_{2k_F}\left(\frac{T - T_{\text{CDW}}^{\text{MF}}}{T_{\text{CDW}}^{\text{MF}}}\right)^{1/2}$$

The figure shows a measurement of the phonon dispersion in ZrTe3 [Hoesch et al., PRL 102, 086402 (2009)]. What phenomenon is seen here? How is it measured? What information can you deduce from the figure? How is this discussed in the paper?

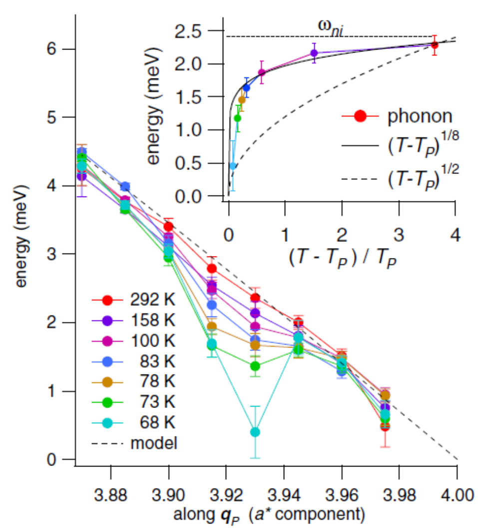

FIG. 2 (color online). Phonon dispersion from $(40\bar{1})$ in the direction of $\vec{q}_P$ at various temperatures $T > T_P$ above the transition. The inset shows the phonon energy $\hbar\omega_q$ at $\vec{q}_P$ as a function of reduced temperature $(T - T_P)/T_P$. The solid and dashed lines represent a 1/8 and a 1/2 power law, respectively.

discussion date: January 16th

2. Phase Transitions I

1. Consider a Landau expansion of the free energy of the form

$$F = \frac{a}{2}m^2 + \frac{b}{4}m^4 + \frac{c}{6}m^6$$

with $c > 0$. Examine the phase diagram in the $a - b$ plane, and show that there is a line of critical transitions $a = 0$, $b > 0$ which joins a line of first order transitions $b = -4(ca/3)^{1/2}$ at a point $a = b = 0$ known as a tricritical point.

Supposing that a varies linearly with temperature and that b is independent of temperature, compare the value of the exponent β at the tricritical point with its value on the critical line.

From Yeomans, *Statistical Mechanics of Phase Transitions*

3. Phase Transitions II

2. Consider a system with a modified expression for the Landau free energy, namely

$$\psi_h(t,m) = -hm + q(t) + r(t)m^2 + s(t)m^4 + u(t)m^6,$$

with $u(t)$ a fixed positive constant. Minimize ψ with respect to the variable m and examine the spontaneous magnetization m_0 as a function of the parameters r and s. In particular, show the following:[21]

(a) For $r > 0$ and $s > -(3ur)^{1/2}, m_0 = 0$ is the only real solution.

(b) For $r > 0$ and $-(4ur)^{1/2} < s \leq -(3ur)^{1/2}, m_0 = 0$ or $\pm m_1$, where $m_1^2 = \frac{\sqrt{(s^2-3ur)}-s}{3u}$. However, the minimum of ψ at $m_0 = 0$ is lower than the minima at $m_0 = \pm m_1$, so the ultimate equilibrium value of m_0 is 0.

(c) For $r > 0$ and $s = -(4ur)^{1/2}, m_0 = 0$ or $\pm(r/u)^{1/4}$. Now, the minimum of ψ at $m_0 = 0$ is of the same height as the ones at $m_0 = \pm(r/u)^{1/4}$, so a nonzero spontaneous magnetization is as likely to occur as the zero one.

[21] To fix ideas, it is helpful to use (r,s)-plane as our "parameter space."

(d) For $r > 0$ and $s < -(4ur)^{1/2},\ m_0 = \pm m_1$ — which implies a *first-order* phase transition (because the two possible states available here differ by a *finite* amount in m). The line $s = -(4ur)^{1/2}$, with r positive, is generally referred to as a "line of first-order phase transitions."

(e) For $r = 0$ and $s < 0,\ m_0 = \pm(2|s|/3u)^{1/2}$.

(f) For $r < 0,\ m_0 = \pm m_1$ for all s. As $r \to 0,\ m_1 \to 0$ if s is positive.

(g) For $r = 0$ and $s > 0,\ m_0 = 0$ is only solution. Combining this result with (f), we conclude that the line $r = 0$, with s positive, is a "line of second-order phase transitions," for the two states available here differ by a *vanishing* amount in m.

The lines of first-order phase transitions and second-order phase transitions meet at the point $(r = 0, s = 0)$, which is commonly referred to as a *tricritical point* (Griffiths, 1970).