II. 2. PEIERLS TRANSITION

Consider a one-dimensional chain (period a) of atoms. Each atom gives one electron to the conduction band, thus normally we expect that this chain is metallic. However, due to electron-phonon interaction, the atoms of the chain can rearrange themselves. Consider the following rearrangement (Fig. 2): Every second atom is displaced by u

from its equilibrium position. Obviously, this costs elastic energy due to atomic interactions; for low displacements, this energy is quadratic in u, $V_{el} = \alpha u^2/2$. On the other hand, there is also energy gain due to electron-electron interactions. In the second order perturbation theory (almost free electrons), calculate this energy gain and conclude whether the rearrangement occurs.

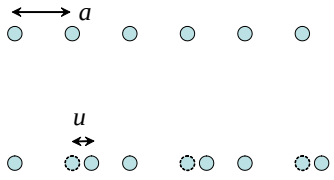

FIG. 2: Top: Unperturbed atomic chain. Bottom: The atomic rearrangement leading to a chain with a doubled lattice period.

In the unperturbed problem, the electrons are almost free, with the spectrum $E_0 = \hbar^2 k^2/(2m)$. The energy only deviates from this expression close to the points $k = \pi/a$, where the gap in the spectrum opens. In the ground state, all states below the Fermi energy are full. The Fermi energy lies at the middle of the band, since only one electron per atom is supplied. In one dimension, the "Fermi surface" consists of just two points, $k = \pm\pi/(2a)$.

If the atoms are rearranged, the period of the lattice doubles. Thus, at $k = \pi/(2a)$ the gap in the spectrum must open. In the free electron approximation, close to this point, one has

$$E(k) = \frac{E_0(k) + E_0(k - \pi/(2a))}{2} \pm \sqrt{\left(\frac{E_0(k) - E_0(k - \pi/(2a))}{2}\right)^2 + |V|^2} \,, \tag{3}$$

where V is the matrix element of the periodic atomic potential (after the rearrangement) calculated at $k = \pi/(2a)$. The signs $\pm$ corresponds to the states above and below the gap, respectively. But only the states below the gap are full. Due to the opening of the gap the total energy of electron lowers. This energy gain is given by

$$E_{kin} = \int_{-\pi/(2a)}^{\pi/(2a)} (E_0(k) - E_-(k)) \, \frac{L dk}{2\pi} \,,$$

where L is the length of the chain, and E_- denotes the renormalized energy (3) with the minus sign. To calculate the integral, we linearize $E(k)$ in the vicinity of $\pi/(2a)$, $E(k) = E_F + v_F q$, $q = k - \pi/(2a)$,

$$E_{kin} = 2\int_{-\pi/(2a)}^{0} \left(\hbar v_F q + \sqrt{\hbar^2 v_F^2 q^2 + |V|^2}\right) \frac{L dq}{\pi} \,,$$

We can calculate the integral by splitting it into two: for $|\hbar v_F q| \lesssim |V|$ (giving $|V|/\hbar v_F$) and for $|\hbar v_F q| \gtrsim |V|$. The second integral diverges logarithmically and has to be cut off at low momenta q. Summing up, we obtain

$$E_{kin} = -\frac{L|V|^2}{\hbar v_F} \ln \frac{|V|}{B} \,,$$

where B is the energy cut-off. Note that in the weak coupling limit ($V \to 0$), the logarithmic kinetic energy is always greater than the quadratic elastic energy, and thus the rearrangement of atome is always profitable. But the rearrangement means that there are no electron states at the Fermi surface — the material becomes an insulator. One-dimensional metals do not exist.