

PHYS 551 Lecture #28

Title: Instabilities in the Electron Gas

Both the free electron gas and tight binding approximations give extreme limits in the various simplifications that are made in order to solve the Schrödinger equation in a periodic crystal potential. One might be tempted to be satisfied to solving these equations in the context of a rigid (or perhaps vibrating crystal) lattice. Even this is non-trivial since the *precise* form of the potential does not permit an exact solution. In addition, nature seldom does what is asked; for it is possible to observe numerous instabilities which give “new” physics in an “old” system.

One of the most straightforward of these instabilities occurs in quasi-one-dimensional conductors. It was discovered theoretically by R. E. Peierls in 1939 and it shows some of the subtlety between electrons and phonons in solids. (There are many others, such as the Jahn-Teller distortion.)

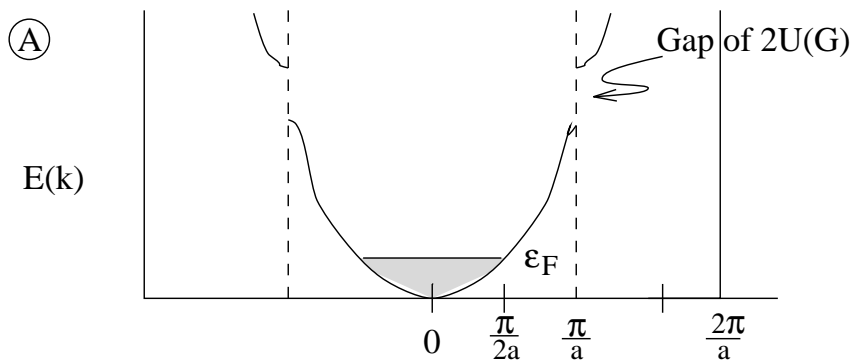
Recall for the FEG (free electron gas) that the form of $E(k)$ in the region $E \leq \frac{\pi}{a}$. (Recall $G = \frac{2\pi}{a}$

$$\begin{vmatrix} E - U_0 - \frac{\hbar^2}{2m} k^2 & -U(G) \\ -U(-G) & E - U_0 - \frac{\hbar^2}{2m} |\vec{k} - \vec{G}|^2 \end{vmatrix} = 0$$

or

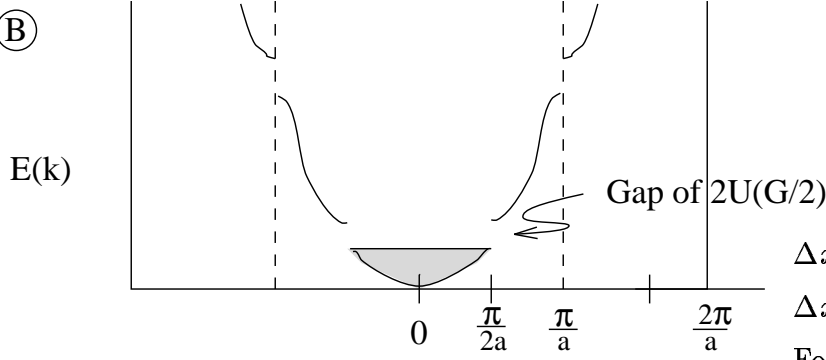
$$E(k) = U_0 + \frac{\hbar^2}{4m} [k^2 + |\vec{k} - \vec{G}|^2] \pm \frac{1}{2} \left[\left(\frac{\hbar^2}{2m} \right)^2 (|\vec{k} - \vec{G}|^2 - k^2)^2 + 4|U(G)|^2 \right]^{1/2}$$

Here, for a one-electron per unit cell lattice, there is a band gap at $2k_F$ or $\frac{\pi}{a}$.



Now suppose the lattice distorts to form a period structure $2a$.

(B)



$$\Delta x = \frac{\Delta}{2} \cos 2k_F x$$

$$\Delta x = \frac{\Delta}{2} \cos \frac{\pi x}{a}$$

$$\text{For } x = 0 \quad \Delta x = +\frac{\Delta}{2}$$

$$\text{For } x = a \quad \Delta x = -\frac{\Delta}{2} - 2a$$

$$\text{For } x = 2a \quad \Delta x = +\frac{\Delta}{2}$$

Notice for (A) $E_A = \int_0^{\epsilon_F} \epsilon \mathcal{D}(\epsilon) d\epsilon = \frac{n}{3} \epsilon_F$ (Ground State)

Since all (B) occupied states for $k \approx k_F$ have lowered their energy,

$$E_B = \int_0^{\epsilon_F - U(G/2)} \epsilon \mathcal{D}(\epsilon) d\epsilon < E_A.$$

Thus, this distortion should occur spontaneously. Since $k_F = \frac{\pi}{2a}$ and $d = 2\pi/G/2 = 2a$ is the real space periodity.

In this case

$$E(k) = U_0 + \frac{\hbar^2}{4m} \left[k^2 + \left| \vec{k} - \frac{\vec{G}}{2} \right|^2 \right] - \frac{1}{2} \left[\left(\frac{\hbar^2}{2m} \right)^2 \left(\left| \vec{k} - \frac{\vec{G}}{2} \right|^2 - k^2 \right)^2 + 4|U(G/2)|^2 \right]^{1/2}$$

Since we have $E(k)$, $E_{\text{electronic}} = \frac{L}{\pi} \int_0^{k_F} dk E(k)$, and let $A\Delta \equiv |U(G/2)|$ and $U_0 \equiv 0$

$$E_{\text{lowered}} = \frac{L}{\pi} \int_0^{k_F} dk \frac{\hbar^2 k^2}{2m} - \frac{L}{\pi} \int_0^{k_F} dk \left[\frac{\hbar^2}{2m} \left(k^2 - \frac{\pi k}{a} + \frac{\pi^2}{2a^2} \right) - \frac{1}{2} \left\{ \left(\frac{\hbar^2}{2m} \right)^2 \left(-\frac{\pi 2k}{a} + \frac{\pi^2}{a^2} \right)^2 + 4A^2 \Delta^2 \right\}^{1/2} \right]$$

$$\text{Now } k_F = \frac{\pi}{2a}$$

$$E_{\ell} = -\frac{L}{\pi} \int_0^{k_F} dk \left[\frac{\hbar^2}{2m} (-2k_F k + 2k_F^2) - \frac{1}{2} \left\{ \left(\frac{\hbar^2}{2m} \right)^2 (-4k_F k + 4k_F^2)^2 + 4A^2 \Delta^2 \right\}^{1/2} \right]$$

so

$$\frac{dE_{lowered}}{d\Delta} = +\frac{L}{\pi} \int_0^{k_F} \frac{A^2 \Delta}{\left(\left(\frac{\hbar^2}{m} \right)^2 (-k_F k + k_F^2)^2 + A^2 \Delta^2 \right)^{1/2}}$$

Let $k' = -k + k_F$

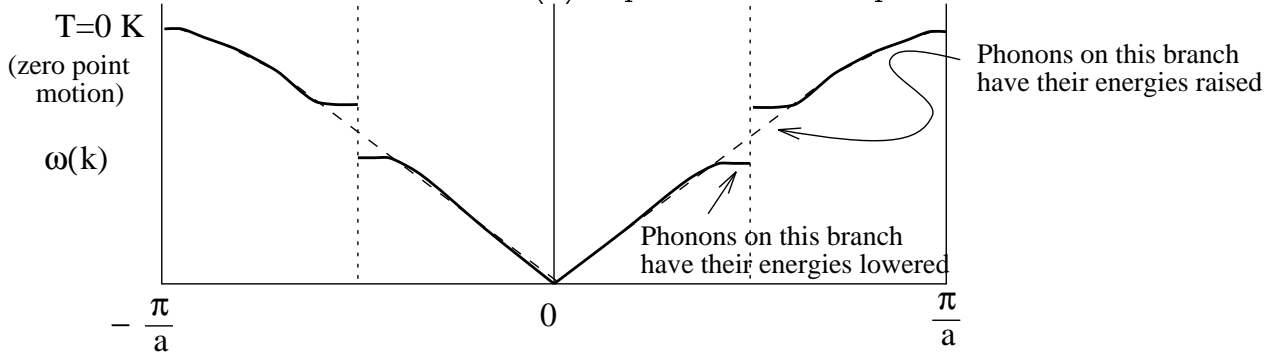
$$\frac{dE_\ell}{d\Delta} = +\frac{L}{\pi} \int_0^{k_F} \frac{dk' A^2 \Delta}{\left(\left(\frac{\hbar^2}{m} \right)^2 (k_F k')^2 + A^2 \Delta^2 \right)^{1/2}}$$

Let $\begin{aligned} x_F &= k_F^2 \frac{\hbar^2}{m} \\ \frac{x_F}{k_F} &= \frac{\hbar^2}{m k_F} \\ x &= k_F k' \frac{\hbar^2}{m} \\ dk' &= \frac{m dx}{k_F \hbar^2} \end{aligned}$

$$\frac{dE_\ell}{d\Delta} = \frac{A^2 \Delta L}{\pi} \int_0^{x_F} \frac{dx}{(x^2 + A^2 \Delta^2)^{1/2}} \frac{k_F}{x_F}$$

$$\frac{dE_\ell}{d\Delta} = \frac{A^2 \Delta L}{\pi} \frac{k_F}{x_F} \sinh^{-1} \left(\frac{x_F}{A \Delta} \right) \text{ for } E_{\text{initial}} - E_{\text{final}} \text{ from } E_{\text{electronic}}$$

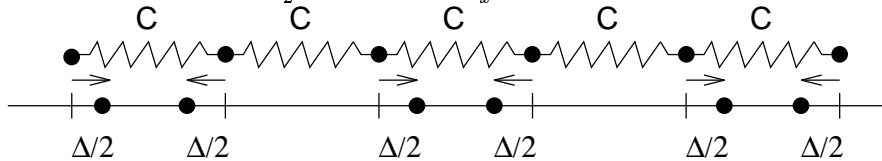
Now we must determine the consequence of this $2a$ distortion on E_{elastic} . Recall for a one-dimensional chain of atoms the $\omega(k)$ dispersion relationship.



In principle, we could calculate $E_{\text{elastic}} = \int_0^{\omega_{max}} \mathcal{D}(\omega) \hbar \omega < n >_\omega$

but it is easier (and equivalent at $T = 0$) to state that the change in energy is $\frac{1}{4} C \Delta^2$.

This is because $E_{\text{elastic}} = \frac{1}{2} C \Delta^2 < \cos^2 \frac{2k_F x}{x} >$



$$\begin{aligned} < \Delta E_{\text{elastic}} > &= \frac{1}{2} C \Delta^2 < \cos^2 2k_F x > \text{ for each "spring"} \\ &= \frac{1}{4} C \Delta^2 \end{aligned}$$

$$\text{So } \frac{d}{d\Delta} < \Delta E_{\text{elastic}} > = \frac{1}{2} C \Delta$$

To find equilibrium, the energy must be at a minimum with respect to Δ .

OR

$$\frac{1}{2} C \Delta - \left[\frac{A^2 m \Delta}{\pi \hbar^2 k_F} \sinh^{-1} \left(\frac{\hbar^2 k_F^2}{m A \Delta} \right) \right] = 0$$

$$\text{or} \quad \sinh^{-1} \left(\frac{\hbar^2 k_F^2}{m A \Delta} \right) = - \frac{\hbar^2 k_F \pi C}{2 m A^2}$$

$$\frac{\hbar^2 k_F^2}{m a \Delta} = \sinh \left(- \frac{\hbar^2 k_F \pi C}{2 m A^2} \right)$$

$$\text{or} \quad \frac{\hbar^2 k_F^2}{m a \Delta} \simeq \frac{1}{2} \exp(\hbar k_F \pi C / 2 m A^2)$$

$$A |\Delta| = \frac{2 \hbar^2 k_F^2}{m} \exp(-\hbar^2 k_F \pi C / 2 m A^2)$$

Notice $W = \frac{\hbar^2 k_F^2}{2m}$ is the band width and $m / \pi \hbar^2 k_F = \mathcal{D}(\epsilon_F)$

So $A |\Delta| = 4W \exp[-c / \mathcal{D}(\epsilon_F) 2A^2] \rightarrow A$ is hard to determine

Notice also the two possible *Ground States*. This leads to some very interesting electronic and structural properties.