Charge density wave
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Sir Rudolf Ernst Peierls, CBE (June 5, 1907, Berlin – September 19, 1995, Oxford) was a German-born British physicist. Rudolf Peierls had a major role in Britain's nuclear program, but he also had a role in many modern sciences. His impact on physics can probably be best described by his obituary in *Physics Today*: "Rudolph Peierls...a major player in the drama of the eruption of nuclear physics into world affairs.

http://en.wikipedia.org/wiki/Rudolf_Peierls

((John Bardeen (1941)))
Many ideas of CDWs were developed in early attemmpts to explain superconductivity. In 1941, John Bardeen suggested that "in the superconducting state there is a small periodic distortion of the lattice" that produces energy gaps, and that these gaps would lead to enhanced diamagnetism. Bardeen abandoned this idea when he realized the difficulty of obtaining an appropriate arrangement of gaps on the three-dimensional Fermi surfaces of common superconductors.

((J. Bardeen, Phys. Rev. 59, 928 (1941)))
Proceedings of the American Physical Society, Minutes of Washington DC, Meeting May 1-3, 1941.
The energy discontinuities produced by the zone structure yield a decrease in the energy of the electrons at the expense of the increase in energy of the lattice resulting from the distortion. A rough estimate of the interaction between the electrons and the lattice obtained from the electrical conductivity in the normal state indicates that the superconducting state may be stable at low temperatures. The most favorable metals are those which have a high

density of valence electrons in a wide energy band and which have a large interaction between electrons and lattice (low conductivity).

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1. One-dimensional energy band
(1) Regular lattice

Suppose that the system consists of N atoms, forming a linear chain along the x direction. They are periodically arranged such that the distance between the nearest neighbor atoms is a. The size of the system is $L = Na$.
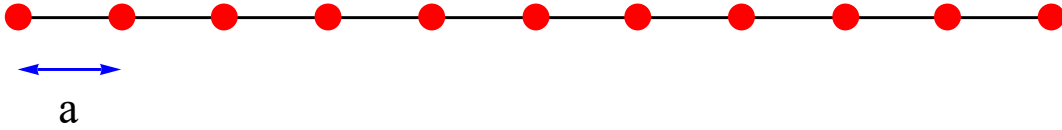

a

Fig.   One dimensional chain of atoms where the nearest neighbor distance is a.

The energy gap appears at the Brillouin zone boundary $(k = \pm \frac{\pi}{a})$. The energy gap is fixed at this reciprocal lattice point. In this case there are $2N$ states for the first Brillouin zone $(|k| \leq \frac{\pi}{a})$. The factor 2 comes from the spin of electrons. When each atom has two electrons, there are $2N$ electrons in the system. Then the band is filled up to the Brillouin zone (insulator). When each atom has one electrons, there are N electrons in the system. Then the band is half-filled in the energy band (metal).
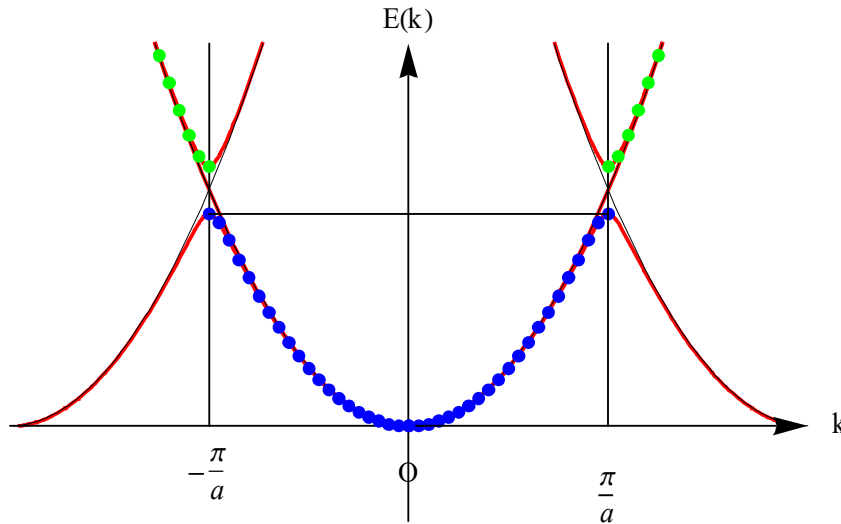

Fig.   Energy band for the system where there are two electrons per atom. All states are occupied up to the zone of the Brillouin zone (insulator)
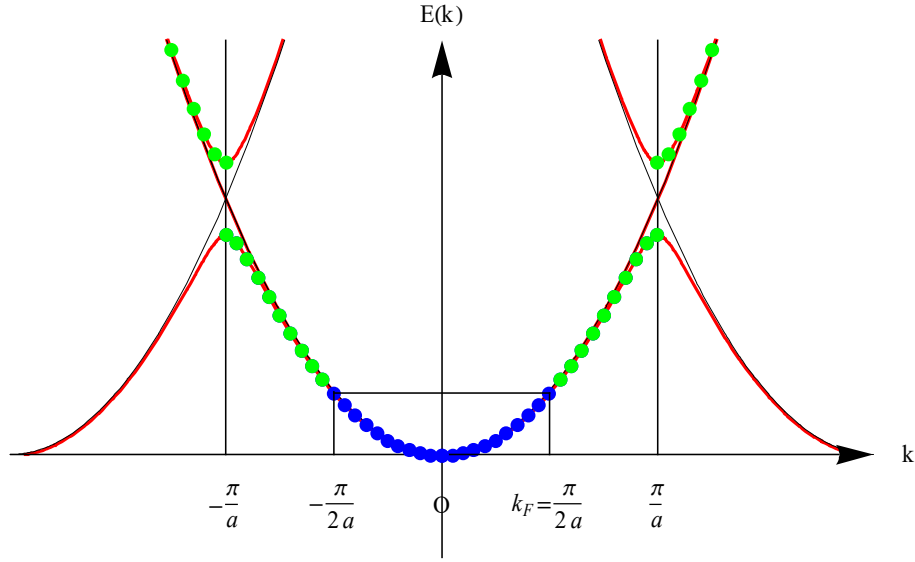
Fig.   Energy band for the system with one electron per atom. All states are occupied for $|k| < k_F$ $(= \pi/a)$ in the Brillouin zone (metal)

(ii)   Effect of lattice distortion

    We still assume that there is one electron per atom in the linear chain. Now let us displace every second atom by a small distance δ.
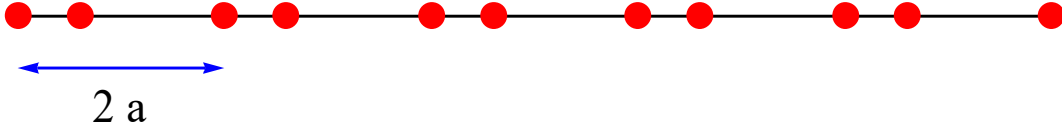

2 a

Fig.   Lattice constant changes from a to $2a$ due the lattice distortion.

This reduces the symmetry to that of a chain with spacing $2a$, and the potential acquires a Fourier component of wave number π/a which in this case is equal to $2k_F$. This results in an energy gap at $k = k_F = \pi/2a$, in accordance with the change in the periodicity from a to 2a. In this case, all states raised by the change are empty, and all states lowered are occupied, so the system becomes insulator.
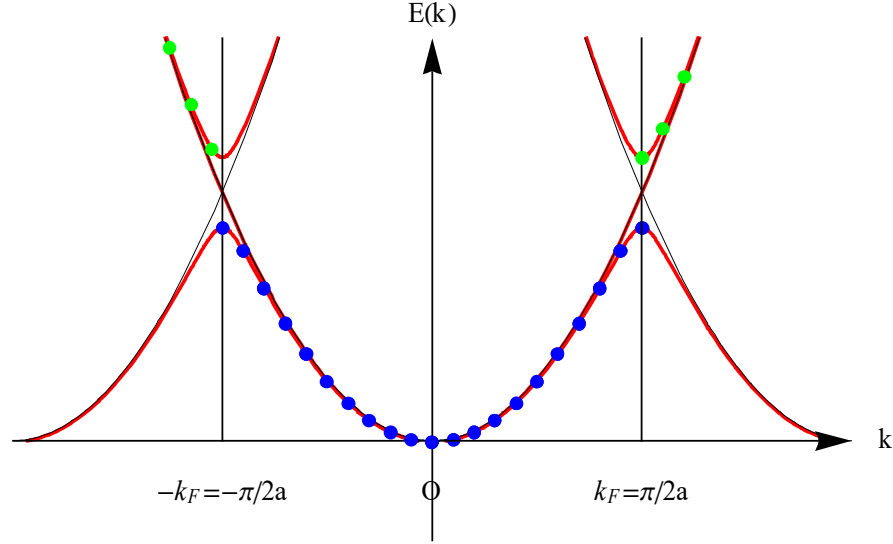
Fig. Energy band for the system with one electron per atom, after the lattice distortion. The energy gap appears at $k=k_F = \pm\pi/2a$. The system changes from metal to insulator (Peierls instability).

((**Peierls, More surprise in theoretical physics, 1991**))

This instability came to me as a complete surprise when I was tidying material for my book (Peierls 1955), and it took me a considerable time to convince myself that the argument was sound. It seemed of only academic significance, however, since there are no strictly one-dimensional systems in nature (and if there were, they would become disordered at any finite temperature. I therefore did not think it worth publishing the argument, beyond a brief remark in the book, which did not even mention the logarithmic behavior.

It must also be remembered that the argument relies on the adiabatic approximation, in which the atomic nuclei are assumed fixed. If their zero-point motion were taken into account, the answer might change, but this would be a difficult problem to deal with, since it involves a strongly nonlinear many-body problem.

2. Elastic energy due to the lattice distortion

Then change of the total energy of the system consists of

(i) the change of energy in electrons ($\Delta E_{electronic} < 0$) which decreases because of the appearance of energy gap.

(ii) the change of energy associated with the lattice distortion ($\Delta E_{elastic} > 0$)

The total energy ΔE is given by

$$\Delta E = \Delta E_{electronic} + \Delta E_{lattice} .$$

If $\Delta E < 0$, the lattice distortion occurs. This is predicted by Peierls for an ideal one dimensional conductor.

The charge density wave has a periodic function of x with the periodicity λ. We consider the elastic strain

$$\delta \cos(Qx) = \delta \cos(2k_F x),$$

where

$$Q = \frac{2\pi}{\lambda} = \frac{2\pi}{\dfrac{\pi}{k_F}} = 2k_F$$

Note that k_F is a general value and is not always equal to $\pi/2a$. The spatial-average elastic energy per unit length is

$$
\begin{aligned}
\Delta E_{elastic} &= \frac{1}{2} C \delta^2 \left\langle \cos^2(2k_F x) \right\rangle \\
&= \frac{1}{2} \frac{C\delta^2}{\lambda} \int_0^\lambda \cos^2(2k_F x) dx \\
&= \frac{1}{4} \frac{C\delta^2}{\lambda} \int_0^\lambda [1 - \cos(\frac{4\pi}{\lambda} x)] dx \\
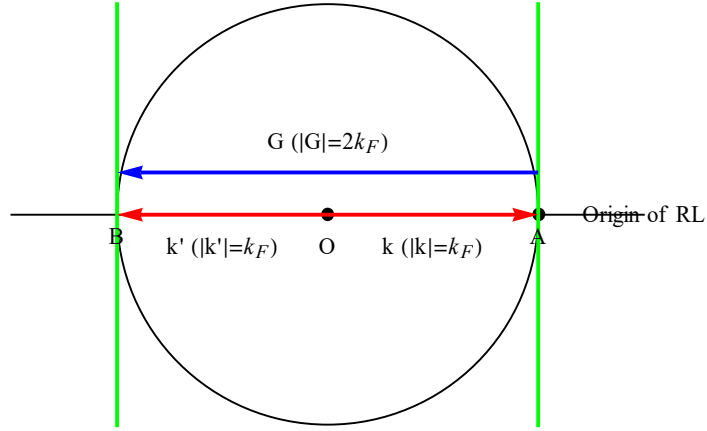&= \frac{1}{4} \frac{C\delta^2}{\lambda} \lambda = \frac{C\delta^2}{4}
\end{aligned}
$$

where C is the force constant of the linear metal. We next calculate $E_{electronic}$. Suppose that the ion contribution to the lattice potential seen by a conduction electron is proportional to the deformation,

$$U(x) = 2V_0 \cos(2k_F x) = V_0 e^{iQx} + V_0 e^{-iQx}$$

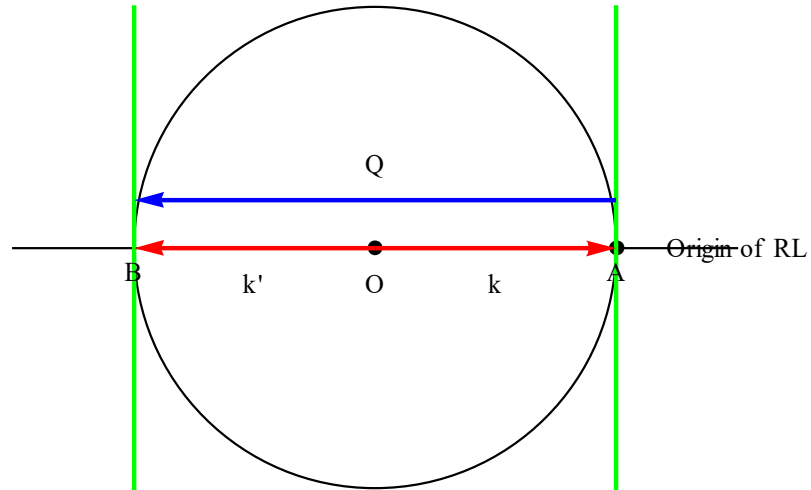where $\qquad U_Q = V_0 = A\delta$ (see Kittel, ISSP, p.422- 423).

3. Bragg diffraction; Ewald sphere
(a)   Typical Bragg reflections:

Fig. Ewald sphere: $q = k'-k$; $k'=k$. The Bragg reflection occurs when $q = $ G. q is the scattering vector and G is the reciprocal lattice vector

(b) The case for the charge density waves;

Fig. Ewald sphere: $q = k'-k$; $k'=k$. The Bragg reflection occurs when $q = Q$. q is the scattering vector and Q is equal to $2k_F$.

Experimentally the Bragg reflection appear at

$$q = la^* \pm 2k_F$$

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where $a^* = \dfrac{2\pi}{a}$ is the reciprocal lattice and a is the lattice constant in the absence of the lattice distortion. The Bragg intensity is proportional the square of the order parameter (energy gap). Note that

$$\frac{\lambda}{a} = \frac{2\pi}{a}\frac{1}{2\pi}\frac{\pi}{k_F} = \frac{a^*}{2k_F}.$$

If this ratio is a rational number ($= p/q$; p and q are integers).

$$\frac{\lambda}{a} = \frac{p}{q}.$$

There are q CDW waves in the p lattice distances. This is called the commensurate CDW. If this ratio is irrational, this is called the incommensurate CDW.

4.   Calculation of the change of energy near the regions at $k = k_F$
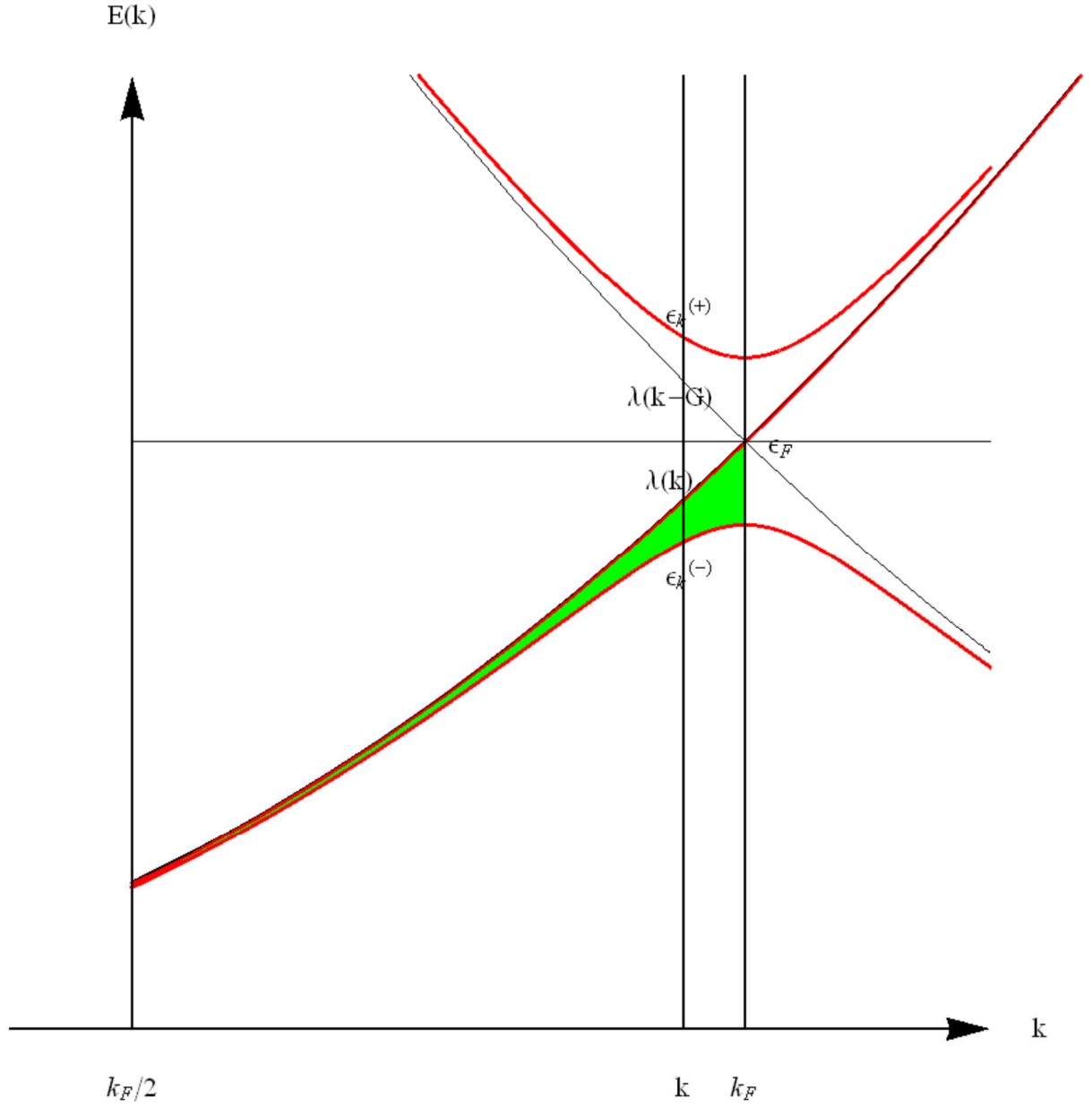
Now we consider the simplest case: mixing of only the two states: $|k\rangle$ and $|k-G\rangle$ ($k \approx k_F$), $k - G \approx -k_F$, $G = 2k_F$). The wavefunction is approximated by

$$|\psi\rangle = C_k|k\rangle + C_{k-G}|k-G\rangle.$$

where only the coefficients C_k and C_{k-G} are dominant. The central equation (eigenvalue problems) is

$$\begin{pmatrix} \lambda_k - \varepsilon & U_G^* \\ U_G & \lambda_{k-G} - \varepsilon \end{pmatrix} \begin{pmatrix} C_k \\ C_{k-G} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

where

$$\lambda_k = \frac{\hbar^2}{2m} k^2, \quad \lambda_{k-G} = \frac{\hbar^2}{2m} (k-G)^2$$

From the condition that the determinant is equal to 0, we have

$$(\lambda_k - \varepsilon)(\lambda_{k-G} - \varepsilon) - |U_G|^2 = 0,$$

or

$$\varepsilon_k^{(\pm)} = \frac{\lambda_k + \lambda_{k-G} \pm \sqrt{(\lambda_k - \lambda_{k-G})^2 + 4|U_G|^2}}{2}.$$

Note that the potential energy $U(x)$ is described by

$$U(x) = U_0 + U_G e^{-iGx} + U_G e^{iGx} = U_0 + 2U_G \cos(Gx),$$

where we assume that U_G is real:

$$U_G = U_{-G}^* = U_{-G} = V_0 \quad.$$

Then we have

$$\varepsilon_k^{(-)} = \frac{\hbar^2}{4m}[k^2 + (k-G)^2] - \sqrt{\frac{\hbar^4}{16m^2}\{[k^2 - (k-G)^2]^2 + V_0^2}$$

We retain the minus sign to get minimum energy. The reduction of the lower energy is

$$\Delta E_{electronic}^{(1)}(k) = -\lambda_k + \varepsilon_k^{(-)}$$

$$= -\frac{\hbar^2}{2m}k^2 + \frac{\hbar^2}{4m}[k^2 + (k-G)^2] - \sqrt{\frac{\hbar^4}{16m^2}\{[k^2 - (k-G)^2]\}^2 + V_0^2}$$

$$= -\frac{\hbar^2}{4m}[k^2 - (k-G)^2] - \sqrt{\frac{\hbar^4}{16m^2}\{[k^2 - (k-G)^2]\}^2 + V_0^2}$$

To get the reduction of the total energy per unit length, we have to integrate from -k_F to k_F, multiplied by $(1/2\pi)$, The main contribution comes from the neighborhood of $k = k_F$. We assume that V_0 is constant. Using the relation

$$k^2 - (k-G)^2 = (k+k-G)(k-k+G) = 2G(k-k_F) = 4k_F(k-k_F)$$

we get

$$\Delta E_{electronics}(k) = \alpha\kappa - \sqrt{\alpha^2\kappa^2 + V_0^2}$$
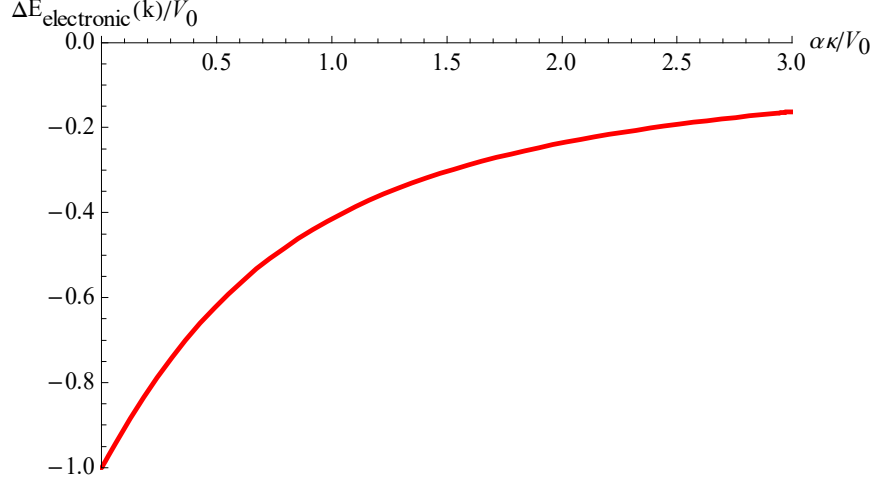
where

$$\alpha = \frac{\hbar^2 k_F}{m}, \qquad \kappa = k_F - k$$

We note that

$$\frac{\Delta E_{electronics}(k)}{V_0} = \frac{\alpha\kappa}{V_0} - \sqrt{\frac{\alpha^2\kappa^2}{V_0^2} + 1}$$

As is expected, the value of $\dfrac{\Delta E_{electronics}(k)}{V_0}$ is negative. It increases with increasing $\dfrac{\alpha\kappa}{V_0}$.

The approximations are valid only in the neighborhood of $k = k_F$. So we need to restrict the integration to a maximum value of k, k_0, such that

$$\frac{V_0}{\alpha} << k_0 << k_F$$

Then we have

$$\Delta E_{electronic}^{(1)} = \frac{2}{2\pi} \int_{k_0}^{k_F} (\alpha\kappa - \sqrt{\alpha^2\kappa^2 + V_0^2})dk = \frac{1}{\pi} \int_{0}^{\kappa_1} (\alpha\kappa - \sqrt{\alpha^2\kappa^2 + V_0^2})d\kappa$$

where the factor 2 comes from the spin degree of the electron.

$$\kappa_1 = k_F - k_0$$

5.   Calculation of change of energy in the regions near $k = -k_F$.

Here we show that the contribution from the regions near $k = -k_F$ is the same as that from the regions near $k = k_F$ as shown in the above. give equal contributions

We consider the case when $k \approx -k_F$ (<0), $k+G = k_F$ with $G = 2k_F$. Since

$$\varepsilon_k^{(-)} = \frac{\lambda_k + \lambda_{k+G} - \sqrt{(\lambda_k - \lambda_{k+G})^2 + 4V_0^2}}{2}$$

we have

$$\Delta E_{electronic}^{(2)}(k) = -\lambda_k + \varepsilon_k^{(-)}$$

$$= -\frac{\hbar^2}{2m}k^2 + \frac{\hbar^2}{4m}[k^2 + (k+G)^2] - \sqrt{\frac{\hbar^4}{16m^2}\{[k^2 - (k+G)^2]\}^2 + V_0^2}$$

$$= -\frac{\hbar^2}{4m}[k^2 - (k+G)^2] - \sqrt{\frac{\hbar^4}{16m^2}\{[k^2 - (k+G)^2]\}^2 + V_0^2}$$

Noting that

$$k^2 - (k+G)^2 = (k+k+G)(k-k-G) = -2G(k+k_F) = -4k_F(k+k_F)$$

we get

$$\Delta E_{electronics}{}^{(2)}(k) = \alpha\kappa - \sqrt{\alpha^2\kappa^2 + V_0{}^2}$$

where

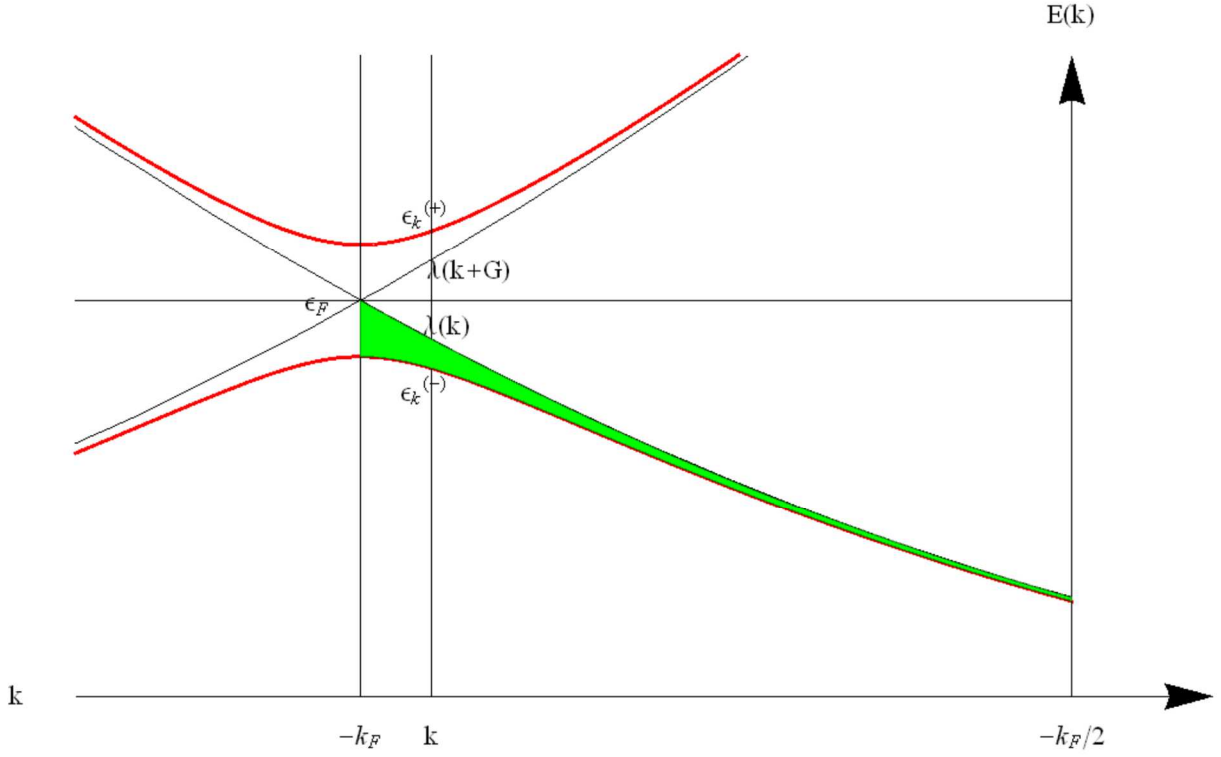$$\alpha = \frac{\hbar^2 k_F}{m}, \qquad \kappa = k_F + k$$

Then we get

$$\Delta E_{electronic}{}^{(2)} = \frac{2}{2\pi}\int_{-k_F}^{-k_0}(\alpha\kappa - \sqrt{\alpha^2\kappa^2 + V_0{}^2})dk = \frac{1}{\pi}\int_0^{\kappa_1}(\alpha\kappa - \sqrt{\alpha^2\kappa^2 + V_0{}^2})d\kappa$$

where the factor 2 comes from the spin degree of the electron.

$$\kappa_1 = k_F - k_0$$

So it is found that

$$\Delta E_{electronic}{}^{(2)} = \Delta E_{electronic}{}^{(1)}$$

6. The change in the total energy due to the lattice distortion

The total energy is given by

$$\Delta E_{electronic} = \Delta E_{electronic}^{(1)} + \Delta E_{electronic}^{(1)}$$

$$= 2\frac{2}{2\pi}\int_0^{\kappa_1}(\alpha\kappa - \sqrt{\alpha^2\kappa^2 + V_0^2})d\kappa$$

$$= \frac{\kappa_1}{\pi}(\alpha\kappa_1 - \sqrt{V_0^2 + \alpha^2\kappa_1^2}) - \frac{V_0^2}{\pi\alpha}\ln(\frac{\alpha\kappa_1 + \sqrt{V_0^2 + \alpha^2\kappa_1^2}}{V_0})$$

$$= \frac{\alpha\kappa_1^2}{\pi}(1 - \sqrt{\frac{V_0^2}{\alpha^2\kappa_1^2} + 1}) - \frac{V_0^2}{\pi\alpha}\ln\left(1 + \sqrt{\frac{V_0^2}{\alpha^2\kappa_1^2} + 1}\right) + \frac{V_0^2}{\pi\alpha}\ln\left(\frac{V_0}{\alpha\kappa_1}\right)$$

$$\approx -\frac{V_0^2}{\pi\alpha}(\frac{1}{2} - \frac{1}{8}\frac{V_0^2}{\alpha^2\kappa_1^2}) + \frac{V_0^2}{\pi\alpha}\ln\left(\frac{V_0}{\alpha\kappa_1}\right)$$

$$-\frac{V_0^2}{\pi\alpha}(\ln 2 + \frac{V_0^2}{4\alpha^2\kappa_1^2})$$

$$\approx -\frac{V_0^2}{2\pi\alpha}[1 + \frac{1}{4}\frac{V_0^2}{\alpha^2\kappa_1^2} + 2\ln\left(\frac{2\alpha\kappa_1}{V_0}\right)]$$

or

$$\Delta E_{electronic} \approx -\frac{V_0^2}{2\pi\alpha}[1 + \frac{1}{4}\frac{V_0^2}{\alpha^2\kappa_1^2} + 2\ln\left(\frac{2\alpha\kappa_1}{V_0}\right)]$$

The important feature of this result is that it behaves for small V_0 as

$$E_{electronic} = -\frac{V_0^2}{\pi\alpha}\ln\left(\frac{2\alpha\kappa_1}{V_0}\right)$$

$$\approx -\frac{V_0^2}{\pi\alpha}\ln\left(\frac{\alpha\kappa_1}{V_0}\right) - \frac{V_0^2}{\pi\alpha}\ln(2)$$

$$\approx \frac{V_0^2}{\pi\alpha}\ln\left(\frac{V_0}{\alpha\kappa_1}\right)$$

For small displacement, V_0 is proportional to the displacement δ.

$$V_0 = A\delta ,$$

where A is constant (see Kittel, ISSP, p.422- 423). The behaviors of the reduction in electronic energy for small displacement is

$$E_{electronic} \approx \frac{A^2 \delta^2}{\pi \alpha} \ln(A\delta) < 0$$

This is interesting because there may be other effects favoring the regular spacing, $\delta = 0$, such as the repulsion between the atomic cores, but these will have an energy varying δ^2. Thus the electronic energy must dominate for small displacement. This suggests that the periodic chain must always be unstable.

The change in the total energy ΔE is given by

$$\Delta E = \Delta E_{electronic} + \Delta E_{elastic}$$
$$= -\frac{A^2 \delta^2}{2\pi\alpha}[1 + \frac{1}{4}\frac{A^2\delta^2}{\alpha^2 \kappa_1^2} - 2\ln\left(\frac{A\delta}{2\alpha\kappa_1}\right)] + \frac{C\delta^2}{4}$$
$$\approx \frac{A^2\delta^2}{\pi\alpha}\ln\left(\frac{A\delta}{2\alpha\kappa_1}\right) + \frac{C\delta^2}{4}$$

In order to find the minimum value of ΔE, we take a derivative of ΔE with respect to δ.

$$\frac{d(\Delta E)}{d\delta} = \frac{1}{2\pi\alpha}\delta[2A^2 + C\pi\alpha + 4A^2\ln(\frac{A\delta}{2\alpha\kappa_1})] = 0.$$

Then we get

$$A\delta = 2 \times \exp(-\frac{1}{2})\alpha\kappa_1 \exp(-\frac{\pi C\alpha}{4A^2})$$
$$= 1.21306\alpha\kappa_1 \exp(-\frac{\pi C\alpha}{4A^2})$$
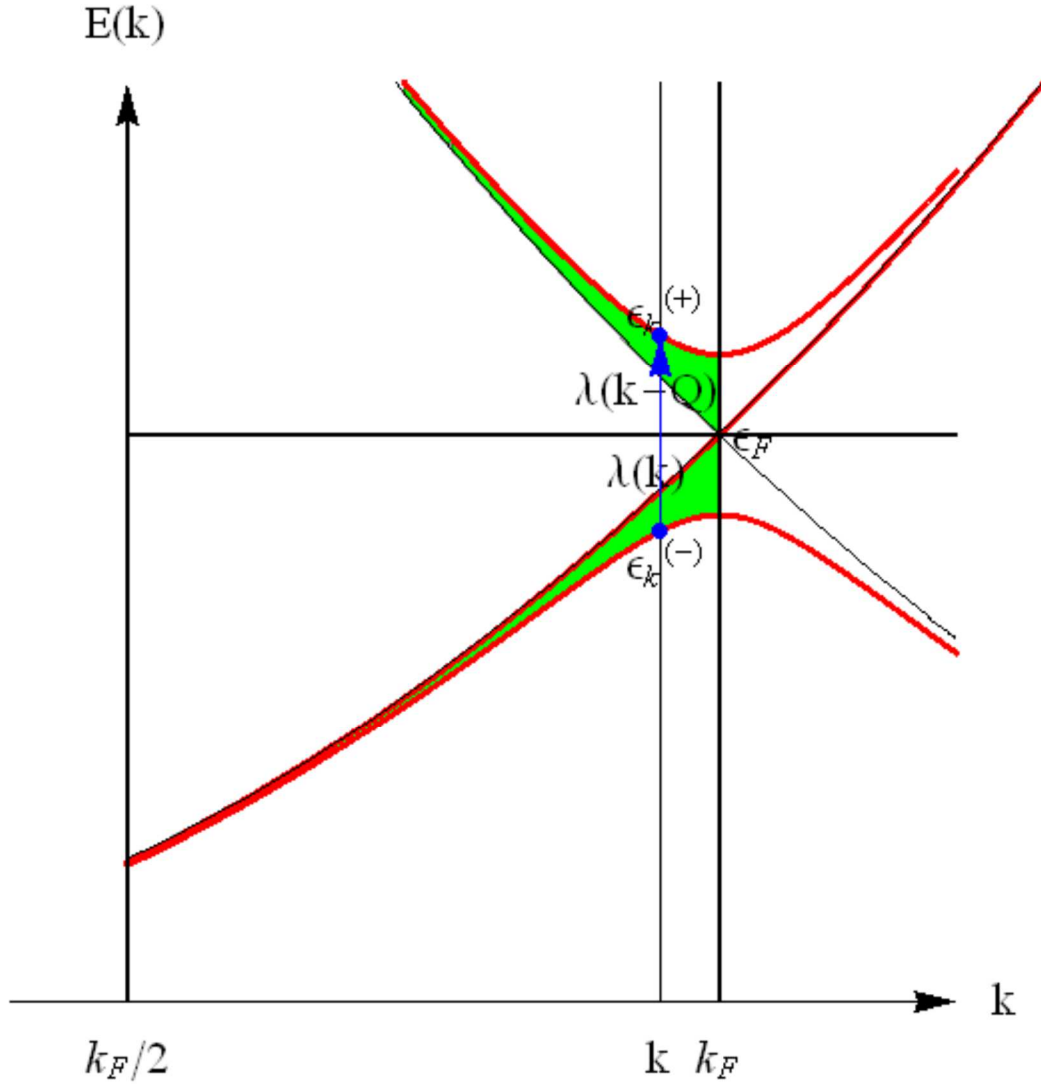
or

$$A\delta = 1.21306\frac{\hbar^2 k_F \kappa_1}{m}\exp(-\frac{\hbar^2 k_F \pi C}{4mA^2})$$

This expression is almost the same as that derived by Kittel,

$$A\Delta \approx \frac{2\hbar^2 k_F^2}{m}\exp(-\frac{\hbar^2 k_F \pi C}{4mA^2}) \qquad\qquad \text{(Kittel, ISSP)}$$

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7. Electronic density $\rho(x)$

$E(k)$

At finite temperatures, there is a finite probability that a part of electrons is excited from the lower state ($\varepsilon_k^{(-)}$) to the higher state ($\varepsilon_k^{(+)}$).

We consider the state given by

$$\left|\psi^{(\pm)}\right\rangle = C_k^{(\pm)}\left|k\right\rangle + C_{k-Q}^{(\pm)}\left|k-Q\right\rangle$$

or

$$\psi_k^{(\pm)}(x) = \left\langle x\middle|\psi^{(\pm)}\right\rangle = C_k^{(\pm)}e^{ikx} + C_{k-Q}^{(\pm)}e^{i(k-Q)x}$$

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where

$$\begin{pmatrix} \lambda_k - \varepsilon & U_Q^* \\ U_Q & \lambda_{k-Q} - \varepsilon \end{pmatrix}\begin{pmatrix} C_k \\ C_{k-Q} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

The eigenvalues are $\varepsilon_k^{(+)}$ and $\varepsilon_k^{(-)}$, defined by

$$\begin{aligned} \varepsilon_k^{(\pm)} &= \frac{\lambda_k + \lambda_{k-Q} \pm \sqrt{(\lambda_k - \lambda_{k-Q})^2 + 4|U_Q|^2}}{2} \\ &= \frac{\lambda_k + \lambda_{k-Q}}{2} \pm \frac{|\lambda_k - \lambda_{k-Q}|}{2}[1 + \frac{2|U_Q|^2}{(\lambda_k - \lambda_{k-Q})^2}] \end{aligned}$$

and

$$\left|C_k^{(\pm)}\right|^2 + \left|C_{k-Q}^{(\pm)}\right|^2 = 1. \qquad \text{(Normalization)}.$$

The charge density at x is given by

$$\rho(x) = \frac{1}{N}\sum_k \{f(\varepsilon_k^{(-)})\left|\psi_k^{(-)}\right|^2 + f(\varepsilon_k^{(+)})\left|\psi_k^{(+)}\right|^2\},$$

where f is the Fermi-Dirac distribution function. When $\lambda_k < \lambda_{k-Q}$,

$$\begin{aligned} \varepsilon_k^{(-)} &= \frac{\lambda_k + \lambda_{k-Q}}{2} - \frac{(\lambda_{k-Q} - \lambda_k)}{2}[1 + \frac{2|U_Q|^2}{(\lambda_k - \lambda_{k-Q})^2}] \\ &= \lambda_k - \frac{|U_Q|^2}{(\lambda_{k-Q} - \lambda_k)} \end{aligned}$$

and

$$\varepsilon_k^{(+)} = \frac{\lambda_k + \lambda_{k-Q}}{2} + \frac{(\lambda_{k-Q} - \lambda_k)}{2}[1 + \frac{2|U_Q|^2}{(\lambda_k - \lambda_{k-Q})^2}]$$

$$= \lambda_{k-Q} + \frac{|U_Q|^2}{(\lambda_{k-Q} - \lambda_k)}$$

When $|U_Q|^2 \approx 0$,

$$f(\varepsilon_k^{(-)}) = f(\lambda_k), \qquad f(\varepsilon_k^{(+)}) = f(\lambda_{k-Q}).$$

The probability is given by $|\psi_k^{(\pm)}(x)|^2$,

$$|\psi_k^{(\pm)}(x)|^2 = |C_k^{(\pm)} e^{ikx} + C_{k-Q}^{(\pm)} e^{i(k-Q)x}|^2$$

$$= |C_k^{(\pm)} + C_{k-Q}^{(\pm)} e^{-iQx}|^2$$

$$= |C_k^{(\pm)}|^2 + |C_{k-Q}^{(\pm)}|^2 + C_k^{(\pm)*} C_{k-Q}^{(\pm)} e^{-iQx} + C_k^{(\pm)} C_{k-Q}^{(\pm)*} e^{iQx}$$

$$= 1 + C_k^{(\pm)*} C_{k-Q}^{(\pm)} e^{-iQx} + C_k^{(\pm)} C_{k-Q}^{(\pm)*} e^{iQx}$$

Then the density is

$$\rho(x) = \frac{1}{N} \sum_k \{f(\lambda_k)|\psi_k^{(-)}|^2 + f(\lambda_{k-Q})|\psi_k^{(+)}|^2\}$$

$$= \frac{1}{N} \sum_k \{f(\lambda_k)[1 + C_k^{(-)*} C_{k-Q}^{(-)} e^{-iQx} + C_k^{(-)} C_{k-Q}^{(-)*} e^{iQx}]$$

$$+ f(\lambda_{k-Q})[1 + C_k^{(+)*} C_{k-Q}^{(+)} e^{-iQx} + C_k^{(+)} C_{k-Q}^{(+)*} e^{iQx}]\}$$

What is the value of $C_k^{(-)} C_{k-Q}^{(-)*}$? We note that

$$\begin{pmatrix} \lambda_k - \varepsilon_k^{(-)} & U_Q^* \\ U_Q & \lambda_{k-Q} - \varepsilon_k^{(-)} \end{pmatrix} \begin{pmatrix} C_k^{(-)} \\ C_{k-Q}^{(-)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

or

$$(\lambda_k - \varepsilon_k^{(-)})C_k^{(-)} + U_Q^* C_{k-Q}^{(-)} = 0,$$

or

$$C_{k-Q}^{(-)} = -\frac{(\lambda_k - \varepsilon_k^{(-)})C_k^{(-)}}{U_Q^*}.$$

Then we get

$$
\begin{aligned}
C_k^{(-)}C_{k-Q}^{(-)*} &= \frac{(\varepsilon_k^{(-)} - \lambda_k)\left|C_k^{(-)}\right|^2}{U_Q} \\
&= \frac{\left|C_k^{(-)}\right|^2}{U_Q}\frac{\left|U_Q\right|^2}{\left(\lambda_k - \lambda_{k-Q}\right)} \\
&= \frac{U_Q^*\left|C_k^{(-)}\right|^2}{\lambda_k - \lambda_{k-Q}}
\end{aligned}
$$

since

$$\varepsilon_k^{(-)} = \lambda_k - \frac{\left|U_Q\right|^2}{\left(\lambda_{k-Q} - \lambda_k\right)}$$

Similarly,

$$
\begin{pmatrix} \lambda_k - \varepsilon_k^{(+)} & U_Q^* \\ U_Q & \lambda_{k-Q} - \varepsilon_k^{(+)} \end{pmatrix}
\begin{pmatrix} C_k^{(+)} \\ C_{k-Q}^{(+)} \end{pmatrix} =
\begin{pmatrix} 0 \\ 0 \end{pmatrix},
$$

or

$$U_Q C_k^{(+)} + (\lambda_{k-Q} - \varepsilon_k^{(+)})C_{k-Q}^{(+)} = 0.$$

Then we get

$$C_k^{(+)} C_{k-Q}^{(+)*} = \frac{(\varepsilon_k^{(+)} - \lambda_{k-Q})^* \left| C_k^{(+)} \right|^2}{U_Q^*}$$

$$= \frac{\left| C_k^{(+)} \right|^2}{U_Q^*} \frac{\left| U_Q \right|^2}{(\lambda_{k-Q} - \lambda_k)}$$

$$= \frac{U_Q \left| C_k^{(+)} \right|^2}{\lambda_{k-Q} - \lambda_k}$$

since

$$\varepsilon_k^{(+)} - \lambda_{k-Q} = \frac{\left| U_Q \right|^2}{(\lambda_{k-Q} - \lambda_k)}.$$

The electron density can be rewritten as

$$\rho(x) = \frac{1}{N} \sum_k \{ f(\lambda_k)[1 + \frac{\left| C_k^{(-)} \right|^2}{\lambda_k - \lambda_{k-Q}} (U_Q e^{-iQx} + U_Q^* e^{iQx}]$$

$$+ f(\lambda_{k-Q})[1 + \frac{\left| C_k^{(+)} \right|^2}{\lambda_{k-Q} - \lambda_k} (U_Q^* e^{-iQx} + U_Q e^{iQx}] \}$$

Suppose that U_Q is real. Thus we have

$$\rho(x) = \frac{1}{N} \sum_k \{ f(\lambda_k)[1 + \frac{2 \left| C_k^{(-)} \right|^2 U_Q}{\lambda_k - \lambda_{k-Q}} \cos(Qx)]$$

$$+ f(\lambda_{k-Q})[1 + \frac{2 \left| C_k^{(+)} \right|^2 U_Q}{\lambda_{k-Q} - \lambda_k} \cos(Qx)] \}$$

It is appropriate that $\left| C_k^{(+)} \right|^2 \approx \left| C_k^{(-)} \right|^2 \approx \frac{1}{2}$ for $\left| U_Q \right| \approx 0$.

$$\rho(x) = \frac{1}{N}\sum_k [f(\lambda_k) + f(\lambda_{k-Q})]$$
$$+ \frac{1}{N}\sum_k [\frac{f(\lambda_k) - f(\lambda_{k-Q})}{\lambda_k - \lambda_{k-Q}}]U_Q \cos(Qx)$$

We define $\chi(Q, T)$ as

$$\chi(Q,T) = \frac{1}{N}\sum_k \frac{f(\lambda_{k-Q}) - f(\lambda_k)}{\lambda_k - \lambda_{k-Q}}.$$

Then we have

$$\rho(x) = \rho_0 - \chi(Q,T)U_Q \cos(Qx).$$

The Fourier component of $\rho(x)$ is given by

$$\rho_Q = -\chi(Q,T)U_Q.$$

We note that the potential energy is given by

$$U(x) = 2U_Q \cos(Qx) = U_Q e^{iQx} + U_{-Q}e^{-iQx}.$$

where

$$U_{-Q} = U_Q^* = U_Q = V_0 = A\Delta = real.$$

8.   Calculation of $\chi(Q, T = 0)$
We now calculate the susceptibility

$$N\chi(Q,T) = \sum_k \frac{f(\lambda_k) - f(\lambda_{k-Q})}{\lambda_{k-Q} - \lambda_k} = \sum_k \frac{f(\lambda_k)}{\lambda_{k-Q} - \lambda_k} - \sum_k \frac{f(\lambda_{k-Q})}{\lambda_{k-Q} - \lambda_k}$$

$$= \sum_k \frac{f(\lambda_k)}{\lambda_{k-Q} - \lambda_k} - \sum_{k'} \frac{f(\lambda_{k'})}{\lambda_{k'} - \lambda_{k'+Q}}$$

$$= \sum_k \frac{2m}{\hbar^2} f(\lambda_k)[\frac{1}{Q^2 - 2kQ} + \frac{1}{Q^2 + 2kQ}]$$

$$= \sum_k \frac{2m}{\hbar^2 Q} f(\lambda_k)(\frac{1}{Q - 2k} + \frac{1}{Q + 2k})$$

At $T = 0$ K, $f(\lambda_k) = 1$ for $k < k_F$ and 0 for $k > k_F$.

$$N\chi(Q,T) = \sum_k \frac{f(\lambda_k) - f(\lambda_{k-Q})}{\lambda_{k-Q} - \lambda_k}$$

$$= \frac{2L}{2\pi} \frac{2m}{\hbar^2 Q} 2\int_0^{k_F} dk(\frac{1}{Q - 2k} + \frac{1}{Q + 2k})$$

$$= \frac{2L}{2\pi} \frac{2m}{\hbar^2 Q} 2\int_0^{k_F} \frac{1}{2} dk(\frac{1}{k + \frac{Q}{2}} - \frac{1}{k - \frac{Q}{2}})$$

$$= \frac{2mL}{\pi\hbar^2 Q} \ln\left|\frac{k_F + \frac{Q}{2}}{k_F - \frac{Q}{2}}\right| = \frac{2mL}{\pi\hbar^2 Q} \ln\left|\frac{Q + 2k_F}{Q - 2k_F}\right|$$

or

$$\chi(Q,T) = \frac{2mL}{N\pi\hbar^2 Q} \ln\left|\frac{k_F + \frac{Q}{2}}{k_F - \frac{Q}{2}}\right| =$$

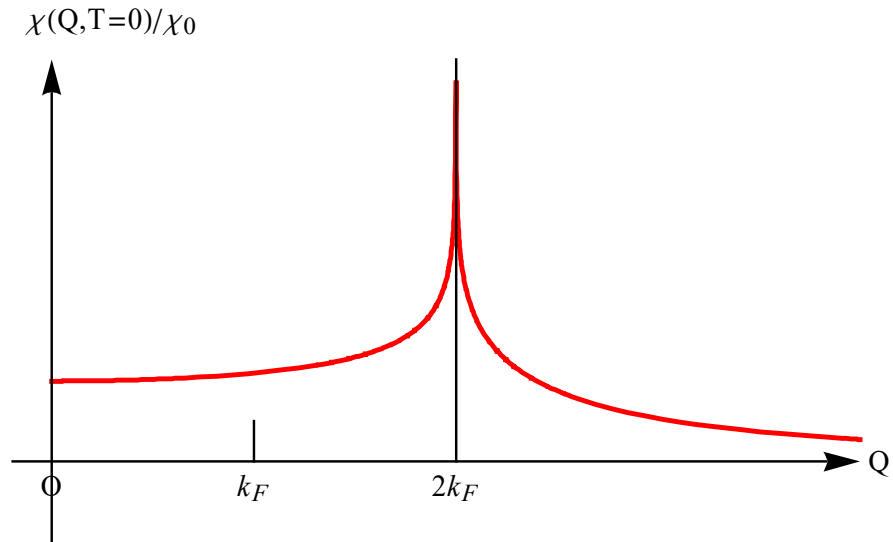$$= \frac{m}{\pi n k_F \hbar^2 \frac{Q}{2k_F}} \ln\left|\frac{\frac{Q}{2k_F} + 1}{\frac{Q}{2k_F} - 1}\right|$$

where we take into account of the degree of spin (the factor 2). We make a plot of the function defined by

$$f(x) = \frac{\chi(Q,T)}{\chi_0} = \frac{1}{x} \ln\left|\frac{x+1}{x-1}\right|$$
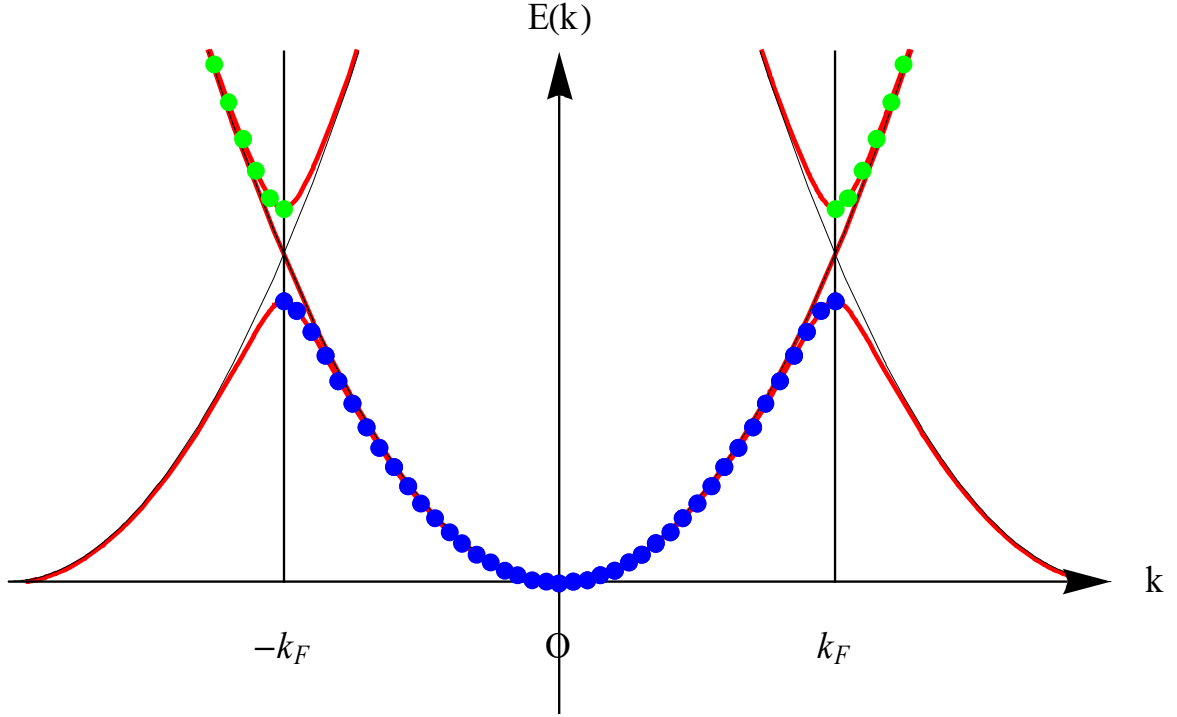
where $x = Q/(2k_F)$, and

$$\chi_0 = \frac{m}{\pi n k_F \hbar^2}$$

The susceptibility is found to diverge at $Q = 2k_F$.

Fig. Scaling plot of $f(x) = \frac{1}{x} \ln\left|\frac{x+1}{x-1}\right|$ with $x = \frac{Q}{2k_F}$.

9.   The density of state at the Fermi energy for the 1D system

Fig. Peierls instability. Electrons with wave number k near $k = k_F$ have their energy lowered by a lattice deformation. When the length of the system is L, the allowed value of k is $k = l\,(2\pi/L)$, where l is 0, ±1, ±2,.... In this figure ($T = 0$ K), the states in the lower energy band is fully occupied, while the states in the upper energy band are empty.

The lattice distortion with wavelength λ gives rise to an energy gap at $k = \dfrac{\pi}{\lambda}$. If $k = k_F$,

$$\lambda = \frac{\pi}{k_F}.$$

Then the system changes from conductor to insulator. All the states $\left|k,\uparrow\right\rangle$ (spin-up state) and $\left|k,\downarrow\right\rangle$ (spin-down state) with $|k|\leq k_F$ are occupied in the lower band. Then we have

$$N = 2\frac{L}{2\pi}(2k_F) = \frac{2L}{\pi}k_F,$$

where the factor 2 comes from the spin degree, and N is the total number of electrons in the system (L). Note that N is not the number of unit cell in this case. The number density n is defined by
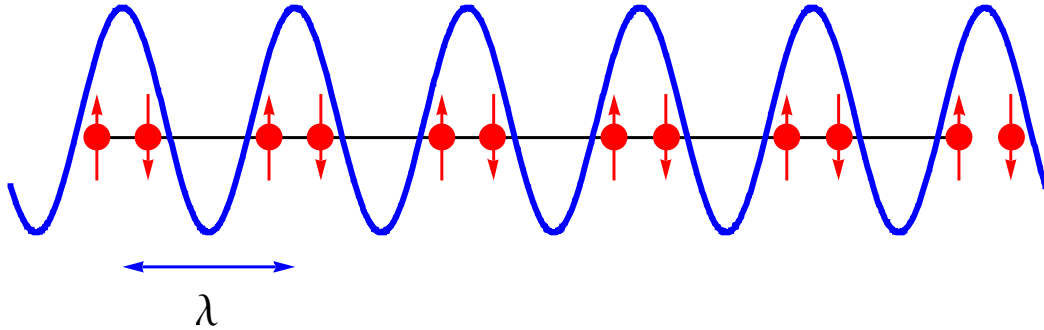
$$n = \frac{N}{L}.$$

Using the above relation, we get

$$n = \frac{2k_F}{\pi}, \qquad \text{or} \qquad , \; k_F = \frac{\pi n}{2}.$$

We note that

$$\frac{2}{\lambda} = \frac{2}{\frac{\pi}{k_F}} = \frac{2k_F}{\pi} = \frac{2}{\pi}\frac{\pi n}{2} = n.$$

This means that here are two electrons per wavelength λ.

The density of states is defined by

$$D(\varepsilon)d\varepsilon = 2\frac{2L}{2\pi}dk = \frac{2L}{\pi}dk,$$

where we take into account of (i) the spin factor (2) and (ii) the even function of k for the energy dispersion. The energy dispersion of the free electron is

$$\varepsilon = \frac{\hbar^2}{2m}k^2, \qquad\qquad dk = \sqrt{\frac{2m}{\hbar^2}}\frac{d\varepsilon}{2\sqrt{\varepsilon}}.$$

Using the relation

$$D(\varepsilon)d\varepsilon = \frac{2L}{\pi}dk = \frac{2L}{\pi}\sqrt{\frac{2m}{\hbar^2}}\frac{d\varepsilon}{2\sqrt{\varepsilon}} = \frac{L}{\pi}\sqrt{\frac{2m}{\hbar^2\varepsilon}}d\varepsilon ,$$

we have the density of states as

$$D(\varepsilon) = \frac{L}{\pi}\sqrt{\frac{2m}{\hbar^2\varepsilon}} = \frac{2\sqrt{m}L}{\sqrt{2}\pi\hbar}\frac{1}{\sqrt{\varepsilon}} .$$

The density of states at the Fermi energy is

$$D(\varepsilon_F) = \frac{L}{\pi}\sqrt{\frac{2m}{\hbar^2\varepsilon_F}} = \frac{L}{\pi}\sqrt{\frac{2m}{\hbar^2\varepsilon_F}} = \frac{2mL}{\pi\hbar^2 k_F} = \frac{mN}{\hbar^2 k_F^2} = \frac{N}{2\varepsilon_F} .$$

10.   The relation $\chi(Q = 2k_F, T) = \dfrac{1}{\lambda_0}$

What is the temperature dependence of the susceptibility?

$$\chi(Q = 2k_F, T) = \frac{1}{N}\sum_k \frac{f(\lambda_{k-2k_F}) - f(\lambda_k)}{\lambda_k - \lambda_{k-2k_F}}$$

We assume that $\kappa = k_F - k$

$$\lambda_k = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}(k_F - \kappa)^2$$

$$= \frac{\hbar^2 k_F^2}{2m}(1 - \frac{\kappa}{k_F})^2$$

$$\approx \frac{\hbar^2 k_F^2}{2m}(1 - \frac{2\kappa}{k_F}) = \varepsilon_F(1 - \frac{2\kappa}{k_F}) = \varepsilon_F - \varepsilon$$

$$\lambda_{k-2k_F} = \frac{\hbar^2}{2m}(k - 2k_F)^2$$

$$= \frac{\hbar^2}{2m}(k_F - \kappa - 2k_F)^2$$

$$= \frac{\hbar^2 k_F^2}{2m}(1 + \frac{\kappa}{k_F})^2$$

$$\approx \frac{\hbar^2 k_F^2}{2m}(1 + \frac{2\kappa}{k_F}) = \varepsilon_F(1 + \frac{2\kappa}{k_F}) = \varepsilon_F + \varepsilon$$

where

$$\varepsilon = \frac{2\varepsilon_F}{k_F}\kappa = \frac{2\varepsilon_F}{k_F}(k_F - k) = \frac{\hbar^2 k_F}{m}(k_F - k)$$

This leads to

$$\lambda_k - \lambda_{k-2k_F} = \varepsilon_F - \varepsilon - (\varepsilon_F + \varepsilon) = -2\varepsilon .$$

The numerator:

$$f(\lambda_{k-2k_F}) = \frac{1}{\exp[\beta(\lambda_{k-2k_F} - \varepsilon_F) + 1} = \frac{1}{e^{\beta\varepsilon} + 1}$$

$$f(\lambda_k) = \frac{1}{\exp[\beta(\lambda_k - \varepsilon_F) + 1} = \frac{1}{e^{-\beta\varepsilon} + 1}$$

Then we get

$$f(\lambda_{k-2k_F}) - f(\lambda_k) = \frac{1}{e^{\beta\varepsilon} + 1} - \frac{1}{e^{-\beta\varepsilon} + 1} = \frac{1 - e^{\beta\varepsilon}}{e^{\beta\varepsilon} + 1} = -\tanh(\frac{\beta\varepsilon}{2})$$

and

$$\frac{f(\lambda_{k-2k_F}) - f(\lambda_k)}{\lambda_k - \lambda_{k-2k_F}} = \frac{\tanh(\frac{\beta\varepsilon}{2})}{2\varepsilon}$$

Then we have

$$\chi(Q = 2k_F, T) = \frac{1}{N} \sum_k \frac{\tanh(\frac{\beta\varepsilon}{2})}{2\varepsilon} \approx \frac{1}{N} D(\varepsilon_F) \int_0^{\varepsilon_0} d\varepsilon \frac{\tanh(\frac{\beta\varepsilon}{2})}{2\varepsilon}$$

$$= \frac{1}{N} D(\varepsilon_F) \int_0^{\varepsilon_0} d\varepsilon \frac{\tanh(\frac{\beta\varepsilon}{2})}{2\varepsilon}$$

$$= \frac{D(\varepsilon_F)}{2N} \int_0^{\varepsilon_0} dx \frac{\tanh(\frac{\beta\varepsilon}{2})}{\varepsilon}$$

or

$$\chi(Q = 2k_F, T) = \frac{D(\varepsilon_F)}{2N} \frac{1}{\lambda_0}$$

$$= \frac{D(\varepsilon_F)}{2N} \ln(1.13387 \frac{\varepsilon_0}{k_B T})$$

where

$$\frac{1}{\lambda_0} = \int_0^{\varepsilon_0} dx \frac{\tanh(\frac{\beta\varepsilon}{2})}{\varepsilon} = \ln(1.13387 \frac{\varepsilon_0}{k_B T})$$

Note that

$$d\varepsilon = -\frac{\hbar^2 k_F}{m} dk$$

$$\varepsilon_0 = \frac{\hbar^2 k_F}{m} (k_F - k_0)$$

k_0 is the lower limit of k (which was discussed above). The magnitude of ε_0 is not essential in our discussion.

11.   The critical temperature T_c

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The energy gap is equal to zero at $T = T_c$. The critical temperature Tc is derived from the energy gap equation. The derivation of Tc is almost the same as that derived for the BCS model of the superconductivity. We start with the energy gap equation with zero energy gap,

$$\frac{1}{\lambda_0} = \int_0^{\varepsilon_0} \frac{d\varepsilon}{\varepsilon} \tanh(\frac{\varepsilon}{2k_B T_c}) = \int_0^{\varepsilon_0/(2k_B T_c)} \frac{d\varepsilon}{\varepsilon} \tanh(\varepsilon)$$

$$= [\ln\varepsilon \tanh(\varepsilon)]_0^{\varepsilon_0/(2k_B T_c)} - \int_0^{\varepsilon_0/(2k_B T_c)} \frac{\ln\varepsilon d\varepsilon}{\cosh^2(\varepsilon)}$$

$$= [\ln\varepsilon \tanh(\varepsilon)]_0^{\varepsilon_0/(2k_B T_c)} - \int_0^{\infty} \frac{\ln\xi d\xi}{\cosh^2(\xi)} \qquad ,$$

$$= \ln(\frac{\varepsilon_0}{2k_B T_c}) \tanh(\frac{\varepsilon_0}{2k_B T_c}) - [\ln(\frac{\pi}{4}) - \gamma]$$

$$= \ln(\frac{\varepsilon_0}{k_B T_c} \frac{2e^{-\gamma}}{\pi})$$

where $\gamma = 0.577216$ is the Euler's constant. Then we get

$$\frac{1}{\lambda_0} \approx \ln(\frac{\varepsilon_0}{2k_B T_c}) + 0.81878$$

since $-[\ln(\frac{\pi}{4}) - \gamma] = 0.81878$. This equation can be rewritten as

$$\frac{\varepsilon_0}{k_B T_c} = 2\exp[\frac{1}{\lambda_0}]\exp(-0.81878)$$

$$\approx 0.881939\exp[\frac{1}{\lambda_0}]$$

or

$$k_B T_c = 1.13387\varepsilon_0 \exp(-\frac{1}{\lambda_0}).$$

12.   The energy difference at finite temperatures

$$\Delta E_{electronic} = \sum_k \{\varepsilon_k^{(-)} f(\varepsilon_k^{(-)}) + \varepsilon_k^{(+)} f(\varepsilon_k^{(+)})\} - \sum_k \{\lambda_k f(\lambda_k) + \lambda_{k-Q} f(\lambda_{k-Q})\}$$

$$\approx \sum_k \{[\lambda_k - \frac{|U_Q|^2}{\lambda_{k-Q} - \lambda_k}] f(\lambda_k) + [\lambda_{k-Q} + \frac{|U_Q|^2}{\lambda_{k-Q} - \lambda_k}] f(\lambda_{k-Q})\}$$

$$- \sum_k \{\lambda_k f(\lambda_k) + \lambda_{k-Q} f(\lambda_{k-Q})\}$$

$$= \sum_k [-\frac{|U_Q|^2 f(\lambda_k)}{\lambda_{k-Q} - \lambda_k} + \frac{|U_Q|^2 f(\lambda_{k-Q})}{\lambda_{k-Q} - \lambda_k}]$$

$$= -|U_Q|^2 \sum_k [\frac{[f(\lambda_k) - f(\lambda_{k-Q})]}{\lambda_{k-Q} - \lambda_k}]$$

$$= -|U_Q|^2 N\chi(Q,T)$$

where

$$\varepsilon_k^{(-)} = \lambda_k - \frac{|U_Q|^2}{\lambda_{k-Q} - \lambda_k}, \qquad \varepsilon_k^{(+)} = \lambda_{k-Q} + \frac{|U_Q|^2}{\lambda_{k-Q} - \lambda_k}$$

$$f(\varepsilon_k^{(-)}) \approx f(\lambda_k), \qquad f(\varepsilon_k^{(+)}) \approx f(\lambda_{k-Q})$$

and

$$\chi(Q,T) = \frac{1}{N} \sum_k \frac{f(\lambda_{k-Q}) - f(\lambda_k)}{\lambda_k - \lambda_{k-Q}} = \sum_k \frac{f(\lambda_k) - f(\lambda_{k-Q})}{\lambda_{k-Q} - \lambda_k}.$$

Then we have

$$\Delta E_{electronic} = -|U_Q|^2 N\chi(Q,T)$$

The total energy of both electron and lattice is given by

$$\Delta E = \Delta E_{electronic} + \Delta E_{elastic}$$

$$= N\chi(Q,T) + \frac{C}{4}\delta^2$$

$$= N\chi(Q,T) + \frac{C}{4A^2}|U_Q|^2$$

$$= -|U_Q|^2 \{N\chi(Q,T) - \frac{C}{4A^2}\}$$

where $U_Q = V_0 = A\delta$. When $Q \to 2k_F$ and $T \to 0$, $\chi(Q,T)$ shows a logarithmic divergence. Therefore, below a characteristic temperature T_p, ΔE becomes negative, leading to the Peierls instability. Using the expression for $\chi(2k_F, T)$,

$$\chi(Q = 2k_F, T) = \frac{D(\varepsilon_F)}{2N} \ln(1.133887 \frac{\varepsilon_0}{k_B T})$$

we get

$$\chi(Q = 2k_F, T) = \frac{C}{4NA^2} = \frac{D(\varepsilon_F)}{2N} \ln(1.13387 \frac{\varepsilon_0}{k_B T})$$

or

$$T_c = 1.13387\varepsilon_0 \exp[-\frac{C}{2A^2 D(\varepsilon_F)}] = 1.13387\varepsilon_0 \exp(-\frac{1}{\lambda_0})$$

where λ_0 is a dimensionless electron-lattice interaction parameter,

$$\lambda_0 = \frac{2A^2 D(\varepsilon_F)}{C}.$$

13.   Kohn anomaly

At temperature which is sufficiently higher than the Peierls transition temperature, the angular frequency $\Omega(k = 2 k_F)$ of the phonon dispersion curve drastically decreases, showing the softening of the phonon mode. This behavior is called the Kohn anomaly. This behavior can be explained qualitatively as follows. The electrons are influenced through the potential U_Q. due to the lattice distortion. The electronic charge is newly generated in the form of

$$\rho_Q = -\chi(Q,T)U_Q.$$

The force exerted on the phonon is weakened by the electron-phonon interaction. This leads to the decrease in the restoring force of the lattice distortion. The angular frequency of phonon at Q becomes softening and is reduced to zero at the critical temperature. In summary, the lattice wave with Q gives rise to the electric potential with Q, which works for the electric charge ρ_Q, turns back to the lattice wave with Q as a positive feedback. This leads to the restoring force of the lattice.

We discuss the time dependence of the displacement η_Q of the phonon mode with Q and ω_Q. Noting that

$$\rho_Q = -\chi(Q,T)U_Q, \qquad U_Q = v_Q\eta_Q$$

we get the equation of motion for η_Q as

$$\frac{d^2}{dt^2}\eta_Q = -\omega_Q{}^2\eta_Q - v_Q{}^2\rho_Q$$
$$= -\omega_Q{}^2\eta_Q + v_Q{}^2\chi(Q,T)\eta_Q$$
$$= -[\omega_Q{}^2 - v_Q{}^2\chi(Q,T)]\eta_Q$$

where v_Q is the strength of the electron-phonon interaction, and $\langle U_Q \rangle = A\delta$ in thermal equilibrium. Then we have the characteristic angular frequency

$$\Omega_Q{}^2 = \omega_Q{}^2 - v_Q{}^2\chi(Q,T)$$

Ω_Q reduces to zero when

$$\chi(Q,T) = \frac{\omega_Q{}^2}{v_Q{}^2}$$

at $Q = 2k_F$. Using

$$\chi(Q = 2k_F,T) = \frac{D(\varepsilon_F)}{2N}\ln(1.13387\frac{\varepsilon_0}{k_BT})$$

we have

$$\frac{\omega_Q^{\,2}}{v_Q^{\,2}} = \frac{D(\varepsilon_F)}{2N} \ln(1.13387 \frac{\varepsilon_0}{k_B T})$$

or

$$T_c = 1.13387\varepsilon_0 \exp[-\frac{1}{\lambda_0}],$$

where

$$\lambda_0 = \frac{v_Q^{\,2} D(\varepsilon_F)}{2N\omega_Q^{\,2}}.$$

This is equal to

$$\lambda_0 = \frac{2D(\varepsilon_F)}{CA^2},$$

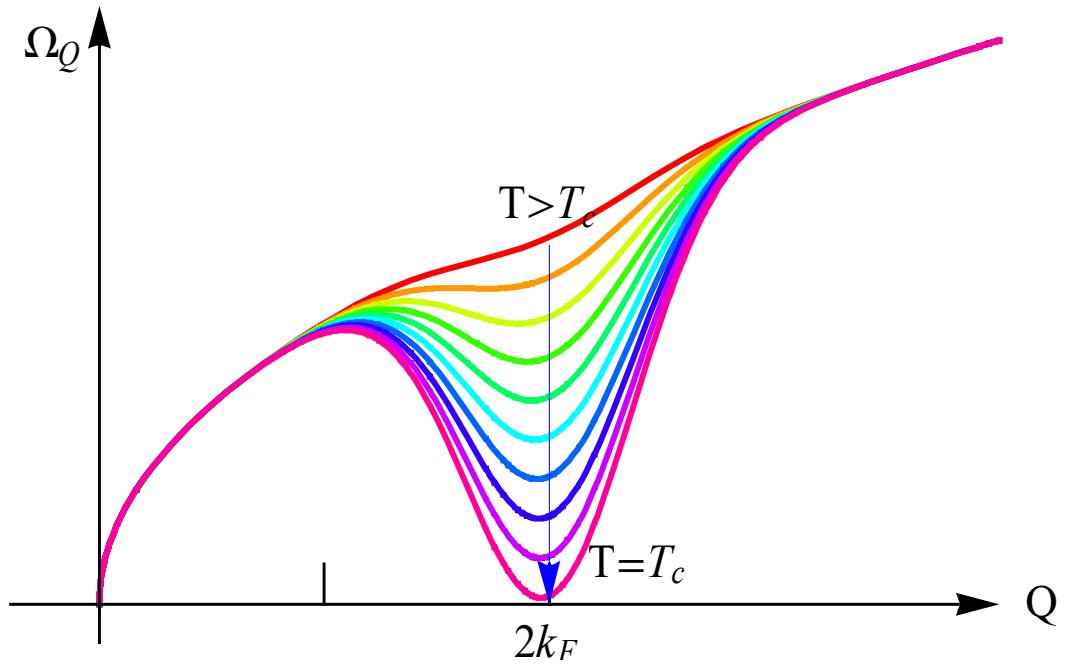which is obtained in the previous section.

Fig.   Schematic diagram of acoustic phonon dispersion relation of a one dimensional metal at various temperatures above T_c.

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14. Order parameter

The Peierls instability occurs in a one-dimensional metal. This instability gives rise to the combination of the electronic density wave and lattice wave with the same wave number $2k_F$. This combined waves are called the charge density wave (CDW). The appearance of the CDW state can be experimentally found by x-ray and neutron scattering.

In the CDW state, the order parameter is the energy gap. This gap is equal to zero at $T = T_c$ and increases with decreasing temperature. We consider the temperature dependence of the energy gap below the critical temperature. We start with

$$\chi(Q,T) = \frac{\omega_Q^2}{v_Q^2}$$

We need to calculate the T dependence of $\chi(Q,T)$.

$$\chi(Q = 2k_F, T) = \frac{1}{N} \sum_k \frac{f(\varepsilon_k^{(+)}) - f(\varepsilon_k^{(-)})}{\varepsilon_k^{(-)} - \varepsilon_k^{(+)}}$$

$$\varepsilon_k^{(\pm)} = \frac{\lambda_k + \lambda_{k-G} \pm \sqrt{(\lambda_k - \lambda_{k-G})^2 + 4|U_G|^2}}{2}$$

$$\begin{aligned}
\lambda_k &= \frac{\hbar^2}{2m}(k^2 - k_F^2) + \varepsilon_F \\
&= \frac{\hbar^2}{2m}(k + k_F)(k - k_F) + \varepsilon_F \\
&\approx \frac{\hbar^2 k_F}{m}(k - k_F) + \varepsilon_F \\
&= \alpha(k - k_F) + \varepsilon_F = -\varepsilon + \varepsilon_F
\end{aligned}$$

$$\begin{aligned}
\lambda_{k-G} &= \frac{\hbar^2}{2m}[(k - G)^2 - k_F^2] + \varepsilon_F \\
&= \frac{\hbar^2}{2m}(k - G + k_F)(k - G - k_F) + \varepsilon_F \\
&\approx -\frac{\hbar^2 k_F}{m}(k - k_F) + \varepsilon_F \\
&= -\alpha(k - k_F) + \varepsilon_F = \varepsilon + \varepsilon_F
\end{aligned}$$

$$\lambda_k + \lambda_{k-G} = 2\varepsilon_F, \qquad \lambda_k - \lambda_{k-G} = 2\alpha(k - k_F)$$

Here we assume that

$$\alpha = \frac{\hbar^2 k_F}{m}, \qquad G = 2k_F \qquad k \approx k_F$$

$$\varepsilon = \alpha(k_F - k), \qquad |U_Q| = \Delta$$

Then we get

$$\varepsilon_k^{(\pm)} = \varepsilon_F \pm \sqrt{\varepsilon^2 + \Delta^2}$$

$$f(\varepsilon_k^{(-)}) = \frac{1}{\exp(-\beta\sqrt{\varepsilon^2 + \Delta^2}) + 1} = \frac{\exp(\beta\sqrt{\varepsilon^2 + \Delta^2})}{\exp(\beta\sqrt{\varepsilon^2 + \Delta^2}) + 1}$$

$$f(\varepsilon_k^{(+)}) = \frac{1}{\exp(\beta\sqrt{\varepsilon^2 + \Delta^2}) + 1}$$

$$f(\varepsilon_k^{(-)}) - f(\varepsilon_k^{(+)}) = \frac{\exp(\beta\sqrt{\varepsilon^2 + \Delta^2}) - 1}{\exp(\beta\sqrt{\varepsilon^2 + \Delta^2}) + 1}$$

$$= \tanh(\frac{\beta\sqrt{\varepsilon^2 + \Delta^2}}{2})$$

$$\chi(Q = 2k_F, T) = \frac{1}{2N}\sum_k \frac{\tanh(\frac{\beta\sqrt{\varepsilon^2 + \Delta^2}}{2})}{\sqrt{\varepsilon^2 + \Delta^2}} = \frac{1}{2N}\sum_k \frac{\tanh(\frac{\beta E}{2})}{E}$$

where

$$E = \sqrt{\varepsilon^2 + \Delta^2}$$

$$\varepsilon_0 = \alpha(k_F - k_0)$$

$$d\varepsilon = -\alpha dk$$

$$\chi(Q,T) = \frac{1}{2N}\sum_k \frac{\tanh(\frac{\beta\sqrt{\varepsilon^2 + \Delta^2}}{2})}{\sqrt{\varepsilon^2 + \Delta^2}}$$

$$= \frac{1}{2N}\int_0^{\varepsilon_0} D(\varepsilon)d\varepsilon \frac{\tanh(\frac{\beta E}{2})}{E}$$

$$= \frac{D(\varepsilon_F)}{2N}\int_0^{\varepsilon_0} d\varepsilon \frac{\tanh(\frac{\beta E}{2})}{E}$$

We note that

$$\frac{2N}{D(\varepsilon_F)}\chi(Q = 2k_F, T) = \frac{1}{\lambda_0} = \ln(1.14\frac{\varepsilon_0}{k_B T})$$

Then we have

$$\frac{1}{\lambda_0} = \int_0^{\varepsilon_0} d\varepsilon \frac{\tanh(\frac{\beta\varepsilon}{2})}{\varepsilon} = \ln(1.14\frac{\varepsilon_0}{k_B T})$$

and

$$\frac{1}{\lambda_0} = \int_0^{\varepsilon_0} d\varepsilon \frac{\tanh(\frac{\beta E}{2})}{E}.$$

14. Calculation of order parameter

$$\frac{1}{\lambda_0} = \int_0^{\varepsilon_0} d\varepsilon \frac{\tanh(\frac{\sqrt{\varepsilon^2 + \Delta^2}}{2k_B T})}{\sqrt{\varepsilon^2 + \Delta^2}}$$

$$= \int_0^{\varepsilon_0} d\varepsilon \{\frac{\tanh(\frac{\sqrt{\varepsilon^2 + \Delta^2}}{2k_B T})}{\sqrt{\varepsilon^2 + \Delta^2}} - \frac{\tanh(\frac{\varepsilon}{2k_B T})}{\varepsilon}\} + \int_0^{\varepsilon_0} d\varepsilon \frac{\tanh(\frac{\varepsilon}{2k_B T})}{\varepsilon}$$

Then we get

$$\frac{1}{\lambda_0} = \int_0^{\varepsilon_0} d\varepsilon \frac{\tanh(\frac{\sqrt{\varepsilon^2 + \Delta^2}}{2k_B T})}{\sqrt{\varepsilon^2 + \Delta^2}}$$

$$= \int_0^{\varepsilon_0} d\varepsilon \frac{\tanh(\frac{\varepsilon}{2k_B T})}{\varepsilon} + \int_0^{\varepsilon_0} d\varepsilon \{\frac{\tanh(\frac{\sqrt{\varepsilon^2 + \Delta^2}}{2k_B T})}{\sqrt{\varepsilon^2 + \Delta^2}} - \frac{\tanh(\frac{\varepsilon}{2k_B T})}{\varepsilon}\} +$$

$$= \ln(\frac{\varepsilon_0}{k_B T} \frac{2e^{-\gamma}}{\pi}) + \int_0^{\varepsilon_0} d\varepsilon [\frac{1}{\sqrt{\varepsilon^2 + \Delta^2}} \tanh(\frac{\sqrt{\varepsilon^2 + \Delta^2}}{2k_B T}) - \frac{1}{\varepsilon} \tanh(\frac{\varepsilon}{2k_B T})]$$

Using the expansion formula

$$\tanh(x) = \sum_{n=0}^{\infty} \frac{8x}{4x^2 + (2n+1)^2 \pi^2}$$

we get

$$\frac{1}{\lambda_0} = \ln(\frac{\varepsilon_0}{k_B T} \frac{2e^{-\gamma}}{\pi}) + \left(\frac{4}{k_B T}\right) \int_0^{\varepsilon_0} \sum_{n=0}^{\infty} [\frac{1}{4\left(\frac{\sqrt{\varepsilon^2 + \Delta^2}}{2k_B T}\right)^2 + (2n+1)^2 \pi^2}$$

$$- \frac{1}{4\left(\frac{\varepsilon}{2k_B T}\right)^2 + (2n+1)^2 \pi^2}]$$

$$= \ln(\frac{\varepsilon_0}{k_B T} \frac{2e^{-\gamma}}{\pi}) - 4\Delta^2 k_B T \sum_{n=0}^{\infty} \int_0^{\varepsilon_0} \frac{d\varepsilon}{[k_B^2 T^2 (2n+1)^2 \pi^2 + \varepsilon^2]^2}$$

Here

$$\int_0^{\varepsilon_0} \frac{d\varepsilon}{[k_B^2 T^2 (2n+1)^2 \pi^2 + \xi^2]^2} = \frac{1}{k_B^3 T^3} \int_0^{\varepsilon_0/k_B T} \frac{dx}{[(2n+1)^2 \pi^2 + x^2]^2}$$

$$= \frac{1}{k_B^3 T^3} \int_0^\infty \frac{dx}{[(2n+1)^2 \pi^2 + x^2]^2}$$

$$= \frac{1}{k_B^3 T^3} \frac{1}{4\pi^2 (2n+1)^3}$$

Then we have

$$\frac{1}{\lambda_0} = \ln(\frac{\varepsilon_0}{k_B T} \frac{2e^{-\gamma}}{\pi}) - \frac{4\Delta^2}{4\pi^2 k_B^2 T^2} \sum_{n=0}^\infty \frac{1}{(2n+1)^3}$$

$$= \ln(\frac{\varepsilon_0}{k_B T} \frac{2e^{-\gamma}}{\pi}) - \frac{\Delta^2}{\pi^2 k_B^2 T^2} \frac{7}{8} \varsigma(3)$$

where

$$\sum_{n=0}^\infty \frac{1}{(2n+1)^3} = \frac{7}{8} \varsigma(3),$$

and $\zeta(3) = 1.2206$. Using the relation

$$\frac{1}{\lambda_0} = \ln(\frac{\varepsilon_0}{k_B T_c} \frac{2e^{-\gamma}}{\pi}),$$

we have

$$\ln(\frac{\varepsilon_0}{k_B T_c} \frac{2e^{-\gamma}}{\pi}) = \ln(\frac{\varepsilon_0}{k_B T} \frac{2e^{-\gamma}}{\pi}) - \frac{\Delta^2}{\pi^2 k_B^2 T^2} \frac{7}{8} \varsigma(3),$$

or

$$\ln(\frac{T}{T_c}) = -\frac{\Delta^2}{\pi^2 k_B^2 T^2} \frac{7}{8} \varsigma(3).$$

or

$$\Delta^2 = \frac{8}{7\varsigma(3)}\pi^2 k_B^2 T_c^2 \frac{T^2}{T_c^2}\ln(\frac{T_c}{T})$$

From this we get the expression for Δ as,

$$\Delta(T) = [\frac{8\pi^2}{7\varsigma(3)}]^{1/2}\pi k_B T_c \frac{T}{T_c}\sqrt{-\ln(\frac{T}{T_c})}$$

$$\approx [\frac{8\pi^2}{7\varsigma(3)}]^{1/2}\pi k_B T_c(1-\frac{T}{T_c})$$

$$= 3.06326 k_B T_c(1-\frac{T}{T_c})^{1/2}$$

((**Mathematical note**))
   Suppose that

$$t = \frac{T}{T_c} = 1-x$$

where x is close to $x \approx 0$ (but $x>0$)

$$\left(\frac{T}{T_c}\sqrt{\ln(\frac{T_c}{T})}\right)^2 = t^2 \ln(\frac{1}{t})$$

$$= -t^2 \ln(t)$$

$$= -(1-x)^2 \ln(1-x)$$

$$= x - \frac{3}{2}x^2 + \frac{1}{3}x^3 + 0(x^4) \approx x$$

In the vicinity of $T = T_c$ (but $T<T_c$), we have a good approximation,

$$\left(\frac{T}{T_c}\sqrt{\ln(\frac{T_c}{T})}\right)^2 \approx (1-t)^{1/2}$$

16.   **Critical behavior of the order parameter (energy gap)**
   The energy gap is obtained as

$$\Delta(T) = \pi k_B T_c \left[\frac{8}{7\varsigma(3)}\right]^{1/2} \frac{T}{T_c} \sqrt{\ln(\frac{T_c}{T})}$$

$$= \pi k_B T_c \left[\frac{8}{7\varsigma(3)}\right]^{1/2} (1-\frac{T}{T_c})^{1/2}$$

$$= 3.06326 k_B T_c (1-\frac{T}{T_c})^{1/2}$$

The energy gap at $T = 0$ K can be evaluated from the energy gap equation at $T = 0$ K

$$\frac{1}{\lambda_0} = \int_0^{\varepsilon_0} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta_0^2}}$$

$$= \ln[\frac{\varepsilon_0 + \sqrt{\Delta_0^2 + \varepsilon_0^2}}{\Delta_0}]$$

$$\approx \ln[\frac{2\varepsilon_0}{\Delta_0}]$$

or

$$\Delta_0 \approx 2\varepsilon_0 \exp(-\frac{1}{\lambda_0}).$$

Together with the relation

$$k_B T_c = 1.13387\varepsilon_0 \exp(-\frac{1}{\lambda_0}),$$

we get the universal relation

$$\frac{2\Delta_0}{k_B T_c} = \frac{4}{1.13387} = 3.52774.$$

The energy gap is the order parameter. Since this order parameter continuously changes with T and reduces to zero. The phase transition is of the second order with the critical exponent $\beta = 1/2$.

$$\frac{\Delta(T)}{\Delta_0} = \frac{2 \times 3.06326 k_B T_c}{3.52774 k_B T_c} (1 - \frac{T}{T_c})^{1/2} = 1.73667(1 - \frac{T}{T_c})^{1/2}$$
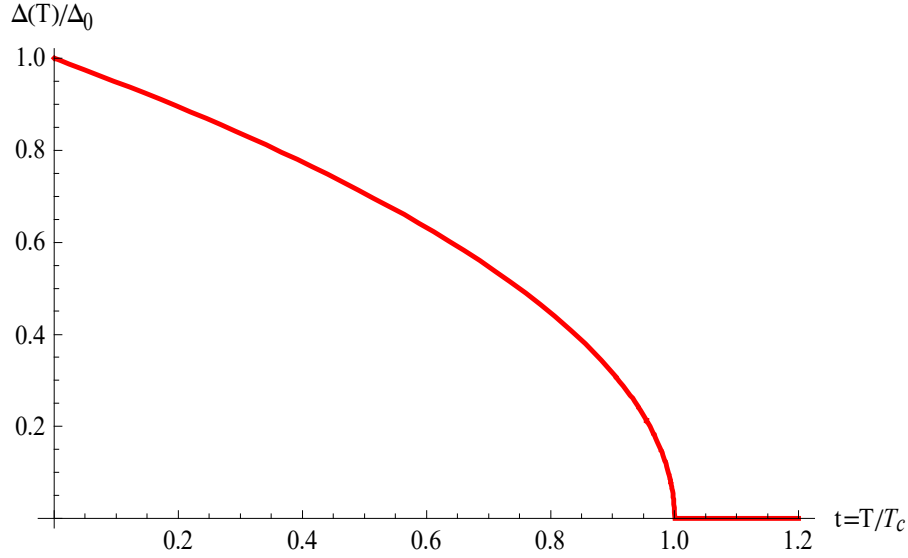
Fig.   Plot of the energy gap Δ/Δ_0 as a function of a reduced temperature $t = T/T_c$.

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APPENDIX   Typical quasi-one dimensional metal

1.   TTF-TCNQ

The tetrathiafulvalene-tetracyanoquinodimethane (TTF-TCNQ) is not a simple metal. Above 58 K, there is an energy gap at $\hbar\omega_g$ = 0.14 eV and an extremely narrow conductivity mode centered at zero frequency. Near 53 K, TTF-TCNQ undergoes a metal-insulator transition to a high-dielectric constant semiconductor in which the oscillator strength is shifted from zero frequency and pinned in the far infrared. In an earlier work.
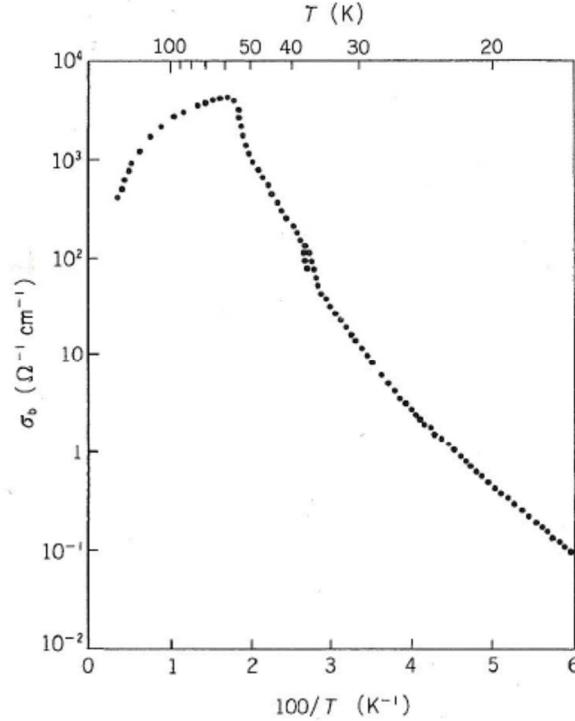
2.   Blue bronze $K_{0.3}MoO_3$

The quasi-one-dimensional (1D) conductor $K_{0.3}MoO_3$ undergoes a Peierls transition at T =183 K. Using cold-neutron scattering, Pouget have succeeded in resolving in frequency and for wave vectors parallel to the chain direction the pre-transitional dynamics and the collective excitations of the phase and of the amplitude of the charge-density-wave (CDW) modulation below T. The pre-transitional dynamics consists of the softening of a Kohn anomaly at the wave vector $2k_F$ together with the critical growth of a central peak in the vicinity of T, . In addition we observed just above T, the beginning of a decoupling between the fluctuations of the phase and of the amplitude of the CDW.