

## Peierls Instability

**Problem.** Consider an ideal one-dimensional electronic system. A weak periodic potential in the form

$$V(x) = V_0 \cos(2k_F x) \quad (1)$$

is added to the Hamiltonian ( $k_F$  is the Fermi momentum;  $\hbar = 1$ ). Calculate the dispersion law for the lowest energy band in the two-band approximation, and evaluate the total ground-state energy of the gas, expressing the result as a difference between the energy of the perturbed and non-perturbed systems.

*Solution*

We start with a general analysis. Our potential is periodic with the period

$$a = \pi/k_F. \quad (2)$$

In 1D, the relation between the number density,  $n$  (of a spin-1/2 system), and the Fermi-momentum is

$$n = 2k_F/\pi. \quad (3)$$

Hence,

$$na = 2, \quad (4)$$

meaning that we have two particles per unit cell, so that the ground state is the band insulator (completely filled lowest band).

Now we find the spectrum of the lowest band in the two-band approximation. The exact system of equations reads

$$\left[ \frac{q^2}{2m} - E \right] C_{\mathbf{q}} + \sum_{\mathbf{G}} U_{\mathbf{G}} C_{\mathbf{q}+\mathbf{G}} = 0. \quad (5)$$

In 1D, and within the two-band approximation, we are left with ( $U_G = V_0/2 \equiv \Delta$ )

$$\left[ \frac{q^2}{2m} - E \right] C_q + \Delta C_{q+G} = 0, \quad G = \pm 2\pi/a. \quad (6)$$

Moreover, in the weak-interaction limit we are interested only in the close vicinities of the resonant points  $q_0 = \pm\pi/a$ , where the hybridization effects are strong enough. Away from these points, for the lowest band we simply have  $C_q \approx 1$ ,  $E \approx q^2/2m$ . By periodicity, it is sufficient to consider the point  $q_0 = -\pi/a$  (for which the resonating  $G$  is  $2\pi/a$ ). Introducing a convenient variable

$$k = q - q_0 \quad (7)$$

and expressing the non-perturbed energies in terms of it,

$$q^2 = (k + q_0)^2 = k^2 + q_0^2 + 2kq_0, \quad (8)$$

$$(q + G)^2 = (k - q_0)^2 = k^2 + q_0^2 - 2kq_0, \quad (9)$$

we get the system of equations

$$\begin{bmatrix} (k^2 + q_0^2 + 2kq_0)/2m - E & \Delta \\ \Delta & (k^2 + q_0^2 - 2kq_0)/2m - E \end{bmatrix} \begin{bmatrix} C_q \\ C_{q+G} \end{bmatrix} = 0. \quad (10)$$

The spectrum is found from the requirement that the determinant be zero. We get two solutions:

$$E = \frac{k^2 + q_0^2}{2m} \pm \sqrt{\left(\frac{kq_0}{m}\right)^2 + \Delta^2}, \quad (11)$$

of which we are interested only in the lowest one:

$$E = \frac{k^2 + q_0^2}{2m} - \sqrt{\left(\frac{kq_0}{m}\right)^2 + \Delta^2} \quad (\text{lowest band}). \quad (12)$$

Within the same parameterization, the spectrum of the non-perturbed system is obtained by simply setting  $\Delta = 0$ :

$$E^{(0)} = \frac{k^2 + q_0^2}{2m} - \left| \frac{kq_0}{m} \right|, \quad (13)$$

leading to the following expression for the energy difference

$$E(k) - E^{(0)}(k) = |v_0 k| - \sqrt{(v_0 k)^2 + \Delta^2} \quad (|k| \ll |q_0|), \quad (14)$$

where

$$v_0 = \left. \frac{dE^{(0)}(k)}{dk} \right|_{k=-0}. \quad (15)$$

Note that replacing  $q_0/m$  with  $v_0$  defined by Eq. (15) renders Eq. (14) more general: now it applies to the case of arbitrary dispersion of the electrons. In particular, Eq. (14) works for the case of any periodic external potential, on top of which the weak potential (1) is imposed.

The system energy (expressed as the energy difference between the energy of the system with and without weak potential per unit length) is:

$$\delta E_{\text{el}} = 2 \int \left[ E(k) - E^{(0)}(k) \right] \frac{dk}{2\pi} = 2 \int \left[ |v_F k| - \sqrt{(v_F k)^2 + \Delta^2} \right] \frac{dk}{2\pi}. \quad (16)$$

(At this point we recall that  $q_0 = k_F$ , meaning that  $v_0$  is the Fermi velocity,  $v_F$ .) Introducing the dimensionless variable

$$x = \frac{kv_F}{\Delta} \quad (17)$$

and taking into account the  $x \rightarrow -x$  symmetry, we get

$$\delta E_{\text{el}} = \frac{2\Delta^2}{\pi v_F} \int_0^{x_*} \left( x - \sqrt{1+x^2} \right) dx, \quad x_* = \frac{v_F k_F}{\Delta} \gg 1. \quad (18)$$

The main contribution to the integral comes from  $x \gg 1$ , where

$$\sqrt{1+x^2} \approx x + \frac{1}{2x} \quad (19)$$

so that with the logarithmic accuracy

$$\int_0^{x_*} \left( x - \sqrt{1+x^2} \right) dx \approx -\frac{\ln x_*}{2}, \quad (20)$$

and the final result is

$$\delta E_{\text{el}} = -\frac{\Delta^2}{\pi v_F} \ln \frac{v_F k_F}{\Delta}, \quad \frac{v_F k_F}{\Delta} \gg 1. \quad (21)$$

**Peierls instability.** The result we obtained is central for the effect known as *Peierls instability*. The energy gain from a weak potential (1) scales as  $V_0^2$  times the (arbitrarily) large logarithm. This is to be contrasted to the energy cost for creating the potential (1) by slightly changing the distances between ions. This energy cost scales only as  $V_0^2$ . Hence, a sufficiently weak distortion of the ionic lattice is *always favorable* in the otherwise metallic phase. A very common pattern of such distortion is dimerization. It

takes place when there is a chain of identical atoms with an odd number of electrons per atom. Here the distances between adjacent ions alternate (shorter–longer), leading to doubling the lattice period, and, correspondingly, opening the insulating gap. Such a state is called Peierls insulator.

**Peierls transition.** As an instructive example, consider a 1D chain of hydrogen atoms. At zero pressure, the chain is a molecular insulator. While it is legitimate to call this state Peierls insulator, here we should keep in mind that the dimerization effect is so strong that it makes little sense to talk of Peierls instability. The situation changes, however, at high pressure. Here the Coulomb interaction between the electrons and ions (and between electrons themselves) becomes perturbative, the Peierls dimerization gets weaker to the degree that it can easily be suppressed by a moderate temperature. This phenomenon is called *Peierls transition*. Strictly speaking, there are no finite-temperature phase transitions in 1D systems with short-range interactions. We are thus talking of a sharp crossover at a certain temperature  $T_c \sim \Delta_0$ , where  $\Delta_0$  is the optimal value of the parameter  $\Delta$  obtained by minimizing the total energy difference

$$\delta E_{\text{tot}} = \delta E_{\text{el}} + \delta E_{\text{latt}}, \quad (22)$$

where  $\delta E_{\text{latt}}$  is the energy cost of lattice distortion. In accordance with our discussion, we have

$$\delta E_{\text{tot}} \propto -\Delta^2 \left[ \ln \frac{v_F k_F}{\Delta} - B \right], \quad (23)$$

where  $B \gg 1$  is a certain dimensionless constant controlling the weakness of the Peierls effect.<sup>1</sup> Minimizing  $\delta E_{\text{tot}}$  with respect to  $\delta$ , we find

$$\Delta_0 = c \varepsilon_F e^{-B}, \quad (24)$$

where  $\varepsilon_F \sim v_F k_F$  is the Fermi energy and  $c$  is the dimensionless constant of order unity. The precise value of this constant is system dependent, since it requires to go beyond the logarithmic accuracy in calculating the integral (20), which in its turn requires the precise form for  $E(k) - E^{(0)}(k)$  at  $k \sim k_F$ .

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<sup>1</sup>In the model where the lattice is replaced with an elastic medium coupled to the gas of ideal electrons, we have  $B = \pi v_F / g^2$ , with  $g$  the coupling constant.