11 Electron-Phonon Interaction:

In the last chapter we concluded that one needs a virtual exchange of quasi-particles between two electrons in order to render an effective attractive interaction between two electrons. As a concrete example we work out in this chapter the quantum theory of the electron-phonon coupling. To this end we cover at first the lattice vibrations classically. Afterwards, we go over to a quantum mechanical description. In particular, we formulate the electron-phonon coupling within the realm of second quantization. By eliminating perturbatively the phonons from the description, we derive at the end at the residual pairing Hamiltonian for electrons. This procedure for dealing with the lattice vibrations can be considered as being representative for all other quasi-particles as, for instance, excitons or plasmons.

11.1 Lattice Vibrations:

Let us start with summarizing the basic properties of lattice vibrations in a solid.

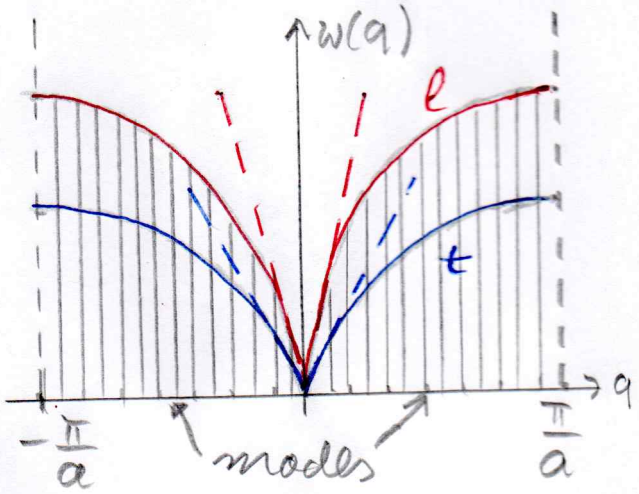
11.1.1 Dispersion Relations:

A dispersion relation $\omega = \omega(\vec{q})$ for lattice vibrations is characterized by two properties. It is usually rotationally symmetric

$$\omega(\vec{q}) = \omega(|\vec{q}|) \tag{11.1}$$

and for small wave vectors it turns out to be linear

$$\omega(\vec{q}) \propto c\,|\vec{q}| \tag{11.2}$$



the latter defining the sound velocity in the continuum limit. One distinguishes between longitudinal lattice vibrations (——) with the dispersion $\omega_l = \omega_l(\vec{q})$ and transversal lattice vibrations (——) with the dispersion $\omega_t = \omega_t(\vec{q})$, which is doubly degenerate. In general we have

$$\omega_l(\vec{q}) > \omega_t(\vec{q}) \tag{11.3}$$

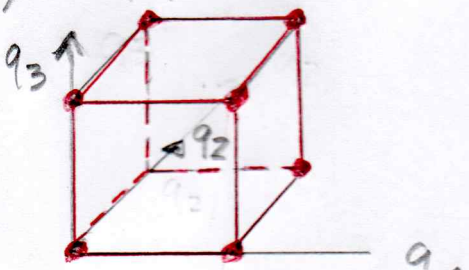
so the sound velocities of longitudinal lattice vibrations is larger than the corresponding one of transversal lattice vibrations.

The N atoms of a solid correspond to 3N degrees of freedom. They are reflected in the wave vector space by N(3N) discrete $\vec{q}$-values and, thus, N(3N) discrete longitudinal (transversal) lattice vibration modes. The continuously drawn dispersion relations have, therefore, to be considered as envelopes of the possible discrete modes of lattice vibrations.

11.1.2 Density of States:

The possible wave vectors $\vec{q}$ for a finite rectangular solid of edge length L have for periodic boundary conditions the discrete values

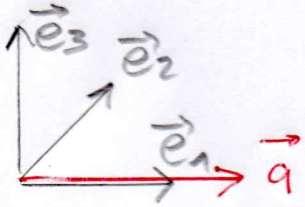
$$\vec{q}(n_1,n_2,n_3) = \frac{2\pi}{L}\begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix} \; ; n_i \in \mathbb{Z} \; ; i=1,2,3 \qquad (11.4)$$



Thus, in $\vec{q}$-space the possible states are represented by a point lattice. The elementary volume is given by

$$\Omega = \left(\frac{2\pi}{L}\right)^3 = \frac{(2\pi)^3}{V} \qquad (11.5)$$

We now denote with the index r the respective polarization directions, so r=1 (r=2,3) describes the polarizations of the longitudinal (transversal) lattice vibrations.



For all three polarization directions one obtains the same homogeneous, isotropic density of states in $\vec{q}$-space via the elementary volume Ω:

$$Z_r(\vec{q}) = \frac{1}{\Omega} \overset{(11.5)}{=\!=} \frac{V}{(2\pi)^3} \qquad (11.6)$$

This density of states in $\vec{q}$-space can now be converted into a corresponding density of states in ω-space denoted by $Z_r(\omega_r)$. To this end one demands that the number of states in the frequency interval $[\omega_r, \omega_r + d\omega_r]$ equals due to the isotropy of the dispersions to the number of states in the interval $[q, q+dq]$:

$$Z_r(\omega_r)d\omega_r = Z_r(q)4\pi q^2 dq \overset{(11.6)}{\Longrightarrow} Z_r(\omega_r) = \frac{V}{2\pi^2} q^2(\omega_r)\frac{dq(\omega_r)}{d\omega_r} \qquad (11.7)$$

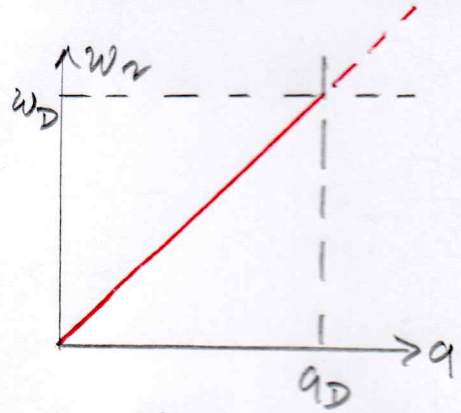
11.1.3 Debye Assumptions:

Debye made the following assumptions for approximately describing lattice vibrations:

1) A crystal is considered to be isotropic continuum. The real dispersion relation sketched on page 156 is approximated to be linear

$$\omega_r(q) = c_r \, q \qquad (11.8)$$

with the corresponding sound velocity c_r of phonon branch r.



2) There is a maximal frequency, the so-called Debye frequency:
   a) Within the spring-mass model mentioned below we can argue that finite number of springs in a solid leads to a finite upper bound of the lattice vibration frequencies.
   b) Via (11.8) a maximal frequency ω_D corresponds to a maximal wave vector q_D. This is reasonable as it does not make sense to consider for lattice vibrations wave lengths, which are smaller than twice the lattice distance a.

3) The lattice structure is indirectly included in the description as the number of degrees of freedom is fixed to be 3N:

$$\int_0^{\omega_D} d\omega \; z(\omega) = 3N \qquad (11.9)$$

11.1.4 Debye Approximation:

Inserting the linear dispersion (11.8) into (11.7) yields for the respective polarization direction

$$z_r(\omega_r) = \frac{V}{2\pi^2} \frac{\omega_r^2}{c_r^3} \qquad (11.10)$$

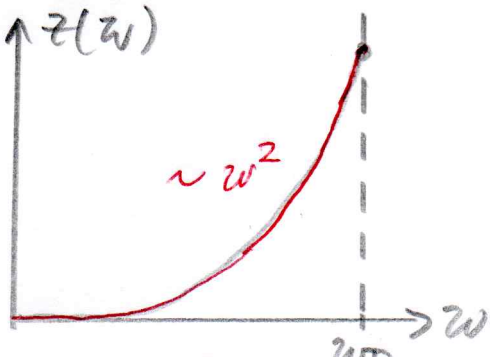
Assuming a degeneracy of the two transversal phonon branches amounts to have just one transversal sound velocity. Adding then the density of states of all three branches

$$z(\omega) = z_l(\omega) + 2 z_t(\omega) \qquad (11.11)$$

we get due to (11.10)

$$z(\omega) = \frac{V}{2\pi^2} \left(\frac{1}{c_l^3} + \frac{2}{c_t^3} \right) \omega^2 \qquad (11.12)$$

Thus the density of states for phonons increases quadratically up to the Debye frequency.



The constraint (11.9) then allows to determine the Da-

Debye frequency according to

$$3N \overset{(11.10)}{\underset{(11.12)}{}} \frac{V}{(2\pi)^2}\left(\frac{1}{c_e^3}+\frac{2}{c_t^3}\right)\frac{\omega_D^3}{3} \Rightarrow \frac{1}{\omega_D^3}=\frac{1}{18\pi^2}\frac{N}{V}\left(\frac{1}{c_e^3}+\frac{2}{c_t^3}\right) \quad (11.13)$$

Here the atomic volume is given by

$$\frac{V}{N}=a^3 \quad (11.14)$$

with the lattice distance a. Thus, defining an average sound velocity c via

$$\frac{1}{c^3}=\frac{1}{3}\left(\frac{1}{c_e^3}+\frac{2}{c_t^3}\right) \quad (11.15)$$

the defining equation (11.13) for the Debye frequency ω_D reduces to

$$\frac{6\pi^2}{a^3}=\left(\frac{\omega_D}{c}\right)^3 \quad (11.16)$$

Introducing a Debye wave vector with

$$q_D \overset{(11.8)}{=\!=} \frac{\omega_D}{c} \quad (11.17)$$

we finally obtain from (11.16)

$$q_D=\frac{(6\pi^2)^{1/3}}{a}\approx\frac{3.9}{a} \quad (11.18)$$

which is of the order of the reciprocal lattice constants. Thus confirms the above statement that it does not make sense to consider lattice vibrations with a wavelength smaller than $2a$.

11.1.5 Remarks:

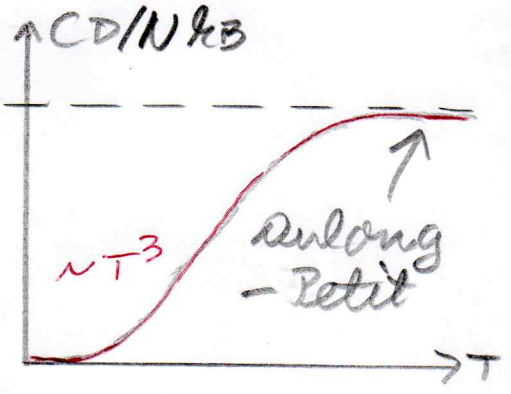
1) In continuum theory it is shown that the sound velocities of longitudinal and transversal lattice vibrations are given by the Lamé constants λ, μ and the mass density ϱ:

$$c_e=\sqrt{\frac{\lambda+2\mu}{\varrho}}\,, \quad c_t=\sqrt{\frac{\mu}{\varrho}} \quad (11.19)$$

2) Within the Debye approximation the adjacent result for the temperature dependence of the heat capacity is obtained:

a) $\lim\limits_{T\to\infty} \frac{C_D}{N k_B}=3$ (11.20)

b) $C_D(T)\sim T^3$, small T (11.21)



3) Considering later on the virtual charge of phonons

between two electrons only those frequencies of the lattice vibrations are taken into account, which are possible due to the Debye assumptions.

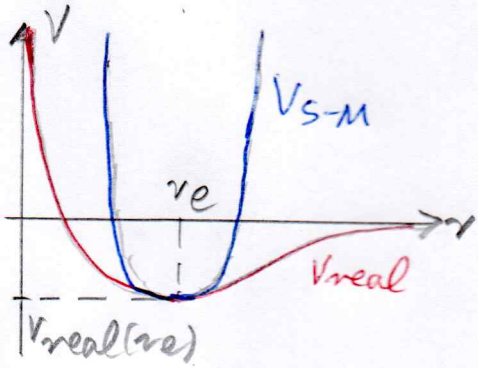
4) Note that high Tc superconductors provide dispersion relations for lattice vibrations, which are highly anisotropic due to the layered crystal structure.

11.2 Lattice vibrations of a linear chain:

In order to make the above discussion of lattice vibrations more concrete, we consider now the versatile model of a linear chain. In this way we introduce a general concept, which turns out to be useful to work out therein the subsequent quantum mechanical description of lattice vibrations.

11.2.1 Spring-mass model:

The positively charged ion cores are glued together by the negatively charged electrons. This yields the adjacent potential curve V_{real} (——), where r denotes the distance between two ion cores. The resulting equilibrium distance is indicated by r_e.



Expanding the potential V_{real} around the equilibrium r_e up to second order, one obtains the harmonic approximation V_{s-m} (——):

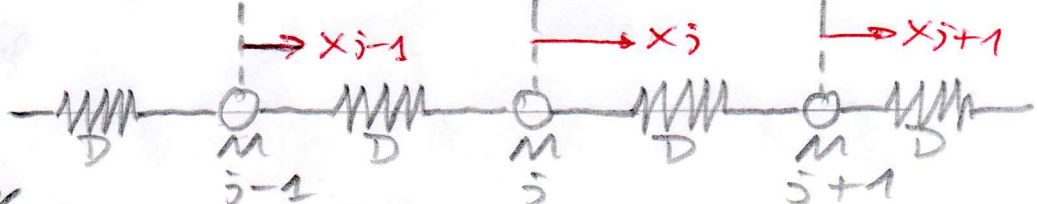
$$V_{s-m}(r) = V_{real}(r_e) + \frac{1}{2} V''_{real}(r_e)(r-r_e)^2 + \dots \qquad (11.22)$$

This harmonic approximation corresponds to a spring-mass model:

1) A positively charged ion core is substituted by a mass point M.
2) The impact of the electrons on the cores is modelled by springs between the cores with the spring constant

$$D = V''_{real}(r_e) \qquad (11.23)$$

The resulting spring-mass model describes a linear chain:



11.2.2 Equations of Motion:

We now embark upon deriving the equations of motion for the elongations out of equilibrium x_j. Due to the spring-mass model we have only to take into account the forces between the considered mass and the neighbouring masses:

$$M \ddot{x}_j = D(x_{j+1} - x_j) - D(x_j - x_{j-1}) \tag{11.24}$$

Here $x_{j+1} - x_j$ ($x_j - x_{j-1}$) represents the relative elongation of the $(j+1)$th and the jth (jth and $(j-1)$th) mass point. Introducing as an abbreviation the eigenfrequency ω_0 of a harmonic oscillator with mass M and spring constant D according to

$$\omega_0 = \sqrt{\frac{D}{M}} \tag{11.25}$$

the equations of motion (11.24) reduce to a set of coupled ordinary differential equations

$$\ddot{x}_j = \omega_0^2 (x_{j+1} - 2x_j + x_{j-1}); \quad j = 1, \dots, N \tag{11.26}$$

It has to be solved with appropriate boundary conditions, which we choose to be periodic

$$x_1 = x_{N+1} \tag{11.27}$$

Here N denotes the number of mass points, which is assumed to be even for later convenience.

11.2.3 Solution:

Due to the periodic boundary condition (11.27) the solutions of (11.26) have the period Na provided that a stands for the equilibrium distance between two adjacent mass points. Therefore, it is appropriate to solve (11.26) with a spatial Fourier transformation as an ansatz:

$$x_j = \frac{1}{\sqrt{N}} \sum_n \xi_n e^{iq_n y_j} \tag{11.28}$$

Here the discrete wave vectors are given by

$$q_n = \frac{2\pi}{aN} n; \quad n = -\frac{N}{2} + 1, \dots, \frac{N}{2} \tag{11.29}$$

and the equilibrium positions read

$$y_j = ja; \quad j = 1, \dots, N \tag{11.30}$$

Indeed, the ansatz (11.28)-(11.30) fulfills the periodic boundary condition (11.27):

$$x_1 = \frac{1}{\sqrt{N}} \sum_n \xi_n e^{i\frac{2\pi}{aN}a} = \frac{1}{\sqrt{N}} \sum_n \xi_n e^{i\frac{2\pi}{aN}(N+1)a} = x_{N+1} \quad \checkmark$$

Therefore, we can now insert the ansatz (11.28) into the equations of motion (11.26):

$$\frac{1}{\sqrt{N}} \sum_n \ddot{\xi}_n e^{iq_n \gamma_j} = \omega_0^2 \frac{1}{\sqrt{N}} \sum_n \xi_n \left(e^{iq_n \gamma_{j+1}} - 2e^{iq_n \gamma_j} + e^{iq_n \gamma_{j-1}} \right)$$

$$\underline{(11.30)} \quad \omega_0^2 \frac{1}{\sqrt{N}} \sum_n \xi_n e^{iq_n \gamma_j} \left(e^{iq_n a} - 2 + e^{-iq_n a} \right) \quad (11.31)$$

Multiplying (11.31) with $e^{-iq_{n'}\gamma_j}/\sqrt{N}$ and summing over j yields

$$\sum_n \left\{ \ddot{\xi}_n - \omega_0^2 \left(e^{iq_n a} - 2 + e^{-iq_n a} \right) \xi_n \right\} \cdot \frac{1}{N} \sum_{j=1}^{N} e^{i(q_n - q_{n'})\gamma_j} \quad (11.32)$$

due to (11.30) the sum over j corresponds to the geometric series:

$$\sum_{j=1}^{N} x^j = \frac{x}{1-x}(1-x^N) \quad (11.33)$$

so we conclude

$$\frac{1}{N} \sum_{j=1}^{N} e^{i(q_n - q_{n'})\gamma_j} \overset{(11.29),(11.30)}{=} \frac{1}{N} \frac{e^{i\frac{2\pi}{N}(n-n')}}{1 - e^{i\frac{2\pi}{N}(n-n')}} \cdot \left(1 - e^{i2\pi(n-n')} \right)$$

$$= \begin{cases} 0 & ; n \neq n' \\ 1 & ; n = n' \end{cases} = \delta_{n,n'} \quad (11.34)$$

Inserting (11.34) in (11.32) yields

$$\ddot{\xi}_n + 4\omega_0^2 \sin^2\left(\frac{q_n a}{2}\right) \xi_n = 0 \quad (11.35)$$

Thus, the spatial Fourier ansatz (11.28) had the effect to decouple the coupled set of differential equations (11.26). The vibrations of the whole chain correspond to elongations of uncoupled harmonic oscillators (11.35), which represent the normal modes.

11.2.4 Dispersion Relation:

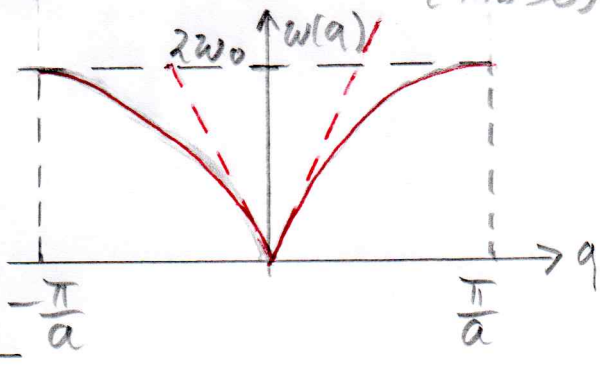
The differential equation of second order (11.35) has the following general solution:

$$\xi_q(t) = A_q^{(1)} e^{-i\omega(q)t} + A_q^{(2)} e^{i\omega(q)t} \quad (11.36)$$

Inserting (11.36) in (11.35) yields the dispersion relation

$$\omega(q) = 2\omega_0 \left| \sin\frac{qa}{2} \right| \quad (11.37)$$

due to (11.29) the range of possible



wave vector values is restricted to the interval $(-\frac{\pi}{a}, +\frac{\pi}{a}]$, which is called Brillouin zone. Let us now discuss the following consequences of (11.37):

1) For long-wave length lattice vibrations we obtain, as assumed by Debye, a linear dispersion relation:

$$\omega(q) \overset{(11.37)}{=\!=} 2\omega_0 \frac{qa}{2} \Rightarrow \omega(q) = c\,q, \quad c = \omega_0 a \tag{11.38}$$

2) The dispersion relation (11.37) allows a maximal frequency $2\omega_0$, which plays the role of the Debye frequency ω_D.

3) From (11.25) and (11.37) we read off

$$\omega(q) \sim \frac{1}{\sqrt{M}} \tag{11.39}$$

which represents a first indication for the isotope effect observed for the critical temperature of superconductivity.

11.2.5 Classical Hamiltonian:

Inserting (11.36) into (11.28) yields for the elongation at site j

$$x_j(t) = \frac{1}{\sqrt{N}} \sum_q \left\{ A_q^{(1)} e^{-i\omega(q)t} + A_q^{(2)} e^{i\omega(q)t} \right\} e^{iqaj} \tag{11.40}$$

However, we have to demand that (11.40) is real:

$$x_j^*(t) = x_j(t) \tag{11.41}$$

By evaluating the complex conjugate of (11.40) we perform the substitution $q' = -q$ in the summation and take into account that the dispersion (11.37) is even:

$$\omega(-q) = \omega(q) \tag{11.42}$$

With this we obtain

$$x_j^*(t) = \frac{1}{\sqrt{N}} \sum_q \left\{ A_{-q}^{(1)*} e^{i\omega(q)t} + A_{-q}^{(2)*} e^{-i\omega(q)t} \right\} e^{iqaj} \tag{11.43}$$

Therefore, we conclude from (11.41) due to (11.40) and (11.43) that the Fourier coefficients $A_q^{(1)}$, $A_q^{(2)}$ have to fulfill

$$A_q^{(1)} = A_q, \quad A_q^{(2)} = A_{-q}^{(1)*} = A_{-q}^* \tag{11.44}$$

so that (11.40) reduces to

$$x_j(t) = \frac{1}{\sqrt{N}} \sum_q \left\{ A_q e^{-i\omega(q)t} + A_{-q}^* e^{i\omega(q)t} \right\} e^{iqaj} \tag{11.45}$$

Correspondingly, the momentum of the elongation at site j reads

$$p_j(t) = M \dot{x}_j(t) = \frac{1}{\sqrt{N}} \sum_q (-i)\omega(q) \left\{ A_q e^{-i\omega(q)t} - A_{-q}^* e^{i\omega(q)t} \right\} e^{iqaj} \tag{11.46}$$

The classical Hamiltonian of the spring-mass model is given by a sum of the corresponding kinetic and potential energy of the linear chain, respectively:

$$H = \sum_{j=1}^{N} \frac{p_j^2}{2m} + \frac{m}{2} \sum_{j=1}^{N} \omega_0^2 (x_{j+1} - x_j)^2 \qquad (11.47)$$

Indeed, the Hamilton equations

$$\dot{x}_j = \frac{\partial H}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial H}{\partial x_j} \qquad (11.48)$$

reduce with the classical Hamiltonian (11.47) to the equations of motion (11.26). On the other hand, inserting the normal mode decompositions (11.46) and (11.47) into (11.48) yields a corresponding decomposition of the classical Hamiltonian. A lengthy but straightforward calculation results in the kinetic energy

$$T = \frac{m}{2} \sum_q \omega(q)^2 \{ A_q A_q^* + A_q^* A_q - A_q^2 e^{-2i\omega(q)t} - A_q^{*2} e^{2i\omega(q)t} \} \qquad (11.49)$$

and, correspondingly, the potential energy

$$V = \frac{m}{2} \sum_q \omega(q)^2 \{ A_q A_q^* + A_q^* A_q + A_q^2 e^{-2i\omega(q)t} + A_q^{*2} e^{2i\omega(q)t} \} \qquad (11.50)$$

Thus, adding both energy contributions we find that the sum terms out to be independent of time, which reflects the conservation of energy:

$$H = T + V = \sum_q m\omega(q)^2 (A_q A_q^* + A_q^* A_q) \qquad (11.51)$$

11.3 Quantization of Lattice Vibrations:

Now we quantize the lattice vibrations of the linear chain. To this end both the elongations (11.45) and their corresponding momenta (11.46) become operators

$$\hat{x}_j(t) = \frac{1}{\sqrt{N}} \sum_q \{ \hat{A}_q e^{-i\omega(q)t} + \hat{A}_{-q}^+ e^{i\omega(q)t} \} e^{iqx_j} \qquad (11.52)$$

$$\hat{p}_j(t) = \frac{1}{\sqrt{N}} \sum_q (-i)\omega(q) m \{ \hat{A}_q e^{-i\omega(q)t} + \hat{A}_{-q}^+ e^{i\omega(q)t} \} e^{iqx_j} \qquad (11.53)$$

and we demand canonical equal-time bosonic commutation relations

$$[\hat{x}_j(t), \hat{x}_{j'}(t)]_- = [\hat{p}_j(t), \hat{p}_{j'}(t)]_- = 0, \quad [\hat{x}_j(t), \hat{p}_{j'}(t)]_- = i\hbar\delta_{jj'} \qquad (11.54)$$

This has consequences for the commutation relations of the normal mode operators A_q, A_q^+ in (11.52), (11.53). In order to deduce them, we have first to invert (11.52),

(11.53) and expresses $\hat{A}_q$ in terms of $\hat{x}_j(t), \hat{p}_j(t)$. To this end we get

$$\frac{1}{\sqrt{N}} \sum_j \hat{x}_j(t) e^{-iqy_j} \underset{(11.52)}{=} \hat{A}_q e^{-i\omega(q)t} + \hat{A}_{-q}^+ e^{i\omega(q)t} \quad (11.55)$$

$$\frac{1}{\sqrt{N}} \sum_j \hat{p}_j(t) e^{-iqy_j} \underset{(11.53)}{=} -i\omega(q)m \{\hat{A}_q e^{-i\omega(q)t} - \hat{A}_{-q}^+ e^{i\omega(q)t}\} \quad (11.56)$$

Adding (11.55) and (11.56) we then obtain

$$\hat{A}_q = \frac{1}{2} \frac{1}{\sqrt{N}} \sum_j \left\{ \hat{x}_j(t) + \frac{i}{\omega(q)m} \hat{p}_j(t) \right\} e^{i\omega(q)t - iqy_j} \quad (11.57)$$

Thus, we conclude immediately

$$[\hat{A}_q, \hat{A}_{q'}]_- = [\hat{A}_q^+, \hat{A}_{q'}^+]_- \underset{(11.54),(11.57)}{=} 0 \quad (11.58)$$

and for the non-trivial commutator we yield

$$[\hat{A}_q, \hat{A}_{q'}^+]_- \underset{(11.54),(11.57)}{=} \frac{1}{4} \frac{1}{N} \sum_j e^{i\omega(q)t - iqy_j} \frac{1}{N} \sum_{j'} e^{-i\omega(q')t + iq'y_{j'}}$$

$$\left\{ \frac{i}{\omega(q)m} [\hat{p}_j(t), \hat{x}_{j'}(t)]_- - \frac{i}{\omega(q')m} [\hat{x}_j(t), \hat{p}_{j'}(t)]_- \right\} \underset{(11.54)}{=} e^{i\{\omega(q) - \omega(q')\}t}$$

$$\cdot \frac{\hbar}{4m} \left\{ \frac{1}{\omega(q)} + \frac{1}{\omega(q')} \right\} \frac{1}{N} \sum_j e^{i(q'-q)y_j} \underset{(11.34)}{=} \frac{\hbar}{2m\omega(q)} \delta_{qq'} \quad (11.59)$$

Thus, in order to obtain at the end canonical bosonic commutation relations for the normal mode operators we define

$$\hat{A}_q = \sqrt{\frac{\hbar}{2m\omega(q)}}\, \hat{b}_q \quad (11.60)$$

and get with this

$$[\hat{b}_q, \hat{b}_{q'}]_- = [\hat{b}_q^+, \hat{b}_{q'}^+]_- \underset{(11.60)}{\overset{(11.58)}{=}} 0, \quad [\hat{b}_q, \hat{b}_{q'}^+]_- \underset{(11.60)}{\overset{(11.59)}{=}} \delta_{q,q'} \quad (11.61)$$

Furthermore, inserting (11.60) into (11.52) yields

$$\hat{x}_j(t) = \frac{1}{\sqrt{N}} \sum_q \sqrt{\frac{\hbar}{2m\omega(q)}} \{\hat{b}_q e^{-i\omega(q)t} + \hat{b}_{-q}^+ e^{i\omega(q)t}\} e^{iqy_j} \quad (11.62)$$

And quantizing the classical Hamiltonian (11.51) by taking into account (11.60) and (11.61), the resulting Hamilton operator reads

$$\hat{H} = \sum_q \hbar\omega(q) \left(\hat{b}_q^+ \hat{b}_q + \frac{1}{2} \right) \quad (11.63)$$

Having obtained in this way the quantization of the vibrations for the linear chain, we now generalize the results directly to the three-dimensional case.

To this end we identify q by the wave vector $\vec{q}$, $y_j = ja$ with the position vector $\vec{r}$ and $\hat{x}_j$ with the shift operator $\vec{s}(\vec{r})$.

Furthermore, we introduce the respective polarisation vectors $\vec{e}_\nu(\vec{q})$ with $\nu = 1,2,3$, which fulfill the orthonormality relation

$$\vec{e}_\nu(\vec{q}) \cdot \vec{e}_{\nu'}(\vec{q}) = \delta_{\nu,\nu'} \tag{11.64}$$

and substitute $\omega(q)$ with the corresponding dispersion relations $\omega_{\vec{q},\nu}$. With this we obtain from (11.62) for the shift operator in the Schrödinger picture with setting $t=0$

$$\hat{\vec{s}}(\vec{r}) = \sum_{\vec{q},\nu} \frac{\vec{e}_\nu(\vec{q})}{\sqrt{N}} \sqrt{\frac{\hbar}{2M\omega_{\vec{q}\nu}}} \left(\hat{b}_{\vec{q}\nu} + \hat{b}^+_{-\vec{q}\nu} \right) e^{i\vec{q}\cdot\vec{r}} \tag{11.65}$$

Here the raising and lowering operators for phonons fulfill canonical commutation relations similar to (11.61):

$$[\hat{b}_{\vec{q}\nu}, \hat{b}_{\vec{q}'\nu'}]_- = [\hat{b}^+_{\vec{q}\nu}, \hat{b}^+_{\vec{q}'\nu'}]_- = 0, \quad [\hat{b}_{\vec{q}\nu}, \hat{b}^+_{\vec{q}'\nu'}]_- = \delta_{\vec{q}\vec{q}'} \delta_{\nu\nu'} \tag{11.66}$$

Thus, $\hat{b}_{\vec{q}\nu}$ and $\hat{b}^+_{\vec{q}\nu}$ describe the annihilation and creation of a phonon with wave vector $\vec{q}$ and mode ν, respectively. And, analogous to (11.63), the corresponding Hamilton operator reads

$$\hat{H} = \sum_{\vec{q},\nu} \hbar\omega_{\vec{q},\nu} \left(\hat{b}^+_{\vec{q}\nu} \hat{b}_{\vec{q}\nu} + \frac{1}{2} \right) \tag{11.67}$$

which represents free phonons.

11.4 Volume Dilatation:

In continuum mechanics one models a local deformation of the material by the coordinate transformation

$$\vec{r}\,' = \vec{r} + \vec{s}(\vec{r}) \tag{11.68}$$

where $\vec{s}(\vec{r})$ represents the local shift. The corresponding Jacobi matrix of the coordinate transformation reads:

$$J_{ij} = \frac{\partial x_i'}{\partial x_j} \overset{(11.68)}{=} \delta_{ij} + \frac{\partial s_i(\vec{r})}{\partial x_j} \tag{11.69}$$

By writing down explicitly the components of the Jacobi matrix (11.69)

$$(J_{ij}) = \begin{pmatrix} 1 + \frac{\partial s_x(\vec{r})}{\partial x} & \frac{\partial s_x(\vec{r})}{\partial y} & \frac{\partial s_x(\vec{r})}{\partial z} \\ \frac{\partial s_y(\vec{r})}{\partial x} & 1 + \frac{\partial s_y(\vec{r})}{\partial y} & \frac{\partial s_y(\vec{r})}{\partial z} \\ \frac{\partial s_z(\vec{r})}{\partial x} & \frac{\partial s_z(\vec{r})}{\partial y} & 1 + \frac{\partial s_z(\vec{r})}{\partial z} \end{pmatrix} \tag{11.70}$$

we recognise the leading change of its determinant for

small shifts $\vec{S}(\vec{r})$:

$$|\det J(\vec{r})| = 1 + \Theta(\vec{r}) \tag{11.71}$$

Here the volume dilatation turns out to be

$$\Theta(\vec{r}) = \operatorname{div} \vec{S}(\vec{r}) \tag{11.72}$$

Thus, in the framework of second quantization, this yield a volume dilatation operator

$$\hat{\Theta}(\vec{r}) = \operatorname{div} \hat{\vec{S}}(\vec{r}) \tag{11.73}$$

which reads with the phonon shift operator (11.65)

$$\hat{\Theta}(\vec{r}) = \sum_{\vec{q},\nu} i \frac{\vec{e}_\nu(\vec{q})\cdot\vec{q}}{\sqrt{N}} \sqrt{\frac{\hbar}{2M\omega_{\vec{q},\nu}}} \left(\hat{b}_{\vec{q},\nu} + \hat{b}^+_{-\vec{q},\nu}\right) e^{i\vec{q}\vec{r}} \tag{11.74}$$

Note that here the scalar product of the wave vector $\vec{q}$ and the respective polarisation vectors $\vec{e}_\nu(\vec{q})$ appear. As the transversal phonons are characterised by polarisation vectors, which are orthogonal to the wave vector and thus fulfill the property

$$\vec{e}_\nu(\vec{q})\cdot\vec{q} = 0, \quad \nu: \text{transversal} \tag{11.75}$$

we conclude from (11.74) that the volume dilatation operator only depends on longitudinal phonons:

$$\hat{\Theta}(\vec{r}) = \sum_{\vec{q}} i \frac{\vec{e}(\vec{q})\cdot\vec{q}}{\sqrt{N}} \sqrt{\frac{\hbar}{2M\omega_{\vec{q}}}} \left(\hat{b}_{\vec{q}} + \hat{b}^+_{-\vec{q}}\right) e^{i\vec{q}\cdot\vec{r}} \tag{11.76}$$

where we simplified the notation according to

$$\vec{e}(\vec{q}) = \vec{e}_\ell(\vec{q}), \quad \omega_{\vec{q}} = \omega_{\vec{q},\ell}, \quad \hat{b}_{\vec{q}} = \hat{b}_{\vec{q}\ell}, \quad \hat{b}^+_{\vec{q}} = \hat{b}^+_{\vec{q}\ell} \tag{11.77}$$

11.5 Electron-Phonon Interaction Hamiltonian:

Based on the above description of phonons we discuss now how their volume dilatation gives rise to the electron-phonon interaction Hamiltonian. With this we obtain the Feynman diagrammatic rules how to treat the electron-phonon interaction perturbatively.

11.5.1 Thomas-Fermi Approximation:

Due to the derivation of the volume dilatation from (11.71) we read off that lattice vibrations lead to local changes of the volume:

$$\Theta(\vec{r}) = \frac{V(\vec{r}) - V}{V} \quad \Rightarrow V(\vec{r}) = V\{1 + \Theta(\vec{r})\} \tag{11.78}$$

On the other hand we know that, according to the jellium model, there must be N electrons in the volume $V(\vec{r})$ pro-

vided there are N ion cores therein in order to guarantee electric neutrality. In this way the lattice vibrations yield local changes of the electron density. In first order we get

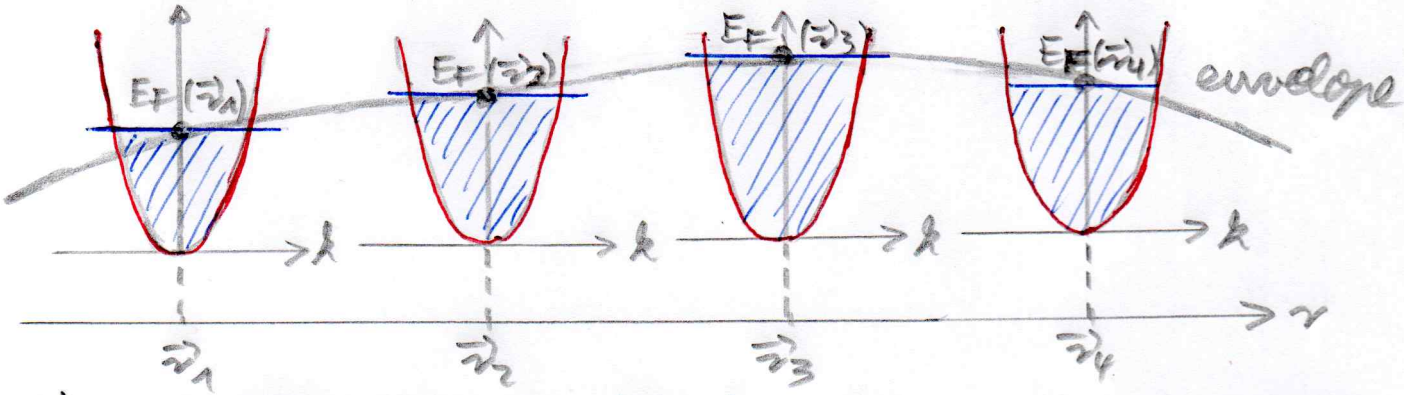
$$n(\vec{r}) = \frac{N}{V(\vec{r})} \overset{(11.78)}{=} \frac{N}{V}\frac{1}{1+\Phi(\vec{r})} \approx n(\vec{r}) = n\{1-\Phi(\vec{r})\} \quad (11.79)$$

Assuming that these local changes of the electron density are small enough, we can invoke the Thomas-Fermi approximation. Thus, at each space point $\vec{r}$ we can imagine for each electron density $n(\vec{r})$ a Fermi-sphere with the Fermi wave vector

$$k_F(\vec{r}) \overset{(9.11)}{=} \{3\pi^2 n(\vec{r})\}^{1/3} \quad (11.80)$$

and the corresponding Fermi energy

$$E_F(\vec{r}) \overset{(9.9)}{=} \frac{\hbar^2 k_F(\vec{r})^2}{2m} \overset{(11.80)}{=} \frac{\hbar^2}{2m}\{3\pi^2 n(\vec{r})\}^{2/3} \quad (11.81)$$



Inserting (11.79) in (11.81) we obtain a local change of the Fermi energy

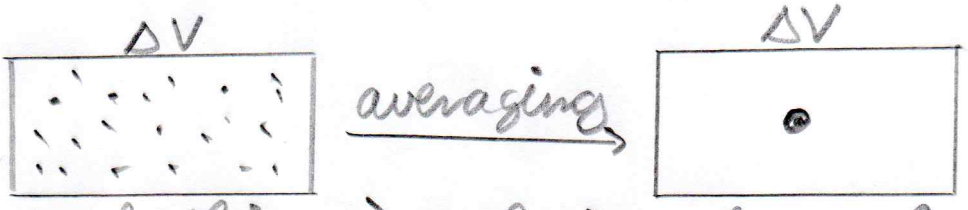
$$E_F(\vec{r}) = \frac{\hbar^2(3\pi^2 n)^{2/3}}{2m}[1-\Phi(\vec{r})]^{\frac{2}{3}} \Rightarrow \delta E_F(\vec{r}) = -\frac{2}{3}E_F\Phi(\vec{r}) \quad (11.82)$$

with the equilibrium Fermi energy E_F defined in (9.17).

11.5.2 Assumptions:

The previous approximations are based on the following assumptions:

1) The transition from a discrete to a quasi-continuum description of a physical quantity is based on performing an averaging over a volume ΔV. The average is then assigned to a mid-point of this volume element:



In order to make this point of view physical

a) the volume element ΔV must be large with respect to the elementary cell so that a continuum description is reasonable.

b) the volume element ΔV must be small with respect to local changes so that the restriction to effects first order is still justified.

2) Provided that a material does not possess a spatially constant Fermi energy, it is no longer at thermodynamic equilibrium. Thus, strictly speaking, we consider with the linear response reasoning a tiny deviation from thermodynamic equilibrium.

3) It is assumed that the electrons can follow the changes of the volume instantaneously.

11.5.3 Hamilton Operator:

The one-particle Hamilton operator of the electrons contains apart from their kinetic energy the local change of the Fermi energy (11.82) as a potential

$$H = \sum_i \left\{ -\frac{\hbar^2}{2m} \Delta_i - \frac{2}{3} E_F \textcircled{11}(\vec{r}_i) \right\} \tag{11.83}$$

This leads in second quantization to the following Hamilton operator:

$$\hat{H} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k})\, \hat{a}^+_{\vec{k},\sigma}\, \hat{a}_{\vec{k},\sigma} + \sum_{\vec{q}} \hbar\omega_{\vec{q}} \left(\hat{b}^+_{\vec{q}}\, \hat{b}_{\vec{q}} + \frac{1}{2} \right)$$
$$- \frac{2}{3} E_F \sum_{\vec{k},\vec{k}',\sigma} \textcircled{11}(\vec{k}-\vec{k}')\, \hat{a}^+_{\vec{k},\sigma}\, \hat{a}_{\vec{k}',\sigma} \tag{11.84}$$

Here the first term represents the free kinetic energy of the electrons and the second term the free energy of the (longitudinal) phonons. The third term describes the electron-phonon interaction via the Fourier transformed

$$\textcircled{11}(\vec{k}-\vec{k}') = \frac{1}{V} \int d^3r\, \textcircled{11}(\vec{r})\, e^{-i(\vec{k}-\vec{k}')\vec{r}} \tag{11.85}$$

Inserting (11.76) in (11.85) yields

$$\textcircled{11}(\vec{k}-\vec{k}') = i\, \frac{\vec{e}(\vec{k}-\vec{k}') \cdot (\vec{k}-\vec{k}')}{\sqrt{N}} \sqrt{\frac{\hbar}{2M\omega_{\vec{k}-\vec{k}'}}} \left(\hat{b}_{\vec{k}-\vec{k}'} + \hat{b}^+_{-(\vec{k}-\vec{k}')} \right) \tag{11.86}$$

Thus, the electron-phonon interaction Hamiltonian follows from (11.84) and (11.86) to be of the form

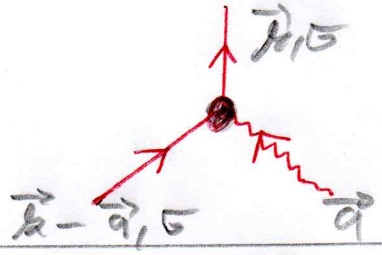
$$\hat{H}_I = \sum_{\vec{k},\sigma} \sum_{\vec{q}} g(\vec{q})\, \hat{a}^+_{\vec{k},\sigma}\, \hat{a}_{\vec{k}-\vec{q},\sigma} \left(\hat{b}_{\vec{q}} + \hat{b}^+_{-\vec{q}} \right) \tag{11.87}$$

where we have substituted the $\vec{k}'$-sum by a sum over $\vec{q} = \vec{k} - \vec{k}'$. The interaction strength turns out to be

$$g(\vec{q}) = -\frac{2}{3} E_F \, i \, \vec{e}(\vec{q}) \cdot \vec{q} \sqrt{\frac{\hbar}{2 M N \omega_{\vec{q}}}} \qquad (11.88)$$

11.5.4 Interpretation:

The respective terms in the electron-phonon interaction Hamiltonian (11.87) represent the following elementary scattering processes:

term	$\hat{a}^+_{\vec{k},\sigma} \hat{a}_{\vec{k}-\vec{q},\sigma} \hat{b}_{\vec{q}}$	$\hat{a}^+_{\vec{k},\sigma} \hat{a}_{\vec{k}-\vec{q},\sigma} \hat{b}^+_{-\vec{q}}$
scattering process		
momentum before	$\vec{k} - \vec{q} + \vec{q}$	$\vec{k} - \vec{q}$
momentum after	$\vec{k}$	$\vec{k} + (-\vec{q})$
characterization	phonon absorption	phonon emission

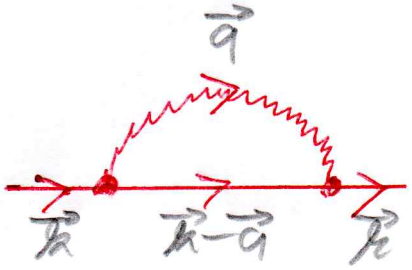
We conclude that the respective phonon absorption and emission processes are characterised by momentum and spin conservation.

11.5.6 Discussion:

Let us finally discuss important consequences of this electron-phonon interaction:

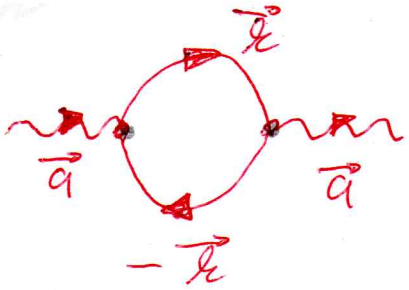
1) The wave vector $\vec{k}$ is no longer a good quantum number as the electron is scattered from one wave vector to the other. As a consequence electrons yield only a finite life time in the state characterised by the wave vector $\vec{k}$. This leads, in particular, to a substantial contribution to the electric resistance.

2) The electronic eigenstates and eigenenergies are modified. In particular, a lattice vibration can move together with the electron. Under certain circumstances this leads to the

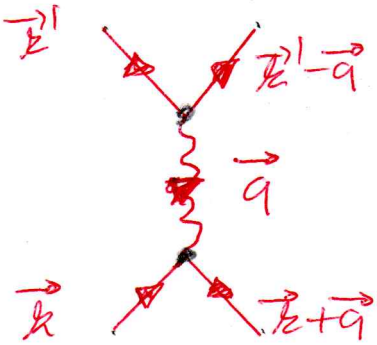


emergence of the new quasi-particle of a polaron, which consists of an electron being surrounded by a cloud of lattice vibrations. Therefore, a polaron has an effective mass, which turns out to be larger than the usual bare electron mass.

3) Conversely, also the phonon properties are renormalized due to the electron-phonon interaction. In particular, there exist processes, where a propagating phonon creates a pair of an electron and a hole.



4) The phonon, which is emitted by a first electron, can be absorped by a second electron, yielding an effective electron-electron interaction. It can be attractive and, thus, leads to the microscopic mechanism of conventional superconductivity.



Finally, we conclude that the electron-phonon interaction occurring in a solid has apparent analogies to quantum electrodynamics, where electrons and photons are coupled in a quite similar way.

11.6. Perturbative Elimination of Phonons:

The Fröhlich Hamiltonian for the electron-phonon interaction has the structure

$$\hat{H} = \hat{H}_0 + \hat{H}_I \tag{11.89}$$

where the unperturbed Hamiltonian is given by both free electrons and free phonons and reads according to (11.84):

$$\hat{H}_0 = \sum_{\vec{k},\sigma} \varepsilon(\vec{k})\, \hat{a}^+_{\vec{k}\sigma} \hat{a}_{\vec{k}\sigma} + \sum_{\vec{q}} \hbar\omega_{\vec{q}}\, \hat{b}^+_{\vec{q}} \hat{b}_{\vec{q}} \tag{11.90}$$

The electron creator and annihilator fulfill the usual anticommutator relations

$$\left[\hat{a}_{\vec{k}\sigma}, \hat{a}_{\vec{k}'\sigma'}\right]_+ = \left[\hat{a}^+_{\vec{k}\sigma}, \hat{a}^+_{\vec{k}'\sigma'}\right]_+ = 0, \quad \left[\hat{a}_{\vec{k}\sigma}, \hat{a}^+_{\vec{k}'\sigma'}\right]_+ = \delta_{\vec{k}\vec{k}'}\delta_{\sigma\sigma'} \tag{11.91}$$

whereas the phonon creator and annihilator are defined by the usual commutator relations

$$[\hat{b}_{\vec{q}\alpha}, \hat{b}_{\vec{q}'\alpha'}]_- = [\hat{b}^+_{\vec{q}\alpha}, \hat{b}^+_{\vec{q}'\alpha'}]_- = 0, \quad [\hat{b}_{\vec{q}\alpha}, \hat{b}^+_{\vec{q}'\alpha'}]_- = \delta_{\vec{q},\vec{q}'} \tag{11.92}$$

Furthermore, the interaction Hamiltonian $\hat{H}_I$ is given by (11.87). In the following we realise an idea, which goes back to Schrieffer and Wolff, and treat the interaction Hamiltonian $\hat{H}_I$ perturbatively by applying a unitary transformation to the Hamiltonian (11.89):

$$\hat{H}' = \hat{U}^+ \hat{H} \hat{U} \tag{11.93}$$

Such a transformation $\hat{U}$ corresponds to a basis change in the underlying Fock space, which does not change the physical meaning of the Hamiltonian. But, due to a suitable choice of $\hat{U}$, one can achieve that in lowest order of perturbation theory virtual phonons no longer appear, but instead an effective electron-electron interaction emerges. This Schrieffer-Wolff transformation represents a standard method in theoretical solid-state physics, which occurs not only in dealing with the electron-phonon interaction but appears also when other types of interactions are analysed. Furthermore, the Schrieffer-Wolff transformation is also used in quantum field theory, for instance by obtaining systematically the non-relativistic limit of the Dirac equation and is called there the Foldy-Wouthuysen transformation.

11.7.1 Lowest Order Calculation:

We start with an exponential ansatz for the unitary transformation:

$$\hat{U} = e^{\hat{S}} \tag{11.94}$$

In order that $\hat{U}$ is unitary, we have to demand $\hat{S}$ is anti-hermitian:

$$\hat{U}^+ \overset{(11.94)}{=\!=} e^{\hat{S}^+} \overset{!}{=} \hat{U}^{-1} \overset{(11.94)}{=\!=} e^{-\hat{S}} \Rightarrow \hat{S}^+ = -\hat{S} \tag{11.95}$$

Inserting (11.94) into (11.93) and expanding up to second order in $\hat{S}$ we obtain

$$\hat{H}' = e^{\hat{S}^+} \hat{H} e^{\hat{S}} \overset{(11.95)}{=\!=} e^{-\hat{S}} \hat{H} e^{\hat{S}} = (1 - \hat{S} + \tfrac{1}{2}\hat{S}^2 + \dots)\hat{H} \cdot (1 + \hat{S} + \tfrac{1}{2}\hat{S}^2 + \dots) = \hat{H} - \hat{S}\hat{H} + \tfrac{1}{2}\hat{S}^2\hat{H} + \hat{H}\hat{S} - \hat{S}\hat{H}\hat{S} + \tfrac{1}{2}\hat{H}\hat{S}^2 + \dots = \hat{H} + [\hat{H}, \hat{S}]_- + \tfrac{1}{2}[[\hat{H}, \hat{S}]_-, \hat{S}]_- + \dots \tag{11.96}$$

Here we have introduced the double commutator

$$[[\hat{A}, \hat{S}], \hat{S}] = [\hat{A}, \hat{S}]_- \hat{S} - \hat{S}[\hat{A}, \hat{S}]_- = \hat{A}\hat{S}^2 - 2\hat{S}\hat{A}\hat{S} + \hat{S}^2\hat{A} \tag{11.97}$$

Now we insert the decomposition (11.89) into (11.96) and assume that $\hat{S}$ is of the same order as $\hat{H}_I$. Up to the second order in $\hat{H}_I$ we then obtain

$$\hat{H}' = \hat{H}_0 + \hat{H}_I + [\hat{H}_0, \hat{S}]_- + [\hat{H}_I, \hat{S}]_- + \frac{1}{2}[[\hat{H}_0, \hat{S}]_-, \hat{S}]_- + \dots \quad (11.98)$$

We choose $\hat{S}$ such that the first-order terms in (11.98) cancel, i.e. we demand

$$[\hat{H}_0, \hat{S}]_- = -\hat{H}_I \quad (11.99)$$

With this we achieve that $\hat{H}'$ in (11.98) has as the lowest-order connection to $\hat{H}_0$ a second order in $\hat{H}_I$, which reads

$$\hat{H}' = \hat{H}_0 + \frac{1}{2}[\hat{H}_I, \hat{S}]_- \quad (11.100)$$

11.7.2 Determining the Unitary Transformation:

Now we determine $\hat{S}$ by solving (11.99) for the unperturbed Hamiltonian (11.90) and the interaction Hamiltonian (11.87). To this end we perform a skeleton ansatz, which consists of similar terms as (11.87) and already respects the anthermiticity restriction (11.95):

$$\hat{S} = \sum_{\vec{k}\vec{q}\sigma} \left\{ A_{\vec{k},\vec{q}}\, \hat{a}^+_{\vec{k}+\vec{q}\sigma}\, \hat{a}_{\vec{k}\sigma}\, \hat{b}^+_{-\vec{q}} - A^*_{\vec{k},\vec{q}}\, \hat{a}^+_{\vec{k}\sigma}\, \hat{a}_{\vec{k}+\vec{q}\sigma}\, \hat{b}_{-\vec{q}} \right\} \quad (11.101)$$

For technical reasons we now perform in the second term the substitution $\vec{k} \to \vec{k}-\vec{q}$ and $\vec{q} \to -\vec{q}$:

$$\hat{S} = \sum_{\vec{k},\vec{q}\sigma} \left\{ A_{\vec{k},\vec{q}}\, \hat{b}^+_{-\vec{q}} - A^*_{\vec{k}+\vec{q},-\vec{q}}\, \hat{b}_{\vec{q}} \right\} \hat{a}^+_{\vec{k}+\vec{q}\sigma}\, \hat{a}_{\vec{k}\sigma} \quad (11.102)$$

Afterwards, we calculate the commutator in (11.99) by taking into account (11.90):

$$[\hat{H}_0, \hat{S}]_- = \sum_{\vec{k}\vec{q}\sigma} \Big\{ \Big(A_{\vec{k},\vec{q}}\, \hat{b}^+_{-\vec{q}} - A^*_{\vec{k}+\vec{q},-\vec{q}}\, \hat{b}_{\vec{q}} \Big) \sum_{\vec{k}'\sigma'} \varepsilon_{\vec{k}'} \Big[\hat{a}^+_{\vec{k}'\sigma'}\, \hat{a}_{\vec{k}'\sigma'},$$
$$\hat{a}^+_{\vec{k}+\vec{q}\sigma}\, \hat{a}_{\vec{k}\sigma} \Big]_- + \hat{a}^+_{\vec{k}+\vec{q}\sigma}\, \hat{a}_{\vec{k}\sigma} \sum_{\vec{q}'} t_{\vec{q}'} \Big(A_{\vec{k},\vec{q}} \Big[\hat{b}^+_{\vec{q}'}\, \hat{b}_{\vec{q}'},\, \hat{b}^+_{-\vec{q}} \Big]_-$$
$$- A^*_{\vec{k}+\vec{q},-\vec{q}} \Big[\hat{b}^+_{\vec{q}'}\, \hat{b}_{\vec{q}'},\, \hat{b}_{\vec{q}} \Big]_- \Big) \Big\} \quad (11.103)$$

In order to calculate the respective commutators, we need the so-called BEC-rule, which exists both in a bosonic and a fermionic version:

$$[\hat{A}, \hat{B}\hat{C}]_- = [\hat{A}, \hat{B}]_- \hat{C} + \hat{B}[\hat{A}, \hat{C}]_- \quad (11.104)$$

$$[\hat{A}\hat{B}, \hat{C}]_- = \hat{A}[\hat{B}, \hat{C}]_+ - [\hat{A}, \hat{C}]_+ \hat{B} \quad (11.105)$$

The validity of (11.104) and (11.105) immediately follows from

explicitly writing down the respective commutators and anticommutators. With this we calculate at first the commutator of the fermionic operators in (11.103):

$$[\hat{a}^+_{\vec{k}'\sigma'}\hat{a}_{\vec{k}'\sigma'}, \hat{a}^+_{\vec{k}+\vec{q}\sigma}\hat{a}_{\vec{k}\sigma}] \overset{(11.104)}{=} [\hat{a}^+_{\vec{k}'\sigma'}\hat{a}_{\vec{k}'\sigma'}, \hat{a}^+_{\vec{k}+\vec{q}\sigma}]_- \hat{a}_{\vec{k}\sigma} + \hat{a}^+_{\vec{k}+\vec{q}\sigma}[\hat{a}^+_{\vec{k}'\sigma'}\hat{a}_{\vec{k}'\sigma'}, \hat{a}_{\vec{k}\sigma}]_- \overset{(11.105)}{=} (\hat{a}^+_{\vec{k}'\sigma'}[\hat{a}_{\vec{k}'\sigma'}, \hat{a}^+_{\vec{k}+\vec{q}\sigma}]_+ - [\hat{a}^+_{\vec{k}'\sigma'}, \hat{a}^+_{\vec{k}+\vec{q}\sigma}]_+\hat{a}_{\vec{k}'\sigma'})\hat{a}_{\vec{k}\sigma} + \hat{a}^+_{\vec{k}+\vec{q}\sigma}(\hat{a}^+_{\vec{k}'\sigma'}[\hat{a}_{\vec{k}'\sigma'}, \hat{a}_{\vec{k}\sigma}]_+ - [\hat{a}^+_{\vec{k}'\sigma'}, \hat{a}_{\vec{k}\sigma}]_+\hat{a}_{\vec{k}'\sigma'}) \overset{(11.91)}{=} (\delta_{\vec{k}',\vec{k}+\vec{q}}\hat{a}^+_{\vec{k}\sigma'}\hat{a}_{\vec{k}\sigma} - \delta_{\vec{k}'\vec{k}}\hat{a}^+_{\vec{k}+\vec{q}\sigma}\hat{a}_{\vec{k}'\sigma'})\delta_{\sigma\sigma'} \tag{11.106}$$

correspondingly, also both commutators of bosonic operators in (11.103) are determined:

1) $$[\hat{b}^+_{\vec{q}'}\hat{b}_{\vec{q}'}, \hat{b}^+_{-\vec{q}}]_- = -[\hat{b}^+_{-\vec{q}}, \hat{b}^+_{\vec{q}'}\hat{b}_{\vec{q}'}]_- \overset{(11.104)}{=} -[\hat{b}^+_{-\vec{q}}, \hat{b}^+_{\vec{q}'}]_-\hat{b}_{\vec{q}'} - \hat{b}^+_{\vec{q}'}[\hat{b}^+_{-\vec{q}}, \hat{b}_{\vec{q}'}]_- \overset{(11.92)}{=} \delta_{\vec{q}',-\vec{q}}\hat{b}^+_{\vec{q}'} \tag{11.107}$$

2) $$[\hat{b}^+_{\vec{q}'}\hat{b}_{\vec{q}'}, \hat{b}_{\vec{q}}]_- = -[\hat{b}_{\vec{q}}, \hat{b}^+_{\vec{q}'}\hat{b}_{\vec{q}'}]_- \overset{(11.104)}{=} -[\hat{b}_{\vec{q}}, \hat{b}^+_{\vec{q}'}]_-\hat{b}_{\vec{q}'} - \hat{b}^+_{\vec{q}'}[\hat{b}_{\vec{q}}, \hat{b}_{\vec{q}'}]_- \overset{(11.92)}{=} -\delta_{\vec{q},\vec{q}'}\hat{b}_{\vec{q}'} \tag{11.108}$$

Inserting (11.106)–(11.108) into (11.103) yields

$$[\hat{H}_0, \hat{S}]_- = \sum_{\vec{k}\vec{q}\sigma}\{(A_{\vec{k},\vec{q}}\hat{b}^+_{-\vec{q}} - A^*_{\vec{k}+\vec{q},-\vec{q}}\hat{b}_{\vec{q}})(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}})\hat{a}^+_{\vec{k}+\vec{q}\sigma}\hat{a}_{\vec{k}\sigma} + \hat{a}^+_{\vec{k}+\vec{q}\sigma}\hat{a}_{\vec{k}\sigma}(\hbar^2\vec{q}\,A_{\vec{k},\vec{q}}\hat{b}^+_{-\vec{q}} + A^*_{\vec{k}+\vec{q},-\vec{q}}\hat{b}_{\vec{q}}\hbar\omega_{\vec{q}})\}$$

$$\overset{(11.99)}{=} -\hat{H}_I \overset{(11.87)}{=} -\sum_{\vec{k}\vec{q}\sigma} g(\vec{q})(\hat{b}_{\vec{q}} + \hat{b}^+_{-\vec{q}})\hat{a}^+_{\vec{k}+\vec{q}\sigma}\hat{a}_{\vec{k}\sigma} \tag{11.109}$$

Identifying the respective coefficients we can solve for the yet unknown coefficients $A_{\vec{k},\vec{q}}$ and $A^*_{\vec{k}+\vec{q},-\vec{q}}$:

$$A_{\vec{k},\vec{q}} = -\frac{g(\vec{q})}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} + \hbar\omega_{\vec{q}}} \tag{11.110}$$

$$A^*_{\vec{k}+\vec{q},-\vec{q}} = \frac{g(\vec{q})}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} - \hbar\omega_{\vec{q}}} \tag{11.111}$$

Note that we can directly read off (11.111) from (11.110):

$$A^*_{\vec{k}+\vec{q},-\vec{q}} \overset{(11.110)}{=} -\frac{g(-\vec{q})^*}{\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}} + \hbar\omega_{\vec{q}}} \overset{(11.88)}{=} \frac{g(\vec{q})}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} - \hbar\omega_{\vec{q}}} \checkmark$$

Here the latter identity follows from (11.81) and a condition for the polarisation vectors

$$\vec{e}(-\vec{q})^* = \vec{e}(\vec{q}) \tag{11.112}$$

which follows from demanding that the shift operator

$\hat{S}(\vec{z})$ in (11.65) is hermitian:

$$\hat{S}(\vec{z}) = \hat{S}^{+}(\vec{z}) \qquad (11.113)$$

11.7.3 Transformed Hamiltonian:

After having determined in lowest order the unitarity transformation according to (11.102) and (11.110), (11.111), it remains to calculate the transformed Hamiltonian (11.100). To this end we have to insert (11.87) and (11.102) into (11.100):

$$\hat{H}'_1 = \hat{H}' - \hat{H}_0 = \frac{1}{2} \sum_{\vec{k}\vec{q}\sigma} \sum_{\vec{k}'\vec{q}'\sigma'} g(\vec{q}) \Big[\big(b_{\vec{q}} + b^{+}_{-\vec{q}} \big) \hat{a}^{+}_{\vec{k}\sigma} \hat{a}_{\vec{k}-\vec{q}\sigma},$$

$$\big(A_{\vec{k}',\vec{q}'} b^{+}_{-\vec{q}'} - A^{*}_{\vec{k}'+\vec{q}',-\vec{q}'} b_{\vec{q}'} \big) \hat{a}^{+}_{\vec{k}'+\vec{q}'\sigma'} \hat{a}_{\vec{k}'\sigma'} \Big]_{-} \qquad (11.114)$$

The commutator to be calculated in (11.114) is of the general form $[\hat{B}\hat{F}, \hat{B}'\hat{F}']_{-}$, where $\hat{B}, \hat{B}'$ and $\hat{F}, \hat{F}'$ denote bosonic and fermionic operators, respectively, which commute. Therefore, we conclude

$$\big[\hat{B}\hat{F}, \hat{B}'\hat{F}'\big]_{-} = \hat{B}\hat{F}\cdot\hat{B}'\hat{F}' - \hat{B}'\hat{F}'\hat{B}\hat{F} = \hat{B}\hat{B}'\hat{F}\hat{F}' - \hat{B}'\hat{B}\hat{F}'\hat{F} \qquad (11.115)$$

$$+ \hat{B}'\hat{B}\hat{F}\hat{F}' - \hat{B}'\hat{B}\hat{F}'\hat{F} = \big[\hat{B}, \hat{B}'\big]_{-}\hat{F}\hat{F}' + \hat{B}'\hat{B}\big[\hat{F}, \hat{F}'\big]_{-}$$

The second term in (11.115) is bilinear in both phonon and electron operator and, thus, describes an interaction between two phonons and two electrons. It is not of the interaction type we are looking for, so we neglect it. Best the first term in (11.115) no longer contains any phonon operators and, thus, represents a residual interaction between two electrons. In the following, we concentrate on that term, which reads

$$\hat{H}''_1 = \frac{1}{2} \sum_{\vec{k}\vec{q}\sigma} \sum_{\vec{k}'\vec{q}'\sigma'} g(\vec{q}) \Big[\hat{b}_{\vec{q}} + \hat{b}^{+}_{-\vec{q}}, A_{\vec{k}',\vec{q}'} \hat{b}^{+}_{-\vec{q}'} - A^{*}_{\vec{k}'+\vec{q}',-\vec{q}'} \hat{b}_{\vec{q}'} \Big]_{-}$$

$$\cdot \hat{a}^{+}_{\vec{k}\sigma} \hat{a}_{\vec{k}-\vec{q}\sigma} \hat{a}^{+}_{\vec{k}'+\vec{q}'\sigma'} \hat{a}_{\vec{k}'\sigma'} \qquad (11.116)$$

The remaining commutator of bosonic operators can directly be evaluated with (11.92). Performing in addition the resummation $\vec{k} \to \vec{k} - \vec{q}$ yields

$$\hat{H}''_1 = \frac{1}{2} \sum_{\vec{k}'\vec{q}\sigma} \sum_{\vec{k}'\vec{q}'\sigma'} g(\vec{q}) \big\{ A_{\vec{k}',\vec{q}'} \delta_{\vec{q},-\vec{q}'} + A^{*}_{\vec{k}'+\vec{q}',-\vec{q}'} \delta_{\vec{q}',-\vec{q}} \big\}$$

$$\cdot \hat{a}^{+}_{\vec{k}+\vec{q}\sigma} \hat{a}_{\vec{k}\sigma} \hat{a}^{+}_{\vec{k}'+\vec{q}'\sigma'} \hat{a}_{\vec{k}'\sigma'} \qquad (11.117)$$

Evaluating the $\vec{q}'$-sum we get

$$\hat{H}''_1 = \sum_{\vec{k}\sigma} \sum_{\vec{k}'\sigma'} \sum_{\vec{q}} V(\vec{k}', \vec{q})\, \hat{a}^{+}_{\vec{k}+\vec{q}\sigma} \hat{a}_{\vec{k}\sigma} \hat{a}^{+}_{\vec{k}'-\vec{q}\sigma'} \hat{a}_{\vec{k}'\sigma'} \qquad (11.118)$$

where the matrix element reads

$$V(\vec{k}',\vec{q}) = \frac{1}{2} g(\vec{q}) \left\{ H_{\vec{k}',-\vec{q}} + H^*_{\vec{k}'-\vec{q},\vec{q}} \right\} \quad \text{(11.110), (11.111)}$$

$$= \frac{1}{2} g(\vec{q}) \left\{ - \frac{g(-\vec{q})}{\varepsilon_{\vec{k}'-\vec{q}} - \varepsilon_{\vec{k}'} + \hbar\omega_{\vec{q}}} + \frac{g(-\vec{q})}{\varepsilon_{\vec{k}'-\vec{q}} - \varepsilon_{\vec{k}'} - \hbar\omega_{\vec{q}}} \right\} \quad (11.119)$$

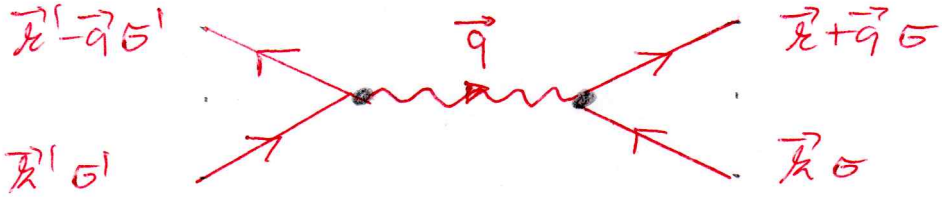
due to (11.88) and (11.112) we have

$$g(-\vec{q}) = g^*(\vec{q}) \quad (11.120)$$

so that (11.119) reduces to

$$V(\vec{k}',\vec{q}) = |g(\vec{q})|^2 \cdot \frac{\hbar\omega_{\vec{q}}}{(\varepsilon_{\vec{k}'-\vec{q}} - \varepsilon_{\vec{k}'})^2 - (\hbar\omega_{\vec{q}})^2} \quad (11.121)$$

The resulting Hamilton operator (11.118) describes an interaction between two electrons via the exchange of a phonon, which is depicted by the Feynman diagram



Note that we have already obtained this result based on a phenomenological discussion in section 10.3. And from chapter 9 we know that an interaction Hamiltonian of the type (11.118) leads to the formation of Cooper pairs only for an attractive interaction, i.e. the interaction strength (11.121) must be negative. This leads to the condition

$$|\varepsilon_{\vec{k}'-\vec{q}} - \varepsilon_{\vec{k}'}| < \hbar\omega_{\vec{q}} < \hbar\omega_D \quad (11.122)$$

Thus, an attractive interaction due to the virtual exchange of phonons is only possible in a small neighborhood around the Fermi edge.

Although the effective electron-electron interaction strength depends according to (11.121) both on $\vec{k}'$ and $\vec{q}$, a useful model for the interaction Hamiltonian (11.118) is given by

$$\hat{H} = V \sum_{\vec{k}\sigma} \sum_{\vec{k}'\sigma'} \sum_{\vec{q}} \hat{a}^+_{\vec{k}+\vec{q}\sigma} \hat{a}_{\vec{k}\sigma} \hat{a}^+_{\vec{k}'-\vec{q}\sigma'} \hat{a}_{\vec{k}'\sigma'} \quad (11.123)$$

where the $\vec{k}',\vec{q}$-dependencies in (11.121) are approximately neglected. Furthermore, from the discussion of the Cooper problem in chapter 9 we know that the interaction model (11.123) can be simplified. The most important contributions from (11.123) in view of the formation of Cooper pairs are those where

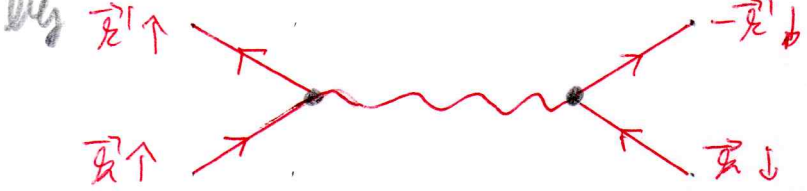
1) $\vec{k}'$ is restricted to $-\vec{k}$.
2) σ and σ' are specialized to $\uparrow$ and $\downarrow$, respectively.
Then (11.118) reduces with the renumeration $\vec{k}' = \vec{k} + \vec{q}$ to

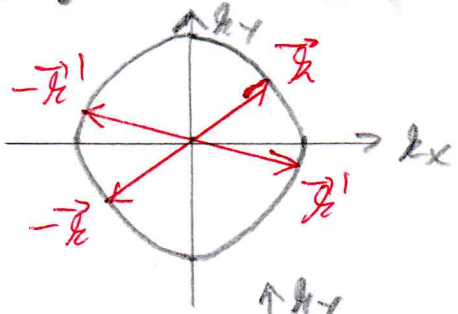
$$\hat{H} = V \sum_{\vec{k}\,\vec{k}'} \hat{a}^+_{\vec{k}'\uparrow}\, \hat{a}_{\vec{k}\uparrow}\, \hat{a}^+_{-\vec{k}'\downarrow}\, \hat{a}_{-\vec{k}\downarrow} \qquad (11.124)$$

In order to convert (11.124) into the normal form of an interaction Hamiltonian, the second fermionic operator has to be moved by two anti-commutations to the very left. As this yields two minus signs, the overall sign is not changing and we get

$$\hat{H} = V \sum_{\vec{k}\,\vec{k}'} \hat{a}^+_{\vec{k}'\uparrow}\, \hat{a}^+_{-\vec{k}'\downarrow}\, \hat{a}_{-\vec{k}\downarrow}\, \hat{a}_{\vec{k}\uparrow} \qquad (11.125)$$

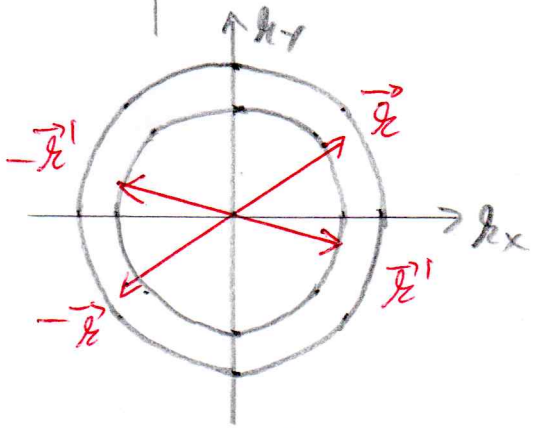
The Feynman diagrammatic content of (11.125) is depicted by





But, note that, in order to take into account the condition (11.122), the summation in (12.125) has to be restricted to those wave vectors, which satisfy

$$|\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'}| < \hbar\omega_{\vec{q}} \ll \hbar\omega_D \qquad (11.126)$$



Combining the free electron Hamiltonian contained in (11.90) with the interaction Hamiltonian (11.125) we, finally, arrive at the so-called pairing Hamiltonian

$$\hat{H}_P = \sum_{\vec{k}\sigma} \varepsilon(\vec{k})\, \hat{a}^+_{\vec{k}\sigma}\, \hat{a}_{\vec{k}\sigma} + V \sum_{\vec{k},\vec{k}'} \hat{a}^+_{\vec{k}'\uparrow}\, \hat{a}^+_{\vec{k}\uparrow}\, \hat{a}_{-\vec{k}\downarrow}\, \hat{a}_{-\vec{k}'\downarrow} \qquad (11.127)$$

It represents the starting point for the microscopic BCS-theory of superconductivity.