

Theory of high-temperature-superconductivity in Cuprates

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Abstract

The theory presented here is able to explain all attributes of cuprate-based High-temperature-Superconductors in the normal- and in the SC-state as well. For the theoretical calculations parameters gained by experiments only are used. It will be shown that all experimental values connecting to HTSC can be predicted/ calculated by assistance of the equation:

$$k_B T_C \propto 1,14 \cdot \frac{\text{Pseudogap}}{\exp(MPG / E_F)}$$

This equation is derived from the Hubbard-Model. MPG is the maximum pseudogap, received by extrapolating the pseudogap-values to $E_F \rightarrow$ zero. From that Fundamental-Formula one can get seven quantitative connections between superconduction-attributes and doping, all proved by experiment.

Additionally two well-hidden faults in BCS- and McMillan-theories will be shown. Without deleting these mistakes no theory of High-Tc-Superconductivity can be successful.

More than 300 experimentally measured values will be compared with the predictions of theory. In more than 90% there is quantitative, otherwise qualitative accordance between experiment and theory. **Reluctance is senseless:** This theory will succeed.

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I) Introduction

In 1987 superconductors with critical T_c -values above 100 K were discovered. According to some estimations T_c -values exceeding 40 K cannot be explained by electron-phonon interaction, because for creating even higher T_c -values the interactions will be so heavy, that they will cause rearrangements of the lattice. Up to now there does not exist any universally acknowledged theory which explains these T_c -values. Certain is only, that in all superconductors known up to now the superconductivity current is transported by pairs of charge-carriers. Therefore the main task of any theory will be to explain the unusual thermal stability of these pairs in HTSC.

Up to now quite a few possible explanations have been debated. Naturally at first scientists tried to apply the model of electron-phonon-interaction to HTSC despite the difficulties mentioned above¹. For some time a model was debated which was based on the separation of

electron-spin and -charge^{2et3}. At present many scientists assume that magnetic interactions play the dominant part⁴. All these models however are not able to explain simultaneously the superconducting **and** the completely unusual normally conducting attributes of HTSC:

In most cases in the normal state the electrical resistance follows a linear temperature law down to deepest temperatures –in contradiction to the Landau-theory of Fermi-liquid (**chapters 6. to 8.**). The conduction-electrons obviously do not create a Fermi-liquid. Accordingly an anomaly in the thermal conductivity appears too. Oddly enough with most of the HTSC –also in a normally conducting state- there will be an energy gap in the density of states (DOS), the so-called “pseudo-gap”.

In HTSC with a low density of holes a huge isotope effect is noticed: With increasing density of holes the effect decreases continuously for strong increasing again above optimal doping

Therefore an interaction must be discovered which

- a) leads to the formation of hole-pairs at high temperatures
- b) is equally responsible for the “non-Fermi-liquid-behaviour”
- c) also creates a gap in the density of state (DOS) of the mobile charge-carriers in the normal state
- d) permits a sufficiently plausible explanation as regards the isotope effects

All these phenomena (and some more) will be brought in connection and explained by this theory.

2.2. The Hubbard model and HTSC

This abstract is based on the idea that the Hubbard model of theoretical solid state physics⁵ can also be applied to HTSC. According to this model the valence band of HTSC is split into three partial bands: two Cu-3d-bands and one oxygen-2p-band. If each lattice site (of ions) is occupied by exactly one electron , then (if T = 0K) the oxygen band and the lower Cu-3d-band are totally unoccupied. As the bands do not overlap –but are separated from each other by energy gaps –then there will be an antiferromagnetic insulator.

These energy gaps are of a different origin than the energy gaps in semi-conductors: They originate from the mutual Coulomb repel of the electrons. This Coulomb repel prevents the delocalization of the El and links them –similar to atomic rests- to destinated sites in the lattice.

This status is similar to a Wigner lattice in two dimensions. For memory: In **two** dimensions a Wigner lattice will exist at **high** densities of electrons only⁶:

$$\Gamma = \frac{e^2 \sqrt{N_s}}{4\sqrt{\pi} \varepsilon_0 k_B T} = 3 \cdot 10^{-5} \frac{\sqrt{N_s}}{T} \quad (1)$$

Thereby is N_s the density of electrons per square metre. If Γ is large enough the mutual repel will overcome the attraction and it is assumed that there will be a diffraction pattern as a periodic lattice⁶. In HTSC the occupied Cu-3d-band is created in a different way than in band insulators: in a band insulator no states can be occupied immediately above the upper band edge. In HTSC the occupied Cu-3d-band is the result of the mutual Coulomb repel of the El. This repel does not exclude the stimulation of small oscillations of the El. If and when El are stimulated to such “lattice” oscillations, these El will occupy states above the occupied Cu-

3d-bands. Similarly to atomic residues these quasi-crystallized EL, which were studied here, can be excused out of their positions. The fact, that the EL are localized at a lattice site does not prohibit the excursion out of their normal positions.

When the system is doped with oxygen, the oxygen band will loose electrons and the system will be doped with holes. With increasing doping the ferromagnetism disappears, the Fermi-energy moves into the region of the oxygen band, the system becomes metallic. In this system now a band appears which contains freely moving holes. A second band will appear, the lower Cu-3d-band containing electrons which repel each other because of the Coulomb interaction.

The upper Cu-3d-band remains unoccupied. For the understanding of the following please keep in mind that the abbreviation EL used in connection with HTSC always refers to the Cu-3- $d_{x^2-y^2}$ -electrons, quasi-bound to Cu- or O-ions in the lower Cu-3d-band. The mobile charge-carriers in the oxygen band will be referred to as “holes”.

If energy is added, **both** types of charge carriers –holes and El- can be scattered into unoccupied levels of energy.

2.3 Application of the Hubbard-model to HTSC

The existing theories of solid state physics consider a metal as a skeleton of ions surrounded by a gas of charge carriers. By interaction between these charge carriers and the ions the latter will be stimulated to virtual lattice oscillations. In contrast to the ions the mobile charge carriers in a metal cannot cause such oscillations, because there is not any restoring force, having an effect on a gas. (Plasma-oscillations of the charge carriers are no lattice

oscillations.) In this essay it is assumed that the typical theories of metals do not work at the HTSC, but the EL in the Cu-3d-band, charging the highest energy can be shifted relatively to the ions. Because of the special electron-configuration in the HTSC, this quasibounded EL can make fast oscillations relatively to the much inert atomic rests. Because of these oscillations of quasibounded EL a polarization will be generated which is relaying an attraction between two holes. Thereby these oscillations of EL play the same role for HTSC as the oscillations of the atomic lattice play for conventional superconductivity.

In this connection should be remembered that according to the simplest theory of conventional superconductivity the critical temperature is inversely proportional to the root of the mass of oscillating particles⁷. Therefore the small mass of the electrons (EL) can manage to generate very high T_C 's. Thus the high T_C 's can be explained qualitatively at least.

At this point it will be remarked, that the virtual “lattice-oscillations” of Cu-3d-EL are Bosons, not obeying the Pauli-Principle. Perhaps this is a bit puzzling, because the carriers of this “lattice-oscillations are electrons, strictly obeying the Pauli-Principle. But lattice-oscillations do not possess a rest mass. A particle without rest mass possesses a whole-number spin and thereby obeys the Bose-Einstein-statistic. This is valid for lattice-oscillations in frozen hydrogen or in hydrides, too. And this is valid at every temperature, although the protons are fermions. In context with impact processes between protons and electrons, p. e. in Pd-H-systems, the protons appear as classical particles, because the protons are fixed at defined lattice-sites and because of this can be identified. From that the building in of statistical distributed protons in metals only leads to a largely T-independent RRR.

In contrary for impact processes of single movable holes with the Cu-3d-system in the HTSC the Fermi-Dirac-statistic is valid, because the holes and the Cu-3d-EL cannot be identified and possesses rest-masses with half-whole-number spin. Towards it results the dominating contribution to the electrical normal-state-resistance in the HTSC.

III) Shielding in HTSC's

3.1 Preface

In this part the way of pair-building in the HTSC's will be demonstrated: This process can be explained by two pathes: At one hand by dielectrical function, and on the other hand by perturbation-theory.

3.2 The statical shielding

At the begin the statical shielding will be handled: It's well known that the conduction-electrons are shielding one-another. Quantitatively it's calculated with the so-called "Thomas-Fermi-theory":

$$V^* = \frac{1}{Vol.} \cdot \frac{e^2}{\epsilon_0(k^2 + k_{TF}^2)} \cdot \frac{1}{\epsilon(dyn)} \approx \frac{1}{Vol.} \cdot \frac{e^2}{\epsilon_0 k_{TF}^2} \cdot \frac{1}{\epsilon(dyn)} = \frac{2E_F}{3N_{LO}} \cdot \frac{1}{\epsilon(dyn)}$$

This relation is a good approximation for small values of wave-vectors and it is also valid in case of complicate densities of state. (The sense of this remark will be explained in part VI.)

NB: In two-dimensional metals like the HTSC's the TF-wave-vector is a constant, namely:

$$k_{TF} = \frac{e^2 m_{EL}}{\pi \epsilon_0 \hbar^2} = 7,6 \cdot 10^{10} m^{-1}$$

The wave-vector k can be neglected in case of $k < k(TF)$ and then it's valid:

$$V^* \approx \frac{E_F(2 \text{ dim})}{N_{LO}} \cdot \frac{1}{\epsilon(dyn)}$$

3.3 The characteristic Reference-Energy, respectively the dynamical shielding:

The word “characteristic Reference-Energy” describes that, which is represented by Debye-Energy in conventional superconductors. There is a general agreement, that in the HTSC’s the so-called “Hubbard-model” by half-filling is realized. That means, the valence-electrons of copper are reciprocal repulsing each other so strong, that there can’t exist an electron-gas. But the valence-electrons of the copper can “hop” virtually to their neighboured copper-atoms.

Ostentative the process can be imagined as collective vibration of electrons: A hole is repulsing the surrounding electrons. Thereby the electrons are collectively “hopping” to their neighboured lattice-sites by leaving a path of positive density of charge. A second hole “feels” that path of positive density of charge and is attracted from this. An indirect attraction of both holes results and they make an electron-pair. In quantitative description, the “hopping” leads to a reduction of the energy of holes. In the following it will be demonstrated, that exactly this sinking of energy is the characteristical Reference-Energy of the HTSC’s.

An elementary equation of solid state physics runs:

$$\varepsilon(MPG, \varepsilon_k) = \frac{\rho_{ext}}{\rho_{ind} + \rho_{ext}}$$

ρ_{ind} is the sum of two parts: The attractive interaction, called ρ_{ion} and the part of statical shielding, called ρ_{el} . Consequently: $\rho_{ind} = \rho_{ion} + \rho_{el}$

3.4 The Maximum Pseudogap

For beginning the shift of charge, called ρ_{ion} shall be determined. At this point it’s important to note, that this expression can’t be derived. The reason for the attractive interaction has to be guessed. (It should be remembered here, that the reason of conventional SC was guessed, too.) In the underdoped “mother-substances” of HTSC’s the “Hubbard-Model” at half-filling is realized. That’s a well-known fact. Besides it shall be given to you, that the important actions of SC’s are playing in two, not in three dimensions. By that it’s merely obvious, searching the reason of HTSC in the two-dimensional version of Hubbard-interaction.

In the HTSC’s the Cu-3d-Electrons can diminish their energy by virtual hopping between neighboured site-lattices. Quantitatively this will be described by the so-called “Hubbard-Model”:

$$MPG = \frac{t^2}{U}$$

In that equation the numerator is the overlap-integral of neighboured EL and describes the reduction of the kinetic energy on account of the delocalization of the EL. The denominator U presents the simultaneous enhancement of the potential energy. Here the the denominator shall be inquired only. The variation of the potential energy of “hopping” Electrons (= denominator) will be described by an elementar formula, which is used in the BCS-theory also:

$$\frac{1}{A} \cdot \frac{e^2}{\varepsilon_0 \varepsilon(\omega) q} = \frac{1}{A} \cdot \frac{e^2}{\varepsilon_0 q} \cdot \left[1 + \frac{\omega^2(q)}{\omega^2 - \omega^2(q)} \right]$$

In deviation to BCS-theory has been regarded here to the fact, that in Cuprates the superconductivity is playing in two, instead of three dimensions. In the square brackets of that equation the cipher “1” appears. That “1” describes the Coulomb-repulsion of the Electrons, appearing in all metals. Therefore that “1” agrees to the normal metal and doesn’t belong to HTSC.

On the other hand, the expression $\frac{\omega^2(q)}{\omega^2 - \omega^2(q)}$ presents a reduction of Coulomb-repulsion between the Electrons, appearing eventually.

Adding a negative sign to that expression, one will get necessarily an expression for an **augmentation** of Coulomb-IA, that means exactly the denominator U in the formula for MPG:

$$\rho_{ind} = MPG = \pm \frac{t^2}{U} = \pm \frac{t^2}{\frac{1}{A} \cdot \frac{e^2}{\varepsilon_0 q}} \cdot \frac{\omega^2(q) - \omega^2}{\omega^2(q)} \propto \pm \left[1 - \frac{\omega^2}{\omega^2(q)} \right]$$

$$\omega^2(q) \propto \frac{1}{M \cdot Vol.} \Rightarrow MPG = \frac{t^2}{U} \propto t^2 \cdot \left[1 - \omega^2 \cdot M \cdot Vol. \right] [Eqn.36]$$

And now the speciality of the HTSC's arises:

The letter **M** in the square bracket **doesn't** mean the atomic-mass, but the mass of the **Electrons**. So in the HTSC's the Cu-3d-Electrons are vibrating. These oscillations are leading to an energy gap. In exactly words they make two energy-gaps: Applied with negative sign to a diminuation and with positive sign to an enhancement of the energies of the Electrons. In second order that process leads to the electrical reluctance of the holes. (See exactly in the **chapters XI to XIV**) and in third order to the **pair-building** of the holes.

Therefore the “lattice-oscillations” of the Cu-3d-Electrons are conducting on one hand to the pseudogap and otherwise to superconductivity. In that work MPG means “Maximum Pseudogap”, that is the pseudogap in case of doping zero.

By that the shifting of charge ρ_{ion} represents the double pseudogap in case of doping zero. Expressed obvious: The Hubbard-energy-reduction, here called as “Maximum Pseudogap” MPG, is the “gluten”, which is bonding the holes to pairs.

By that equation for the Maximum Pseudogap we can get some results:

A)

Below (**Chapter VIII**) will be shown exactly and in all details, that the maximal critical temperature T_C^{\max} at optimal doping is directly proportional to MPG. By that is valid:

$$T_C^{\max} \propto MPG \propto t^2 \cdot [1 - \omega^2 \cdot M \cdot Vol.]$$

Therefore it's established/ascertained, that T_C^{\max} will be increased by decreasing the volume of the cell unit (p. e. by external pressure). That prediction is confirmed experimentally

[N. Suresh et al., PRB 78 (2008) 100503 (R)]

B)

On account of Pauli-Principle these hopping-processes only can appear parallel to the a- and b-axes, but not in 45° -angle to these axes. Therefore s-wave pairing by this mechanism is impossible.

C)

Furthermore we expect a small influence of atomic mass on T_C^{\max} . Consequently there should appear isotope effects in very small magnitudes. Why in fact there exist huge isotope effects will be explained in **chap. IX**.

D)

The wideness of the isotope effects not only depends on doping, but also on pressure. That means a decreasing IE by increasing pressure. Verifying that prediction by experiment should be able.

3.5 The variable pseudogap

In case of doping this pseudogap is reduced under influence of holes. Just it has been demonstrated: The Hubbard-energy-sinking, here called “Maximum Pseudogap” MPG, is the gluten, bonding holes to pairs. But the conduction-electrons (holes) are not only bound to

pairs, but they also have another effect: They produce bands at the higher and the lower edge of the energy gap. On account of that the energy gap becomes smaller. As more conduction-electrons exist, as bigger the bands are and as smaller the pseudogap becomes. The latitude/largeness of that decrease depends directly proportional on doping. For wide enough doping the pseudogap vanishes totally. In consequence the “variable Pseudogap” is written as:

$$PSL = MPG - E_F$$

IV) The dielectrical function in HTSC

4.1 Elementary formula of the dielectrical function

I will give it to you again: In the foregoing part 3.3 was mentioned:

$$\varepsilon(MPG, k) = 1 - \frac{\rho_{ind}}{\rho_{ind} + \rho_{ext}}$$

With this equation we are available to declare the inter-action between two holes in dependence to MPG and k, if the establishing of the three alterations of charge-density appearing in the formula is possible.

4.2 The external perturbation

ρ_{ext} is the perturbation, ingressing from outside: $\rho_{ext} \propto E_F + \varepsilon_k$

That means, this perturbation from outside is proportional to the kinetic energy of the pairing holes. Because of the Pauli-Principle that's at least the Fermi-Energy. The part of kinetical energy, which is kept over the FE by the holes, will be described in this work as ε_k .

4.3 The statical shielding

The polarization generated by the external perturbation is shielded at once by the conduction-electron-gas. This shielding is described by Thomas-Fermi-theory (s. the chapter before).

4.4 The characteristic Reference Energy

The size ρ_{ind} is proportional to the characteristic reference energy, which is responsible for pair-building. In the HTSC's this characteristic reference energy is identical with the Maximum Pseudogap **MPG** (see the foregoing section).

4.5 The Hamiltonian

A)

With these three sizes belonging to the dielectrical function the Hamiltonian can be constructed:

$$\begin{aligned}
 \varepsilon(MPG, \varepsilon_k) &= 1 - \frac{\rho_{ind}}{\rho_{ind} + \rho_{ext}} = 1 - \frac{MPG}{MPG - \varepsilon_k - E_F} \Rightarrow \\
 \Rightarrow H &\approx \frac{1}{2} \cdot \frac{E_F}{N_{L\delta}} \cdot \sum_{k,k'} \left(\frac{\frac{(MPG - \varepsilon_k - E_F)}{(MPG - \varepsilon_k - E_F) - MPG} - \frac{(MPG - \varepsilon_k - E_F)}{(E_F - MPG + \varepsilon_k) + MPG}}{\frac{(E_F - MPG + \varepsilon_k)}{(E_F - MPG + \varepsilon_k) + MPG} - \frac{(E_F - MPG - \varepsilon_k)}{(MPG - \varepsilon_k - E_F) - MPG}} \right) = \\
 &= \frac{E_F}{N_{L\delta}} \cdot \left[\sum_k \frac{(\varepsilon_k - MPG + E_F)}{E_F + \varepsilon_k} + \sum_{k'} \frac{(\varepsilon_{k'} - MPG + E_F)}{E_F + \varepsilon_{k'}} \right] = \\
 &= \frac{E_F}{N_{L\delta}} \cdot \left[\sum_k \frac{\varepsilon_k - (MPG - E_F)}{E_F + \varepsilon_k} + \sum_{k'} \frac{\varepsilon_{k'} - (MPG - E_F)}{E_F + \varepsilon_{k'}} \right] = \\
 &= \frac{E_F}{N_{L\delta}} \cdot \left(\sum_k \frac{\varepsilon_k - PSL}{E_F + \varepsilon_k} + \sum_{k'} \frac{\varepsilon_{k'} - PSL}{E_F + \varepsilon_{k'}} \right) \approx 2 \frac{E_F}{N_{L\delta}} \cdot \sum_k \frac{\varepsilon_k - PSL}{E_F + \varepsilon_k} [Eqn.43]
 \end{aligned}$$

B)

The holes are scattered from the ground-state ($E_F + \varepsilon_k$) to the intermediate-state. The energy of this intermediate-state mostly is the Maximum Pseudogap **MPG**. That's on account of the fact, that the highest values of the DOS are lying in this energy-region (experimental fact). In the Hamiltonian derived even, the expression **MPG** doesn't mean a singular, determined energy-state. But it means a gathering name of many, various, narrow beneath situated, states. By that the scatter of the hole-energies is equivalent mostly to $(MPG - \varepsilon_k - E_F)$ (and reversibly).

C)

In this formula ε_k doesn't represent the complete kinetic energy of the holes. The expression ε_k takes care, that $(MPG - \varepsilon_k - E_F)$ can possess every value between zero (corresponding to $\varepsilon_k = MPG - E_F$) and $(MPG - E_F)$ (corresponding to $\varepsilon_k = 0$).

By that the limits of allowed kinetic energies of paired holes are zero and $(MPG - E_F)$ ($(MPG - E_F)$) is nothing else, but the well-known pseudogap **PSL**.

D)

After a simple rearranging of the individual contributions to energy, you will see at once, that the dielectrical function gets a positive value, if $\varepsilon_k > MPG - E_F \equiv PSL$

A stronger repulsion of holes is the result in this case. In the contrary, if $\varepsilon_k < PSL$, an attractive interaction between two holes must be expected. The energy shell within an attraction may be possible, reaches from $\varepsilon_{k,k} = 0..to..\varepsilon_{k,k} = MPG - E_F \equiv PSL$

Therefore the pseudogap **PSL** corresponds to the Debye-energy in conventional SC's.

Naturally this statement is of great weight (s. also in **6.3**)

E)

So higher the Fermi-Energy, so smaller the pseudogap **PSL** and so smaller the amount of the matrixelement V^* (that means the Hamiltonian). In case of $E_F > MPG$ becomes positive, resulting in a stronger repulsion.

Therefore the equation [43] presented here, describes the maximal possible size of V^* .

As condition for any attraction results: $0 < \varepsilon_k < PSL$

F)

Consequently there must exist an upper limit of the doping range within an attractive interaction is possible yet. On account of that there must be found an upper limitation of doping for SC in Cuprates. The SC disappears with the pseudogap.

G)

It's a well-known fact, that the contribution of the k-state to pairing is the widest, if $k = -k'$ and in consequence $\varepsilon_{k'} = \varepsilon_k$. That's the reason why in the last line of the Hamiltonian the formula [43] could be simplified in the presented way.

H)

It's rather interesting that there is a coincidence with the denominator of the DOS in HTSC's to the numerator of V^* :

$$D(E) = \frac{2N_{LO}}{|MPG - E_F - \varepsilon_k|} = \frac{2N_{LO}}{|PSL - \varepsilon_k|} [Eqn.46]$$

This coincidence will be very significantly yet (s. **6.2, Cross-over to integration**)

I)

For a first survey here shall be inquired the normal case only (SC and PSL are disappearing together). The special case (HTSC without a pseudogap) shall be contemplated later.

At last it shall be pointed out, that this version of the matrix-element V^* is rather similar to the corresponding matrix-element in the BCS-theory:

The expression $MPG - \varepsilon_k - E_F$ corresponds to the term $\varepsilon_{k+q} - \varepsilon_k$ in the BCS-theory.

And MPG corresponds to the “cut-frequency” $\hbar\omega_D$. Really not so difficult.

4.6 Simplification of the formula of the dielectrical function:

Now the equation (regular form) of the dielectrical function is written again, but in another manner:

$$\begin{aligned}\varepsilon(MPG, k) &= 1 - \frac{MPG}{MPG - E_F - \varepsilon_k} = \frac{MPG - E_F - \varepsilon_k}{MPG - E_F - \varepsilon_k} - \frac{MPG}{MPG - E_F - \varepsilon_k} = \\ &= \frac{(MPG - E_F - \varepsilon_k) - MPG}{MPG - E_F - \varepsilon_k}\end{aligned}$$

One possible simplification is trivially: $\varepsilon(MPG, k) = \frac{-E_F - \varepsilon_k}{MPG - E_F - \varepsilon_k}$

But there exists another, more subtle, simplification, too:

For this purpose it's determined, that $(MPG - E_F - \varepsilon_k) \ll MPG$

This determination is valid nearly always. She doesn't success in the strong underdoped region, in which the FE is very small. In all other doping-regions the term $(MPG - E_F - \varepsilon_k)$ in the numerator of the dielectrical function can be neglected in comparison to MPG. By that it can be written:

$$\varepsilon(MPG, k) \approx \frac{-MPG}{MPG - E_F - \varepsilon_k} = \frac{-MPG}{PSL - \varepsilon_k}$$

Then the Matrix-Element is simplified to: $V^* \propto \frac{(MPG - E_F) - \varepsilon_k}{-MPG} = \frac{PSL - \varepsilon_k}{-MPG}$

Naturally this possible simplification wasn't demonstrated without any reason. But it shall facilitate immensely the comparison between theory and experiment.

At last should be predicted here: By application of this simplification to underdoped substances (i. e. HTSC's with small Fermi-Energies) too big sizes of the dielectrical function are generated. Consequently in the underdoped region the theoretical Tc-values should result to small (that is to say, smaller than the experimental). Indeed that's a matter of fact (s. **chap. VIII, 8.4**).

V) Result for Matrixelement V*

In **chapter 3.2** it was explained, that

$$V^* = \frac{e^2}{A \cdot \varepsilon_0 (k + k_{TF})} \cdot \frac{1}{\varepsilon(MPG)} \approx \frac{E_F(2 \text{ dim})}{N_{LO}} \cdot \frac{1}{\varepsilon(MPG)}$$

In the upshot we get as an expression for the attracting interaction between two holes:

$$V^* \approx \frac{E_F}{N} \cdot \frac{\varepsilon_k - (MPG - E_F)}{MPG} = \frac{E_F}{N} \cdot \frac{\varepsilon_k - PSL}{MPG}$$

The result of **4.3** was applied to this equation.

V* is the Matrixelement of hole-hole-interaction.

This expression is a intermediate result of great weight.

In this equation “MPG” means Maximum Pseudogap for doping zero

(s. **chap. 3.4, “The Maximum Pseudogap”**).

The expression **MPG** describes the characteristic Reference-Energy and presents the energy of the polarization. It's very probably that not only the shift of the Cu-3d-Elektrons, but also the shift of atomic rests, that means the generating of phonons, contributes to this polarization. This additional contribution to polarization-energy depends on the isotope mass. From that the supposition of a -although small- isotope effect in MPG is obvious. Below (**chap. 6.8**) the dependency of the Tc's on MPG will be proved. Indeed for that reason in case of small and high doping the isotope effect of Tc's reaches huge values. Particularities you will see further below in **chap. VIII) (Isotope effects)**.

It should be pointed out that V^* is negative as long as $\varepsilon_k < PSL$. That means, as soon as the kinetic energies of holes are smaller than the pseudogap **PSL**, an attractive interaction between two holes can appear.

VI) Application to the the self-consistence-equation (SCE), plagiarised from BCS-theory

5.1 For calculating the Tc's and many other sizes, the self-consistence-equation (SCE) from BCS-theory [7] is needed:

$$\sum_k -\frac{V^*}{2} \cdot \frac{1}{\sqrt{\varepsilon_k^2 + \Delta^2(T)}} \cdot \tanh \frac{\sqrt{\varepsilon_k^2 + \Delta^2(T)}}{2k_B T} \approx 1 [Eqn.26]$$

With the expresssion for V* from part **4.2 C)**: $V^* \approx \frac{E_F}{N} \cdot \frac{(\varepsilon_k - MPG)}{MPG}$ results:

$$\sum_k \frac{E_F}{2N} \cdot \left(\frac{MPG - \varepsilon_k}{MPG} \right) \cdot \frac{1}{\sqrt{\varepsilon_k^2 + \Delta^2(T)}} \cdot \tanh \frac{\sqrt{\varepsilon_k^2 + \Delta^2(T)}}{2k_B T} \approx 1 [Eqn.26]$$

6.2 Cross-over to integration

When T = Tc, the superconduction-energy-gap $\Delta_{SC}(T_c)$ becomes zero. Now we set $\Delta^2(T) = 0$ in this SCF and additionally we use the result of **4.1** belonging V*.
Then the SCF becomes as following:

$$\sum_k \frac{E_F}{2N_{Lö}} \cdot \left(\frac{MPG - \varepsilon_k}{MPG} \right) \cdot \frac{1}{\varepsilon_k} \cdot \tanh \left(\frac{\varepsilon_k}{2k_B T} \right) \approx 1$$

It shall be pointed out here, that ε_k always has to be smaller than MPG. If ε_k would be greater than MPG, the left side of SCE would be negative, and at the same time the right side would be nearly one. And that's impossible.

At now the cross-over from summation to integration is made. As DOS (for both spin-directions) the following expression is used :

$$D(\varepsilon_k) = \frac{2N_{Lö}}{|MPG - \varepsilon_k|}$$

ε_k is the kinetic energy of holes (resp. of the excess-electrons in electron-doped substances) and is measured from the zero-point of energy. Therefore ε_k can have a positive or a negative value in the equation for DOS .

Naturally in reality the DOS can't become negative. In spite of that this formula is a good approximation to the real DOS's. Especially it foretells that the DOS above the pseudogap is bigger than the DOS below the pseudogap. This prediction is confirmed by experiment.

And here two further statements:

A) The DOS of the holes is inverse proportional to the size of MPG. In consequence a big MPG leads to a small DOS of holes. As smaller this DOS as faster the Fermi-Energy of holes increases with increasing doping. As faster the Fermi-energy is increasing with increasing doping as faster the (variable) pseudogap will be closed with increasing doping. These both effects (big MPG and fast ascending of Fermi-Energy) are compensating each other. That allows a prediction: In total apart HTSC's the pseudogap vanishes at the same doping. A well-known fact is ascertained: The pseudogap vanishes mostly at a doping of 0,27. Indeed this prediction is correct.

B) With enhancing temperatures the energy-states are distributed otherwise, but the **summary** of states in the energy-interval $\varepsilon_k = 0..bis..\varepsilon_k = MPG$ always remains in the same level. Since it must be integrated about the **sum of all states** in the energy-interval $\varepsilon_k = 0..bis..\varepsilon_k = MPG$ the distribution of states inside of this energy-interval doesn't play any role. By that the DOS for T = 0K can be taken in case of all temperatures.

But let us now return to integration:

$$\int_{\varepsilon_k=E_F}^{\varepsilon_k=MPG} \frac{2N_{Lö}}{|PSL - \varepsilon_k|} \cdot \frac{E_F}{2N_{Lö}} \cdot \frac{(MPG - \varepsilon_k)}{MPG} \cdot \frac{1}{\varepsilon_k} \cdot \tanh\left(\frac{\varepsilon_k}{2k_B T}\right) d\varepsilon_k \approx 1$$

[Eqn.22]

It's noted at once: The blocking term $MPG - \varepsilon_k$ is shortening practically itself:

$$\int_{\varepsilon_k=E_F}^{\varepsilon_k=MPG} \frac{E_F}{MPG} \cdot \frac{1}{\varepsilon_k} \cdot \tanh\left(\frac{\varepsilon_k}{2k_B T}\right) d\varepsilon_k \approx 1$$

6.3 Setting of integration limits

The limits of integration are coming about by merely considerations:

A)

It has to be integrated inside the “shell” of kinetic energies in which an attractive interaction appears.

B)

The lower integration limit is -because of Pauli-Principle- the Fermi-Energy of the holes. The paired holes are permanently scattered in other states of energy. The non-occupation of these states must be taken for granted. But the states below Fermi-Energy mostly are occupied. The states above Fermi-Energy mostly are unoccupied. Therefore as the lower integration limit the FE can be taken for granted approximatively. But this lower IL is valid not always. More it is a useful thumbrule (or snap regula), failing at yttrium-holding and electron-doped HTSC`S. Probably in these classes of substances the lower IL lies significantly lower. Probably from that their Tc-values are significantly higher as expected by the plain form of this work. But these few substance-classes are exceptions, confirming the rule. That this theory is also suitable for these exceptions will be demonstrated in **part VII**). For simplicity -and on account of the great success- at first the Fermi-Energy will be used as lower Integration limitation.

So the Fermi-Energy of holes is the lower integration limit.

C)

Upper integration limit:

When in the expression $MPG - \varepsilon_k$ in the SCF the kinetic energy of holes exceeds the MPG, the left side of the SCF becomes negative. At one hand that describes a stronger repulsion between the holes. On the other hand then results mathematical nonsense, because the value of the right side of the SCF always lies near one. On account of that it can be concluded: The kinetic energy of holes ε_k always must be smaller than the MPG. Consequently the Maximum Pseudogap MPG represents the upper integration limit.

Upper integration limit is the Maximum Pseudogap, that means the pseudogap in case of doping zero. This important expression is a constant and especially independent from doping and from the kinetic energy of holes.

D) Result:

It's necessary to integrate from the Fermi-Energy of holes up to the MPG.

6.4 Bringing about of integration

In this section the abbreviation $\frac{\varepsilon_k}{2k_B T_c} \equiv X$ is used. With this abbr. it's got(ten):

$$\frac{E_F}{MPG} \cdot \int_{\frac{E_F}{2k_B T_C}}^{\frac{MPG}{2k_B T_C}} \frac{\tanh x}{x} dx \approx \frac{E_F}{MPG} \cdot \int_0^{\frac{MPG - E_F}{2k_B T_C}} \frac{\tanh x}{x} dx \approx 1$$

The shifting of IL in this expression is not correct totally, but it is a great average. It shall be turned out that in practical application the difference between MPG and Fermi-Energy is significantly greater than $k_B T_c$. By that the value of the integral represents as:

$$\int_0^{\frac{MPG - E_F}{2k_B T_C}} \frac{\tanh x}{x} dx = \ln\left(\frac{MPG - E_F}{2k_B T_c}\right) - \ln 0,44 = \ln\left(1,14 \frac{MPG - E_F}{k_B T_C}\right)$$

By setting this integral into SCE the SCE becomes to:

$$\int_0^{\frac{MPG - E_F}{2k_B T_C}} \frac{E_F}{MPG} \cdot \frac{1}{\varepsilon_k} \cdot \tanh\left(\frac{\varepsilon_k}{2k_B T_C}\right) d\varepsilon_k \approx \frac{E_F}{MPG} \cdot \ln\left(1,14 \cdot \frac{MPG - E_F}{k_B T_C}\right) \approx 1 [Eqn.35]$$

With some elementar transformations the formula for the critical temperatures is go(ten) as:

$$k_B T_C = 1,14 \cdot \frac{(MPG - E_F)}{\exp\left(\frac{MPG}{E_F}\right)} = 1,14 \cdot \frac{Pseudolücke}{\exp\left(\frac{MPG}{E_F}\right)}$$

VII) The Fundamental Equation (FE) of High Temperature Superconductivity

As a fundamental relation between Maximum Pseudogap, variable pseudogap, Fermi-Energy of conduction-electrons and critical temperature the forementioned equation was received:

$$k_B T_C = 1,14 \cdot \frac{(MPG - E_F)}{\exp\left(\frac{MPG}{E_F}\right)} = 1,14 \cdot \frac{Pseudolücke}{\exp\left(\frac{MPG}{E_F}\right)}$$

At now this equation will be called as “**Fundamental Equation**” (FE).

At this point I'm carefully reminding you that MPG is the pseudogap in the undoped state.

At once will be understood the importance of this fact: It's nearlying to identify the term

$MPG - E_F$ (that means Maximum Pseudogap being deduced the Fermi-energy of holes) as **variable pseudogap**. In consequence follows:

$$k_B T_C = 1,14 \cdot \frac{Pseudolücke}{\exp\left(\frac{MPG}{E_F}\right)} = 1,14 \cdot (MPG - E_F) \cdot \exp\left(-\frac{MPG}{E_F}\right)$$

This Formula represents the Fundamental Equation of High Temperature Superconductivity. It is the fundamental quantitative relation between all experimental ascertainable parameters of HTSC. This equation connects the superconductivity with the pseudogap found in all substance-classes of HTSC.

Formulated in other words: The critical temperature is appointed by quantity of pseudogap and by that from density of holes, resp. by doping. Above a certain doping the Fermi-Energy of holes is higher than MPG and the pseudogap reaches (theoretical) negative values. Above this limit of doping superconductivity can't exist.

All these estimations are confirmed by experiment.

Attention: The appearing of a pseudogap in every HTSC isn't pretended here. Here is pointed out only that hole-couples can appear only when the kinetic energies, transported between the paired holes, are smaller than the Maximum Pseudogap.

VIII) Quantitative comparison between theory and experiment

8.1 Inquiring the FE more exactly, ten(!) quantitative and experimental ascertainable relations are received. All of these estimated relations are confirmed quantitatively by experiment. That's very surprising, regarding to the fact that in this work some bold approximations are used. Natural those approximations are not able to describe exactly the reality. Especially the DOS's and the limits of integration (IL) can deviate from theory (how it will be seen lower). It follows:

A summary of the most important comparisons between theory and experiment:

- 1) Correlation between doping and critical temperatures
- 2) Correlation between pseudogap and SC-energy-gap
- 3) Correlation between pseudogap and critical temperature
- 4a) Dependency in doping of pseudogap
- 4b) The maximal critical temperature lies in the neighbourhood of the “Golden Section”
- 5) Relationship between Maximum Pseudogap MPG and the pseudogap found at optimal doping
- 6) Relationship between critical temperature and pseudogap at optimal doping
- 7) The maximal critical temperature (in Kelvin) has the equal numerical value like the Maximum Pseudogap MPG (in meV)
- 8) Isotopic Effects
- 9) Influence of impurity ions
- 10) Prediction of a so-called “Plateau-region” in the underdoped region of LSCO

Annotation: The quantity of $MPG - E_F$ can be received with the assistance of the measured and the maximum pseudogap:

If $MPG - E_F = \text{Pseudogap}$, than $E_F/MPG = 1 - (PSL/MPG) = 1 - \frac{PSL}{MPG}$.

$$\text{And: } MPG/E_F = 1 \left/ \left[1 - \left(\frac{PSL}{MPG} \right) \right] \right.$$

Thereby was used the (not always correct) approach, that the pseudogap disappears, when the Fermi-energy is reaching the energy of the maximum pseudogap.

8.2 The critical temperatures in dependence on doping

In VII) it was derived the Fundamental Formula for HTSC:

$$k_B T_C \propto 1,14 \frac{PSL}{\exp(MPG/E_F)} = 1,14 \frac{MPG - E_F}{\exp(MPG/E_F)} \quad (6)$$

Considering the Fundamental Formula for calculating the critical temperatures, you verify, that the Tc's do not depend on doping like a parabola, but similar to a parabola. That means, with increasing doping, Tc also is increasing in the beginning, to go down at more higher doping. The maximum of Tc will be reached at $E_F/MPG = 0,62$. That means, if superconductivity appears on doping $\leq 0,27$, the maximum is reached at 0,17. Above a discrete doping (that implies above discrete Fermi-energies) all Cuprates only show normal-state-conduction at all temperatures. (Physical explanation see under **6.3 “Setting of Integration Limits”**.

These forecasts of theory are all confirmed by experiments (till now). The following tables allow a comparison between theory and measured quantities.

8.3 Ratio between pseudogap PSL($\equiv \Delta_P$) and superconducting energy gap $\Delta_{SC}(T = 0K)$

The theory presented in this work makes a universal previous statement between the experimental quantities variable pseudogap PSL ($\equiv \Delta_P$) and superconducting energy gap $\Delta_{SC}(T = 0K)$. In concordance with BCS-theory is valid:

$$\Delta_{SC}(T = 0) = \frac{\text{relevante Energieskala}}{\sinh\left[\frac{1}{D(E_F) \cdot V^*}\right]}$$

This well-known formula succeeds totally universal and especially independent of the exact coupling mechanism. “Translated” in the theory designated here, it's given:

$$\Delta SC(T = 0) = 1,213 \cdot \frac{Pseudolücke}{\sinh \left[\frac{MPG}{E_F} \right]}$$

According to this equation the SC-energy gap **doesn't** reach its maximal value at optimal doping (how it should be supposed by intuition), but already at half-maximal doping. That means at $p = 0,27/2 = 0,135$. (Optimal doping is $p = 0,16$.) Now it shall be examined, if these forecasts are suiting well to reality. Because d-wave-pairing is realised in the Cuprates the value of SC-energy gap has to be multiplied with 1,21306 [28wm, 11hüf]:

A) Tabula for ratio between pseudogap and Superconducting gap in case of Hg1201
 (Maximum Pseudogap MPG = 97 meV)

Doping	0,11	0,12	0,13	0,14	0,15
2PSL [meV]	100	90	85	84	74
Doubled experimental SC-energy gap at $T_c = 0$ [meV]	38	43	45	45	47
MPG/E _F	2,06	1,86 5	1,78	1,76 4	1,62
(Theoretical value) $\frac{2\Delta_p}{2\Delta_{sc}} = \frac{1}{1,213} \cdot \sinh \left(\frac{MPG}{E_F} \right)$	3,18	2,6	2,3 75	2,33 5	2
$\frac{2\Delta_p}{2\Delta_{sc}}$ (Experimentell)	2,63	2,1	1,9	1,87	1,57
Deviation between theory and experiment %	21	24	25	25	27

Lit.: [10 ØF, 12nak, 11Hüf, 15sl]

The difference between theory and experiment always amounts roughly to a quarter. Probably a systematical deviation is presented here (particulars see below).

B) Tabula for ratio between pseudogap and Superconducting gap in case of Bi2212
 (Maximum Pseudogap MPG = 93 meV)

Dotierung	0,11 5	0,13	0,16	0,17	0,21 3	0,22
2PSL [meV]	105	97	76	63	45	36,3
Doubled experimental superconducting gap at Tc = 0 [meV]	33	38,3	41	39	36	27
MPG/E _F	2,3	2,1	1,7	1,5	1,32	1,24 5
$\frac{2\Delta_P}{2\Delta_{SC}} = \frac{1}{1,213} \cdot \sinh\left(\frac{MPG}{E_F}\right)$ (theoretetrical value)	4,07	3,3	2,18	1,76	1,43	1,32
$\frac{2\Delta_P}{2\Delta_{SC}}$ (Experimentell)	3,18	2,53	1,85	1,6	1,25	1,34
Deviation of experiment to theory	28 %	30 %	18 %	10 %	14,4 %	-2 %

Lit.: [10 Ø F, 12nak, 11Hüf, 15sl]

At a first glance the coincidence of theory and experiment is enhancing with increasing doping.

C) In case of **Tl2201** and doping p = 0,25 the following values are available:

2 PSL = 20 meV and MPG = 100 meV. A theoretical ratio between pseudogap and superconducting gap in height of 1,12 is calculated by these values. In experiment: 20 meV/18 meV = 1,11[11hüf, fig. 2]. So in this substance the deviation between theory and experiment is imperceptibly small.

D) It shan't have be depressed, that in optimal doped **LSCO** a great deviation between theory and experiment is found. The theoretical ratio amounts to 2,36. In comparison the experimental ratio is 7,5/5 = 1,5. This is a deviation of always 57%. Indeed I dare say, a measuring fault is before us at this point.

Lit.: [Achsaf, N. et al. in Coherence in High Temperature Superconductors, S. 428, World Scientific, Singapur 1996 & Ekino, T. et al., Superconducting energy gap...., Physica C 263 (1996), S. 249]

E) In the article [11hüf] very much superconducting gaps are comparated. Dividing the mean values represented there for pseudogaps and superconducting gaps at optimal dopings the following ratio is received : 75,5 meV/40 meV = 1,89. The theoretical result lies at:

$$\frac{2\Delta_P}{2\Delta_{SC}} = \frac{1}{1,213} \cdot \sinh\left(\frac{MPG}{E_F}\right) = 0,81 * \sinh(1,67) = 2,11.$$

The mean deviation from theory to reality is: $2,11/1,89 = 12\%$.

F) In comparison in case of extreme overdoping a limiting value of $\frac{MPG}{E_F} \rightarrow 1$ results.

$$\text{In consequence for this limit case follows: } \frac{2\Delta_P}{2\Delta_{SC}} \rightarrow \frac{1}{1,213} \cdot \sinh(1) \approx 0,97$$

So in this work a blend of pseudogap and superconducting gap in the very overdoped region is forecasted. Indeed in case of doping higher as roughly 0,26 the converging of pseudogap and superconducting gap is mentioned in the paper of S. Hüfner et al [11hüf, fig. 2 and remark on p. 4]. Here it shall be given to you again: In the cited article [11hüf] a great number of measured quantities is presented. These values were used for proving this theory bespoken here. The predication of this work are satisfied very well by experiment.

G) **NB:** By equation used here: $\Delta SC(T=0) = 1,213 \cdot \frac{\text{Pseudolücke}}{\sinh\left[\frac{MPG}{E_F}\right]}$

the maximum of superconducting gap will **not** be received at the optimal doping, but at a doping of 0,17. The difference between $T_c(\max)$ and the critical temperature belonging to the maximal superconducting gap amounts (by theory) only 1,7 per thousand, that means 0,17%. And the differences in the energy gaps amounts to 1,4 per thousand = 0,14%. That means in case of a maximum T_c of 100 K this difference amounts to plain 0,17 K, resp. to 0,06 meV. Perhaps, instead of its imperceptibility, this effect will be searched and found by experiment in future.

8.4 Previous calculation of the critical temperatures from pseudogap-values.

Previous calculation of the relationship between pseudogap and critical temperature.

Following the Fundamental Equation, we find out: $\frac{2PSL}{k_B T_c} \propto 1,75 \cdot \exp\left(\frac{MPG}{E_F}\right)$.

By simple transformation we get: $\frac{2Psl.}{k_B T_C} \propto 1,75 \cdot \exp\left(\frac{MPG}{E_F}\right)$

Table A): Critical temperatures and the relation between PSL (= Pseudogap) and Tc for
Bi2212MPG (extrapolated) = 90 meV¹⁰⁻¹² [8ren, 10F, 11hüf u. 62Dah]

Doping	$\approx 0,105$	0,12	0,13	UD	0,16	0,18	0,19	0,2	0,21	0,26
Measured PSL [meV]	49	46,4	44	40	36	35,5	31	39,3	25	26
MPG/ E_F (calc., see above)	2,2	2,064	1,96	1,8	1,67	1,65	1,525	1,775	1,38	1,48
Tc (calculated) [K]	72	78	82	87	90	90	89	88	83	60
Tc (experimental) [K]	64	80	85	81	90	88	86	79	76	57
$\frac{2PSL}{k_B T_C} = 1,75 \exp(MPG/ E_F)$, calculated	15,8	13,8	12,4	10,6	9,3	9,1	8,0	10,3	7,0	7,7
$\frac{2PSL}{k_B T_C}$ (experimental)	17,5	13,2	12,0	11,5	10,0	9,35	8,6	11,3	8,7	10,6

Lit.:¹⁰ [8ren, 10F, 11hüf u. 62Dah]

Author: Hans Chr. Haunschild, born Ffm 20. 2. 1964

Table B): Critical temperatures and the relation between PSL (= Pseudogap) and Tc for **LSCO**

MPG(extrapolated) = 38 meV^{10,12}

Doping	0,04	0,05	0,06	0,075	0,08	0,086
Measured PSL [meV]	33	31,5	30	27,5	27	26
MPG/ E_F (calc., s. above)	7,6	5,85	4,75	3,62	3,46	3,17
Tc (calculated) [K]	0,2	1,2	3,4	9,7	11,3	14,5
Tc (experimental) [K]	[Null] ^{13et18}	[Zero] ¹⁵	¹⁴ 5,5 ¹⁵ 8,5 ¹⁵	¹³ 21,2 ¹⁶ 24 ¹⁵ 19	¹⁷ 19,6 ¹⁸ 29,7	¹⁷ 22,25
$\frac{2Psl.}{k_B T_C} = 1,75 \exp(\frac{MPG}{E_F})$	3500	608	202	65	56	42
$\frac{2Psl.}{k_B T_C}$ (experimentell)	∞	∞	103	31	27	30

Doping	0,09	0,1	0,105	0,11	0,113	0,115	0,12
Measured PSL [meV]	25	23	22,75	22,5	22,3	22,25	22
MPG/ E_F (calc., s. above)	2,9	2,53	2,5	2,45	2,42	2,41	2,375
Tc (calculated) [K]	17,8	24	25	25,6	26,2	26,4	27

Tc (experimental) [K]	27,5 ¹⁴ 29,3 ¹⁶ [16 ¹⁵]	29,2 ¹⁶ 26,2 ¹⁹	27,8 ¹⁴	26,1 ²⁰ [13,9 ²¹] 29,1 ¹⁶	29,6 ¹³	27,3 ²⁰	30,2 ²⁰ 29,4 ¹⁶
$\frac{2PSL}{k_B T_C} = 1,75 \exp(MPG/E_F)$	32	22	21,3	20,3	19,7	19,5	18,8
$\frac{2PSL}{k_B T_C}$ (experimental)	22	21	22	20	18,5	19,9	17,75

Doping	0,125	0,13	0,14	0,15	0,16	0,17	0,18
Measured PSL [meV]	21,5	21	20,5	16,6	14	11,75	11
MPG/E_F (calc., s. above)	2,3	2,235	2,17	1,775	1,58	1,44	1,4
Tc (calculated) [K]	28,4	30	31	37	38	35	35,6
Tc (experimental) [K]	28,4 ²² 27,8 ²³	34,4 ¹⁶ 40 ¹² 35 ²⁴	36,9 ¹⁶ 37,0 ¹⁴ 36,5 ¹³ 33,0 ²⁷ 31,5 ¹⁸	34,5 ²² 33,5 ²⁵ 28,6 ¹⁹ 38,0 ²³	39,0 ²⁶	34 ¹⁵	40 ¹² 35 ²⁴
$\frac{2PSL}{k_B T_C} = 1,75 \exp(MPG/E_F)$	18,35	16,4	15,3	10,3	8,5	7,4	7,1
$\frac{2PSL}{k_B T_C}$ (experimental)	18,35	14,6	11,2	11,2	9,5	7,5	6,2

Doping	0,188	0,2	0,225	0,24	0,25	0,263	0,3
Measured PSL [meV]	8,5	7	5	4	3	Ca. 2	Zero
MPG/E_F (calc., s. above)	1,3	1,226	1,15	1,12	1,086	1,06	Ca. 1
Tc (calculated) [K]	31,0	27,2	21	17,3	13,4	9,2	Zero
Tc (experimental) [K]	34,4 ¹³ 33,5 ¹⁵ 30,4 ¹⁸	[18,9] ¹⁹ 25 ¹²	23 ¹³ 19 ¹⁸	10,1 ²¹	8 ¹³	[15,2 ¹⁹]	
$\frac{2PSL}{k_B T_C} = 1,75 \exp(MPG/E_F)$, calculated	6,35	6	5,5	5,4	5,2	5	4,8 (theor. value)
$\frac{2PSL}{k_B T_C}$ (experimental)	6,65	5,8	5,8	5,6	[9,2]	5,8	[1,5]

Literature: The values of pseudogaps are from^{11et12}.

Experimental Tc-values in brackets are "freak values", resp. "runaways", probably measuring faults. Take note of the phenomenon, that a "plateau-region" between the dopings of 0,1 and 0,13 is predicted in theory. Indeed this predicted "plateau-region" is confirmed by experiment. In accordance with these results the depending of Tc on pseudogap and not on hole-concentration is evidently

8.5 The magnitude of the Pseudogap in dependence on doping

In the case of doping zero ($E_F = 0$) is valid: MPG – E_F = MPG - 0 = MPG. Following this theory the pseudogap must reach his maximum -defined as MPG- by zero doping. This assumption is confirmed by experiment^{8,9}.

8.6 The maximum of Tc is situated at the "Golden Section"

The maximal Tc is reached at: $E_F = \frac{\sqrt{5}-1}{2}$ MPG ≈ 0.618 MPG.

This is exactly the formula of the "Golden Section", which cannot be only a coincidence. That means, when superconduction appears at doping ≤ 0.27 , the theoretical Tc-maximum will be reached at a doping of $0.62 * 0.27 = 0.167$. The Tc-maximum is found mostly at a doping of 0.16.

8.7 Special cases YBCO and elektrondoped Cuprates

The Fundamental Equation is applicable to HTSC's without a pseudogap, too.

In part 6.3) the Fermi-Energy was given as a lower limit of energy shell, in which an attracting interaction can be brought about. The reason was, that the states lower as the Fermi-Energy are occupied mostly. This approximation is very successful for the most HTSC's. But in case of YBCO and of electrondoped Cuprates it is not satisfying. The reason why is unknown till now.

8.8 The relation between the maximum pseudogap and that value of pseudogap, found at optimal doping

$$\text{If } \frac{E_F(T_C^{\max})}{\text{MPG}} = 0,62, \text{ then is MPG} - E_F(T_C^{\max}) = 0,38 \text{ MPG.} \quad (8)$$

From the relation: $\text{MPG} - E_F(T_C^{\max}) = 0,38 \text{ MPG} = \text{pseudogap at } T_C^{\max}$, results:

$$\text{MPG} = \frac{PSL(T_C^{\max})}{0,38} = 2,63 \cdot PSL(T_C^{\max}). \quad (9)$$

But that causes, the maximum pseudogap is 2,63 times higher than the pseudogap at optimal doping.

Table III. Relations of pseudogaps

Substance	LSCO	Bi2212	Bi2223	Hg1201	Hg1212	Hg1223	PCCO
PSL(T_C^{\max}) [meV]	14	36	45	33	50	46	11 (?)
Experimental							
$\frac{PSL(T_C^{\max})}{0,38} = \text{MPG}$	37	95	118	87	132	120	29
calculated [meV]							
MPG, extrapolated from experiment [meV]	38	90	110	97	123	131	23

Substance	YBCO	$YBa_2Cu_4O_8$	NdCCO	Tl2201
PSL(T_C^{\max}) [meV]	22	24,4	4,6	35,5
Experimental				37^{15}
$\frac{PSL(T_C^{\max})}{0,38} = \text{MPG}$	58	64	12	93
calculated [meV]				97^{15}
MPG, extrapolated from experiment [meV]	92	81	18,5	100

All values without ¹⁵ are from ^{10 et 12}.

8.9 Ratio between Tc and pseudogap at optimal doping

It shall be given to you again: $k_B T_C = 1,14 \cdot \frac{(MPG - E_F)}{\exp\left(\frac{MPG}{E_F}\right)} = 1,14 \cdot \frac{Pseudolücke}{\exp\left(\frac{MPG}{E_F}\right)}$

In case of optimal doping is valid: $k_B T_C^{\max} = 1,14 \cdot \frac{PSL(T_C^{\max})}{\exp(1,618)} = 0,226 \cdot PSL(T_C^{\max})$

The conversion factor between Kelvin-temperatures and energies in meV runs to 11,6.

Multiplying 0,266 with 11,6, the value of 2,62 is gotten. Consequently the critical temperature in Kelvin amounts to the 2,62-fold of pseudogap measured in meV:

$$k_B T_C^{\max} = 0,226 \cdot PSL(T_C^{\max}) \Rightarrow T_C^{\max} \triangleq 2,62 \cdot PSL(T_C^{\max})$$

B)

Following the simplest assumptions of this work the ratio of doubled pseudogap and critical temperature always is 7,76:

$$\frac{2\Delta_P}{k_B T_C} = \frac{2PSL(T_C^{\max})}{1,14 \cdot PSL(T_C^{\max}) \cdot \exp(-1/1,62)} = \frac{2}{1,14 \cdot 0,226} = 7,76$$

Be regarded that for making of this calculation the experimental values of PSL and Tc(max) not must be known.

Table IV)

Coherence between Tc and pseudogap at optimal doping.

Experimental values are used only.

Substance	LSCO	Bi2212	Bi2223	Hg1201	Hg1212	Hg1223	PCCO
T_C^{\max} experiment.[K]	37	90	111	97	123	131	23
PSL(T_C^{\max}) [meV] Experimental	14	36	45	33	50	46(measuring fault ?)	11 (?)
T_C^{\max} [K] $PSL(at T_C^{\max})$ [meV]	2,64	2,5	2,47	2,9	2,5	2,85	2,1

Substance	YBCO	$YBa_2Cu_4O_8$	NdCCO	Tl2201
T_C^{\max} experim.[K]	92	81	18,5	90

$PSL(T_C^{\max})$ [meV]	22	24,4	4,6	35,5
Experimental				37^{15}
$\frac{T_C^{\max} [K]}{PSL(at T_C^{\max}) [meV]}$	4,2	3,3	4,0	2,54
Lit. ^{10 et 15}				$2,43^{15}$

8.10 The maximum Tc, measured in K, has the same numerical value like the maximum pseudogap, measured in meV.

From **V)** results, that T_C^{\max} [in K] = $2,64 \cdot PSL(T_C^{\max})$ [in meV]

From **IV)** results, that MPG [meV] = $2,63 \cdot PSL(T_C^{\max})$ [meV]

In consequence of the results of **IV)** and **V)** results, that T_C^{\max} [in K] = $\frac{2,64}{2,63} \cdot MPG$ [in meV].

That means, with increasing MPG (by pressure, for example), T_C^{\max} also increases.

Table V. Ratio between MPG and T_C^{\max}

Substance	LSCO	Bi2212	Bi2223	Hg1201	Hg1212	Hg1223	PCCO
T_C^{\max} experiment.[K]	37	90	111	97	123	$\emptyset = 131$	23
MPG [meV]	37	90	Not	deter-	min-	ed	20 (?)
T_C^{\max} /MPG	1,0	1,0					1,15

Substance	YBCO	$YBa_2Cu_4O_8$	NdCCO	Tl2201
T_C^{\max} experiment.[K]	92	81	18,5	90
MPG [meV]	unknown	71	unknown	100
T_C^{\max} /MPG		1,14		0,9

Literature:¹⁰

VII) Relationship between energy-gap of superconduction Δ_{SC} (T=0) and critical temperature Tc.

About the presupposition, that the energy ε_k , transferred between the holes is situated in the area of the pseudogap, results from BCS-theory⁷:

$$\text{Superconducting-energy-gap} = \Delta_{SC}(T=0) = \frac{\text{Pseudogap}}{\sinh[1/D(E_F)V]} = \frac{\text{Pseudogap}}{\sinh[MPG/E_F]}$$

$$\text{Und: } 2\Delta_{SC}(T=0)/k_B T_C = \frac{2 \cdot \text{Pseudogap}}{\sinh[MPG/E_F]} \cdot \frac{\exp(MPG/E_F)}{1,14 \cdot \text{Pseudogap}} \approx \frac{2 \cdot 2 \exp(MPG/E_F)}{1,14 \exp(MPG/E_F)} \approx 3,5.$$

Since in the Cuprates the d-wave-pairing appears, it is necessary to multiply this value with 1,21306²⁸. In consequence appears a value of $3,52 \cdot 1,21306 = 4,27$. This value of 4,27 is valid for underdoped substances. In case of overdoped substances results a value of $4,0 \cdot 1,21306 = 4,85$. That means, with augmenting doping Δ_{SC} increases circa about a seventeenth. Measured are values between 4 and 6^{29et30}, and in fact the experimental mean-values are augmenting with increasing doping about a seventeenth.

On Tl2201 seems to exist a recognizable deviation: Possible here are measured values between 8 and 11³⁰.

3.6 Evaluation

Theory and experiment are in satisfying accordance. Distinct deviations between theoretical predictions and experimental measurements appear at the Yttrium-compounds and at NdCCO. For these classes of substances accordance between theory and experiment is available, if there are used modified formulas of the FF. This theory not only makes qualitatively, but quantitatively exactly right predictions. That is so more surprising, if it is bored in mind, how strong simplifications are included. An unequivocal relation between the pseudogaps, Maximum Pseudogap, doping and superconductivity is demonstrated here.

IV. Explanation of the Isotope-Effects (IE) of the HTSC

For completing, the isotope-effect (IE) in HTSC should be discussed.

That the HTSC at all show an IE, is a sure hint, that phonons are playing an important role in the pair-building. But at a first glance the magnitudes of the observed IE's doesn't have any atom of meaning in it: So smaller the Tc-values, so higher are the IE's. By far the smallest IE's are found at the maximum of Tc. By all ordinary ideas about SC exactly the opposite should be the case. A senseful explanation can be searched with aid of the Fundamental Equation:

How it was demonstrated in the chapters above a variation of Maximum Pseudogap **MPG** leads to variation of Tc. Since a variation of atomic masses varies the Tc-values also, the conclusion is obvious that the size of **MPG**, respectively of pseudogaps also depends in a small amount by atomic mass. By that the Tc's must be varied, too. That means, the **MPG** depends on atomic mass also, leading to an isotope effect.

Now there exist two possible ways of varying the **MPG**: (Probably) by substituting O^{16} by O^{18} . And surely by substituting of Bismut by Lanthan. In both cases the same variation of doping in both substance-classes should variate the relative Tc-values (i. e. T_c/T_c) **in the same way**. Explained easier: When the ratio $T_c(O^{16})/T_c(O^{18})$ shows a relative maximum the ratio of $T_c(\text{Bi}2212)/T_c(\text{LSCO})$ will reach a relative maximum. When the ratio $T_c(O^{16})/T_c(O^{18})$ shows a relative minimum the ratio of $T_c(\text{Bi}2212)/T_c(\text{LSCO})$ will reach a relative minimum, too. (Anyway then, if **MPG** depends really on atomic mass.) After application of the Fundamental Equation the following view is gotten:

$$\frac{T_c(\text{Bi}2212)}{T_c(\text{LSCO})} = \frac{PSL(\text{Bi}2212)}{PSL(\text{LSCO})} \cdot \exp\left(\frac{\text{MPG}(\text{LSCO})}{E_F} - \frac{\text{MPG}(\text{Bi}2212)}{E_F}\right)$$

By application of this formula appears **Table IV**):

Doping	$\frac{PSL(Bi2212)}{PSL(LSCO)}$	$\frac{MPG}{E_F}(LSCO) - \frac{MPG}{E_F}(Bi2212)$	$\frac{T_c(Bi2212)}{T_c(LSCO)}$ theoretical	$\frac{T_c(Bi2212)}{T_c(LSCO)}$ experimentel
0,105	2,154	2,5 - 2,2 = + 0,3	2,9	2,3 (evtl. measuring -fault at Bi)
0,12	2,1	2,375 - 2,064 = + 0,3	2,88	2,65
0,13	2,1	2,235 - 1,95 = + 0,285	2,8	2,47
0,14	2	2,17 - 1,8 = + 037	2,9	2,22 (absolut. Minimum)
0,15	2,35	1,775 - 1,765 = + 0,01	2,38	2,32
0,16	2,6	1,58 - 1,67 = - 0,087	2,36	2,31
0,18	3,23	1,4 - 1,65 = - 0,244	2,53	2,35
0,19	3,65	1,3 - 1,53 = - 0,24	2,9	2,5
0,2	5,6	1,226 - 1,775 = - 0,55	3,2	2,47

Lit.: chap. 3.5, Tabellen I) und II) in this work]

Considering the big differences between the magnitudes of the the pseudogaps of Bi2212 and LSCO the variableness of these magnitudes can hardly falsify the results. The relations of the experimental Tc's are consistent in the framework of measuring-accuracy. Considering the success of the theory till now such a result could be expected. It is more interesting, that the relations of the Tc-values of both substance-classes demonstrate the same behaviour as the IE in dependence of doping: Table V) is showing the experimental OIE in LSCO.

7.2 Quantitative Observation

$$\begin{aligned} \frac{T_c(O16)}{T_c(O18)} &= \frac{PSL(0^{16})}{PSL(0^{18})} \cdot \exp \left[\frac{MPG(0^{18})}{E_F(0^{18})} - \frac{MPG(0^{16})}{E_F(0^{16})} \right] = \\ &= 1,02 \cdot \exp \left[\frac{MPG(0^{16}) - 0,2meV}{E_F(0^{16}) - 0,2meV} - \frac{MPG(0^{16})}{E_F(0^{16})} \right] [Eqn.16] \end{aligned}$$

Considering this corrected, but also complicated formula, the following is gotten:

A)

A)

In the UD region the exponentialfunction is dominating and an augmentation of phonon-frequencies leads to an enhancement of Tc.

B)

In the OD region the phonon-frequencies are appearing fewer in the denominator, but have a big influence to the numerator of the FE (that means to pseudogap), and the Tc-values are growing with decreasing atomic mass.

D)

Compared to it the contradicted influences of phonons are extinguishing each other. By that the influence of isotopic mass is imperceptibly small at optimal doping.

E)

Please keep your attention to the fact, that this work doesn't predict any influence of foreign ions on **MPG** and **PSL**. That doesn't exclude an eventual variation of critical temperatures by incorporation of foreign ions. But the foreign ions are varying critical temperatures in another way. See more in the following **chapter VIII**.

Table V): Survey of the OIE of LSCO

Tabelle V): Übersicht über den OIE des LSCO

Doping	Pseudogap [meV]	$\frac{MPG}{E_F} (0^{16})$	Tc(O16) [K]	$-\Delta T_C$ [K] experim	$-\Delta T_C$ [%] Theorie	$-\Delta T_C$ [%] experim.	Literature
0,06	30	4,75	8	1,0	12,3	12,5	[20,zhao]
0,075	28	3,8	20	0,76	8	3,9	[13cr30ha]
0,08	27	3,46	19,6	1,1	6,2	5,5 und 5,7	[17h/c, 17A]
0,086	26	3,17	20	1,07	5,5	5,3 und 4,8	[17h/c, 17A]
0,09	24,5	2,8	28	1,6	5,4	5,7	[32cr, 20 zhao]
0,105	23,75	2,67	28,5	1,7	4,1	6	[21ph,

							20zhao, 33zhaol
0,11	23,5	2,62	29	1,6	4,4	5,5	[20zhao, 33zhaol]
0,11 4	23,3	2,59	29,6 und 20	1,9 u. 1,46	4,3	6,4 und 7,3	[13cr, 20zhao, 33zhaol]
0,12	23	2,53	25,4**	2,25	4,5	8,9 rel.Max	[31cr, 33zhaol]
0,12 5	22	2,38	28	2,0	3,8	7,15	[22mr, 23jpf]
0,13	21	2,24	29,8	2,0	3,5	6,7	[32cr]
0,14	20,5	2,17	32,4	0,6	3,5	1,85	[32cr]
0,15	16,6	1,78	37	0,7	2,7	1,9	[13,20-23,32]
0,16 6	12	1,46	35	0,5	2,5	1,4 rel.Min.	[35bab]
0,17 5	11,4	1,43	16,2**	0,3	2,3	1,85	[32cr]
0,19	8	1,27	34,4	0,21	2,15	0,6**	[13cr]
0,2	7	1,23	28,4	1,1	2,1	3,9**	[21ph]
0,22 5	5	1,15	23	0,23	2,1	1**	[13cr]
0,25	3	1,09	10,1	0,3	2	3	[21ph]
0,26 3	Ca. 2	1,06	8	0,22	2	2,75	[13cr]

Values of the pseudogaps are shown in **chapter III. in this work**

Naturally the results of tables IV) and V) are not identically. But both agree in one point: If Bi is substituted by La, or if light oxygen is substituted by heavy oxygen, the maxima and minima are situated at similar doping. The highest variation on Tc in dependence on **MPG** is appearing in under- and overdoped Cuprates. The Tc-dependency on **MPG** is the smallest at optimal doping. Remarkably the IE's in LSCO present the same behaviour. Intuitive assuming should lead to the idea of the appearance of the strongest IE at optimal doping. Suiting to this work the reality is in contrary to this assumption.

In consequence I dare say that Maximum Pseudogap shows an isotope effect. And in account of that the variable pseudogap, too. Furthermore I dare say the reason of the isotope effect of HTSC's is this dependency of **MPG** on the IE. Inquiring the tables above a decrease of

Maximum Pseudogap **MPG** by increasing of isotope mass is perceptible. By that the critical temperatures are decreased, too. The reason is probably a small contribution of phonons to polarization (see **ch. V**). Suiting the explanations in **ch. 3.4** the **MPG** is reversely proportionally to the masses of Copper and Oxygen. In the denominator of the Fundamental Formula the Fermi-Energy describes the statical shielding. The phonon-frequencies are describing the contribution of dynamical shielding.

Comparing theory and experiment it is established, that the predictions of theory are generally satisfied. The prediction of a decreasing maximum pseudogap MPG with increasing atomic weight is reliable, in consequence resultant to an Isotope Effect.

VIII) Influence of impurities upon the superconducting parameters

Nearly with discovering of HTSC it was established, that the substitution of copper by paramagnetic ions suppresses the Tc-values. This could be expected by the well-known theories of superconductivity at this time. But it was not provided for a stronger sinking of critical temperatures by substitution of copper by unmagnetically zinc-ions. There are no hints for changing the (maximum) pseudogap by impurities. By that a decreasing of the pair-density by impurities can be supposed. Quantitatively: The impurities increase the argument of the exponential-function in the denominator of the FF. If this assumption is true, than with increasing doping the influence of the impurities is decreasing. Someone very similar we got to know upon the IE. In accordance with the FF is valid: $T_C = \frac{PSL}{\exp\left(\frac{MPG}{E_F}\right)}$

This simple equation only is valid **without substitutions**. With substituting impurities is valid

$$Tc = 1,14 * Psl \cdot \exp\left(-F \cdot \frac{MPG}{E_F}\right)$$

In this formula is $F > 1$ and proportional to the portion of impurities. It is in the nature of such an approximation, that the worth of F depends on the type of impurities, too.

The result is: $\frac{Tc_1}{Tc_2} = \exp\left[\left(1 - F\right) \frac{MPG}{E_F}\right]$. If we point out $1 - F = f$, we get:

$$Tc_2/Tc_1 = \exp[-f(MPG/E_F)]. \quad (15)$$

The size of “ f ” is an other for every metal (and probably for every class of substances, too) and must searched by experiment. In contrary the size of “ f ” should not depend on doping.

For the class of LSCO-substances the following tabulas will show the quantitative comparison between theory and experiment:

Zink: $La_{1,85}Sr_{0,15}Cu_{(1-x)}Zn_xO_4$:

$$MPG/E_F = 1,6 \quad \text{Parameter} = 4 \text{ und } F = 1 + \frac{\%Zn}{4} \quad \text{Therefore is valid:}$$

$$Tc_2/Tc_1 = \exp\left[\left(1 - F\right) \frac{MPG}{E_F}\right] = \exp\left[\left(1 - 1 - \frac{\%Zn}{4}\right) \frac{MPG}{E_F}\right] = \exp\left(-\frac{1,6}{4} \cdot \%Zn\right)$$

Zn-portion in %	$\frac{1,6}{4} \cdot \%Zn$	Tc ₂ /Tc ₁ Theory	Tc ₂ /Tc ₁ Experiment
0,4	0,16	0,85	1,0
0,8	0,32	0,73	0,76
1,2	0,48	0,62	0,63
1,6	0,64	0,53	0,51
2,2	0,9	0,4	0,36

Lit. ^{36et37}

Nickel:

$La_{1,8}Sr_{0,15}Cu_{(1-x)}Ni_xO_4$: MPG/ $E_F = 1,6$ Parameter = six

und $La_{1,8}Sr_{0,2}Cu_{(1-x)}Ni_xO_4$ MPG/ $E_F = 1,25$ Parameter = six

	for opt.	doping	for over-	Doping
Ni-portion in %	Tc2/Tc1 Theory	Tc2/Tc1 Experiment	Tc2/Tc1 Theory	Tc2/Tc1 Experiment
0,5	0,88	0,92	0,9	0,91
1,0	0,77	0,8	0,81	0,82
1,5	0,67	0,69	0,73	0,74
2,0	0,59	0,59	0,66	0,65

Lit. ^{36et37}

Iron:

$La_{1,85}Sr_{0,15}Cu_{(1-x)}Fe_xO_4$ MPG/ $E_F = 1,6$ Parameter = 3,2.

Therefore is valid:

$$Tc2/Tc1 = \exp\left(-\frac{1,6}{3,2} \cdot \%Fe\right) = \exp(-0,5 \text{ multiplied with the \%-portion of Fe})$$

and $La_{1,8}Sr_{0,2}Cu_{(1-x)}Fe_xO_4$ MPG/ $E_F = 1,25$ Parameter = 3,2.

Here is valid: $Tc2/Tc1 = \exp\left(-\frac{1,25}{3,2} \cdot \%Fe\right) = \exp(-0,4 \text{ multiplied with the \%-portion of Fe})$.

Fe-portion in %	Tc2/Tc1 Theory	Tc2/Tc1 Experiment	Tc2/Tc1 Theory	Tc2/Tc1 Experiment
0,3	0,86	0,9	0,89	0,94
0,5	0,78	0,82	0,82	0,85
0,7	0,71	0,7	0,76	0,81
0,8	0,67	0,66		unknown.
0,9	0,64	0,53		unknown
1,0	0,61	0,45 ³⁸	0,68	0,69

Lit. ³⁶⁻³⁸

Result:

The theory predicts a linear decrease of critical temperatures by increasing portions of

impurities. The dependency of the optimal doped HTSC (and probably of the underdoped, too) is bigger than the dependency of the overdoped. Again a nearly quantitative agreement between theory and experiment exists.

Diagrams to these tables you can find in the supplement.

In contrary to copper the zinc possesses a closed 3d-shell. Therefore the substitution with zinc-ions prevents the “conditional-hopping-interaction” of the EL, leading to a decreasing of density of pairs. Naturally the reduction of density of pairs leads to lower critical temperatures.

The explanation of reducing the density of pairs by paramagnetic ions is a part of the BCS-theory and must not discussed here.

VI) The temperature-dependency of normal state resistance of HTSC

It is well-known [Lit. see chapter 7.] that in overdoped HTSC the normal state resistance is increasing **linear** with temperature over a large range of temperature –especially down to the lowest temperatures. This behaviour cannot be explained by the conventional models of electron-phonon- or electron-electron-interactions. In the following a possible explanation of this unusual behaviour will be presented:

In a totally periodical lattice no electrical resistance appears. The electrical resistance always is generated by a disturbance of the periodicity of lattice. Thereby in HTSC must appear disturbances whose number or whose scattering cross-section is increasing linearly with increasing temperature. In a metal the density of charge-carriers, which are thermally excited

above a discrete energy, is increasing linearly with temperature. It's nearby, searching this extra-ordinary temperature-dependence of resistance in this connection.

Therefore it is reasonable to search for the extraordinary temperature-dependence in this context.

As mentioned in **chapter 2.2**, in the HTSC the EL (not the holes) do not behave as part of the electron gas but behave similarly to particles of a lattice. These electrons, which are stimulated about the higher band edge behave similarly to **irregularly** distributed lattice-sites. These irregularly distributed “lattice-sites” disturb the periodicity of lattice. Since the holes are not only particles, but also are waves, they are scattered at these lattice deformations. By that the quasi-impulse $\Delta k\hbar$ is translated upon the total crystal, this means upon all Cu-3d-EL in the crystal. Therefore these thermal stimulated EL act as disturbances of the periodicity of lattice –that means of scattering centres for the holes.

As the mass of all EL is bigger than the mass of one hole, it is a nearly elastic collision. Translating of energy is negligible. In the last resort, the hole will be scattered into a state with similar energy (about E_F), but another (that means a negative) wave-vector. But that means that electrical energy will be converted in warmth, because the translated quasi impulse $\Delta k\hbar$ will be absorbed by the whole crystal. By that, no charge can be transmitted. That means that the charge, which had been transported by the hole, reverses its direction of motion. This process is noted as electrical resistance. Due to the Pauli-principle only these Cu-3d-EL, which are nested in the vicinity or above the upper edge of the band can temporarily take energy and linear momentum. Cu-3d-El in lower levels of the band do not come into consideration as targets for the holes.

In the HTSC the interaction between holes and thermal excited El. gives rise to an electrical resistance.

Although the scattering is nearly elastic, the total angle of impact between hole and pushed EL is always 90° . This results from the conservation of energy and impulse: In the beginning

the hole strikes with the EL and after that the EL translates energy and impulse upon the lattice. By that the total angle of impact between hole and pushed EL always has a size of 90° (classical physic).

Therefore the hole is scattered in an angle smaller than 90° . This small angle scattering between holes and EL only can exist, if one of the partners of scattering (in our case hole or EL) was excited about the band edge before scattering. Otherwise no push is coming about, since the hole would forced to be scattered in already occupied states.

The densities of EL and holes, which are thermally excited about the band edges, are both growing linearly with temperature. Naturally the sum of both densities also grows linearly with temperature. From this fact the equation for the electrical resistance in the HTSC includes the well-known linear therm.

The elastically interaction of holes with thermal excited EL in the HTSC is leading to an electrical resistance, increasing **linear** with temperature.

In conventional metals there is a pure electron gas, whose constituents cannot be excited to (“lattice site”)-oscillations because of absence of restoring force. Therefore the mechanism of resistance –described above- cannot exist in conventional metals.

The density of El which are thermally excited above the Cu-3d-band increases linearly with increasing temperature. Accordingly the density of scattering frequency and because of that the normal state resistance also increases linearly with increasing temperature, what is in agreement with experiments. **[Literature at chapter VII)**

This argumentation assumes that the interaction between mobile holes and immobile but excited El does not depend on temperature and that the density of state of the El does not depend on their energy. The well-known interaction between holes and phonons is more than a factor of hundred smaller than the explained interaction between holes and bound El and does not matter.

For completeness it should be remarked, that this consideration are not available for metallic hydrogen and for palladium-hydrogen-systems. In such systems the protons are installed at fix lattice sites and can be identified by that. Therefore as many as you like of protons can occupy the same state. The conduction electrons of these substances can be scattered on every proton irregularly installed in the lattice. Therefore results a T-independent RRR and no linear T-dependent resistivity can be observed.

VII) Numerical calculation of temperature-dependence of normal state resistivity

7.1 Calculation of the density of thermal above the Fermi-energy stimulated El.

In this section we will make a quantitative calculation of the normal state resistivity.

In a certain subject the number (not the density) of thermal excited El. is:

$$N_{th} = \int_{E_F}^{E-E_F} f(E)D(E)dE$$

In a two-dimensional crystal the electronic density of states $D(E)$ does not depend on the energy of the states of electrons. Therefore $D(E)$ does not depend on carried thermal energy or of temperature. That is why $D(E)$ can be taken before the integral:

$$N_{th} = D(E) \int_{E_F}^{E-E_F} \frac{dE}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1}$$

We now take E_F as zero point of energy and define $E/k_B T = X$. Now it is possible to write:

$$N_{th} = D(E) k_B T \int_0^{\infty} \frac{dx}{e^x + 1} = D(E) k_B T [x - \ln(1 + e^x)]_0^{\infty}$$

The limitation of the integral is received by the following considerations: At very low temperatures x will reach infinite quantity. For high temperatures x will reach zero.

The DOS of a two-dimensional electron gas is: $D(E) = \frac{m_e A}{\hbar^2 \pi}$

(In reality this formula is acceptable only for s- and not for d-electrons. The real DOSes are larger and additionally depending on the density of d-El. in the ground state. But to show that the normal state resistivity really can be brought about by this described mechanism, this primitive formula is sufficient.)

By that $N_{th} \approx 0,7 \frac{m_e A}{\hbar^2 \pi} k_B T$.

And the density n_{th} of thermal excited El.:

$$n_{th} = \frac{N_{th}}{A} = 0,22 \frac{m_e}{\hbar^2} k_B T = 2,5 \cdot 10^{14} \cdot \left(\frac{T}{K}\right) \cdot m^{-2}. \quad (16)$$

Therefore the density of thermal super E_F excited El. the theoretical value of $2,5 \cdot 10^{14}$ El. on square meter and Kelvin. By that the density of excited El. in a CuO_2 -area of a HTSC depends only on temperature, but not on the electronic density in the ground state.

7.2 Probability of interaction between holes and EL

As explained in section 6., the thermal excited El are disturbing the periodicity of the lattice site by which is generated an electrical resistivity. With the results of the density of thermally excited El in section 7.1 it is now possible to make a numerical calculation of the resistivity generated by the hole-El.-scattering:

$$\rho = \frac{m_{\text{hole}}}{n_0 e^2 \tau} \quad \frac{1}{\tau} = \frac{v_F}{l} \quad \text{and} \quad l = \frac{1}{\frac{n_{\text{ofll.}}}{\text{meter}} \cdot n_{\text{th}} \sigma_0}$$

Because of calculation of n_{th} in m^{-2} , it was necessary to convert in m^{-3} . Therefore it was multiplicated with the number of lattice-layers per meter (n. of ll./meter).

Intermediate notice:

n_0 is the concentration of holes in the dimension m^{-3} and τ is the relaxation rate, that is the time between two collisions. Meant are the collisions between the mobile holes and the immobile El. v_F is the Fermi-velocity. As the holes can only move in two directions of space, it is necessary to calculate v_F for a two-dimensional electron gas. That is why

$$v_F = \frac{\hbar}{m_{L\ddot{o}}} \sqrt{2\pi \frac{N}{A}}.$$

n_{th} means the density of thermally excited d-El. at the Cu-sites (not the density of the holes) in two-dimensional metals. σ_0 is the cross-section for interactions between the mobile holes and the thermally excited, but localized El.

With $\sigma_0 = \frac{2 \cdot 10^5}{v_F^4}$ (see **chapter 6.3**) results for reluctance:

$$\frac{d\rho}{dT} = \frac{m_{L\ddot{o}}}{e^2} \cdot \frac{N}{A} \cdot \frac{Z.d.GS}{meter} \cdot v_F \cdot \frac{Z.d.Gs}{meter} \cdot n_{\text{th}} \cdot \frac{2 \cdot 10^5}{v_F^4}$$

With $v_F^3 = \frac{\hbar^3}{m_{L\ddot{o}}} (2\pi)^{3/2} \cdot \left(\frac{N}{A}\right)^{3/2}$ the final result for resistivity is: $\rho = \frac{m_{L\ddot{o}}}{n_0 e^2} \cdot \frac{1}{\tau} = \frac{m_{L\ddot{o}}}{n_0 e^2} \cdot$

$$\frac{\hbar \sqrt{2\pi \cdot N/A}}{m_{L\ddot{o}}} \cdot n_{\text{th}} \cdot \frac{Z.d.Gs.}{meter} \cdot \sigma_0. \quad (17)$$

Example:

In $YBa_2Cu_3O_{6,9}$ $1,7 \cdot 10^9$ current-carrying lattice-layers are paralleled³⁹.

. The density of holes amounts to, what is (numerical): $\frac{N}{A} = \frac{4,6 \cdot 10^{27} m^{-3}}{1,7 \cdot 10^9 m^{-1}} = 2,7 \cdot 10^{18} m^{-2}$.

n_{th} multiplicated by the number of lattice-layers per meter: $2,5 \cdot 10^{14} m^{-2} K^{-1} \cdot 1,7 \cdot 10^9 m^{-1}$.

From this results as conductivity $\rho = 1,57 \cdot 10^9 \frac{\Omega}{meterK} \sigma_0$.

With $\sigma_0 = 3,9 \cdot 10^{-18} m^2$ (For calculation of cross-section σ_0 look at 5.3) results an increase of resistivity of ca. $6 \cdot 10^{-9} \Omega m/K = 0,6 \mu\Omega cm/K$. On assumption, that shielding reduces the resistivity an increase of **0,1 $\mu\Omega cm/K$** results. Measured are values between 0,25 and $1,46 \cdot 10^{-9} \mu\Omega cm/K$ ⁴⁰⁻⁴⁵.

In the middle, this is about $0,85 \mu\Omega cm/K$. Theory and experiment are not in agreement as well. The very strong simplifications made by this model are a possible reason. In the case of LSCO better agreements between theory and experiment are received (look at VIII, Table 11.). It should be remarked, that doping of CuO_2 -planes of the same substance with $2,24 \cdot 10^{17}$ Cobaltions per squaremeter leads to a RRR of ca. $270 \mu\Omega cm$ ⁴⁶.

Therefore $2,5 \cdot 10^{14}$ excited EL per squaremeter and Kelvin should make an increase of resistivity of $0,3 \mu\Omega cm/K$. This result makes confidence into the actual insure calculation.

7.3 Calculation of collision cross-section σ_0 .

σ_0 will be calculated with the following equation from plasmaphysics:

$$\sigma_0 = \frac{\pi Z^2 e^4}{(4\pi \epsilon_0)^2 m_{L\ddot{o}}^2 v_F^4} = 2 \cdot 10^5 v_F^{-4} [\text{squaremeters}] \quad (18)$$

v_F is the Fermi-velocity (in two dimensions), because only the holes on the Fermi-surface can be scattered. Z is equal one (charge of holes) and $m_{L\ddot{o}}$ is the mass of holes (= mass of electrons).

The attentive reader will find fault with something:

1. This equation only considers the large-angle-scattering.
2. In this formula a cross-section is calculated. Consequently in a two-dimensional hole-gas a perimeter ought to be calculated. But the interaction between holes and El. will be produced by the Coulomb-interaction. Although the holes cant leave their lattice-layers, nevertheless they are in interaction with the El from neighbouring lattice-layers and will be shielded by themselves.
3. The Coulomb-interaction of El. with the holes reduces the cross-section of collision. In this work will be used as an approximate calculation the theory of Thomas-Fermi. It's possible to deduce this theory indeed for two dimensions. But this is senseless, because the Coulomb-shielding exists also cross to the lattice-layers. The shielding reduces the resistance to about 15%.

VIII) The temperature-dependence of normal state resistivity of some HTSC at low temperatures for example.

Summarizing all just terms factors for calculation of resistivity, results the following equation:

$$\frac{d\rho}{dT} = 7,27 \cdot 10^{45} \cdot \left(\frac{N}{A} \right)^{-2,5} \mu\Omega cm / K . \quad (19)$$

Apart from shielding, which has to be considered for each HTSC separately, this formula is valid for all HTSC, independently of the chemical composition, the stoichiometry or density of holes. In any case, if the approximation of quasi-free holes is acceptable and conventional scattering mechanisms are only playing a subordinate part. Therefore the formula above is very suitable for proving the usability of the represented theory. With this formula for ρ the plot of the measured resistivity values against $(N / A)^{-2,5}$ will make a straight line with an ascending gradient of $7,35 \cdot 10^{45}$. Additional regarding the shielding (shielding factor see **chapter 7.3 c**), then we should get a straight line with the ascending gradient of $\frac{7,35}{6} \cdot 10^{45} \approx 1,2 \cdot 10^{37} \Omega m^6 K^{-1}$.

With this equal were set up the following schedules. In all cases the hole concentration was calculated with³⁷.

Table 11. $d\rho / dT$ in dependence on the density of holes, by example of LSCO.

Sr-doping x	N/A [$10^{18} m^{-2}$]	$(N / A)^{-2,5}$ [$10^{-46} m^5$]	ρ [$\mu\Omega cm / K$] Calculated without shielding	ρ [$\mu\Omega cm / K$] Calculated with shielding	ρ [$\mu\Omega cm / K$] experimental
0,1	0,7	24,4	18	3,0	$2,2^{47}$
0,12	0,84	15,5	11,4	1,9	$2,0^{47}$
0,15	1,05	8,85	6,5	1,1	$1,3^{47}; 1,4^{48}; 1,4^{49}; 0,8^{49}; 1,3^{18}$
0,17	1,19	6,5	4,78	0,8	$0,9^{48}$
0,20	1,4	4,3	3,16	0,53	$1,0^{49}; 0,8^{18}$
0,22	1,54	3,4	2,5	0,42	$0,45^{48}$
0,24	1,68	2,73	2,0	0,33	$0,9^{18}$
0,25	1,75	2,46	1,8	0,3	$0,66^{51}; 0,7^{51}$

0,3	2,1	1,565	1,15	0,2	0,63 ⁴⁹ ; 0,43 ¹⁸
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Table 12. $d\rho / dT$ for the substance **Bi₂Sr₂CaCu₂O_{8+x}** (=Bi2212)

Oxygen doping x	N/A [$10^{18} m^{-2}$]	$(N / A)^{-2,5}$ [$10^{-46} m^2$]	ρ [$\mu\Omega cm / K$] calculated with shielding	ρ [$\mu\Omega cm / K$] experimental
0,2135	0,73	22	2,7	2,6
0,217	0,74	21,2	2,6	2,3
0,22	0,75	20,5	2,5	1,83
0,24	0,82	16,4	2,0	1,5
0,25	0,85	15	1,84	1,3
0,255	0,87	14	1,7	1,17
0,26	0,887	13,5	1,65	1,08
0,27	0,92	12,3	1,5	0,8

The calculated resistivities already regard the shielding by a factor of six. Experimental values from⁵².

Table 13. Comparison between theory and experiment:

Class of substances	$\frac{\Delta\rho}{\Delta(N / A)^{-2,5}} [10^{37} \Omega m^6 K^{-1}]$	$\frac{\Delta\rho}{\Delta(N / A)^{-2,5}} [10^{37} \Omega m^6 K^{-1}]$
	Experimental	theoretical
LSCO	1,1	1,2
Bi2212	1,26	1,2

According to the formula for ρ , the outline of resistance values in $\mu\Omega cm / K$ against $(N / A)^{-2,5}$ should make a straight line with an ascending gradient of $1,210^{37} \Omega m^6 K^{-1}$.

The deviations between theory and experiment are lower than 10%.

Regarding the amounts on has to take into account that an explicit theoretical and simplified model was taken as a basis. In addition to that, measured values differ between authors.

Nevertheless this model can describe the unusual dependence of the normal state resistivity qualitatively true and quantitatively well.

IX) The heat conduction in HTSC

Preliminary remark:

The following explanations belong to the normal- and not to the SC-state.

9.1 The model of electrical resistivity which was explained in sections **6.-8.** also is applicable to thermal resistance. Hence it follows that the thermal resistance must increase with the density of the thermally excited EL, that means likewise linearly with temperature. As the electronic contribution to thermal conduction likewise proportional follows to the density of the thermally excited El, that means by a linear temperature law, the thermal stipulated increasing of density of thermal conducting particles and the increasing of thermal resistance must counterbalance each other (in the normal state).

But that mean, that the hole-induced part of thermal conduction in HTSC should show a constant quantity. This quantity is independent of temperature. A deviation only will occur at low temperatures: At low temperatures the thermal-resistance will be generated by defects of lattice and impurities. Therefore in the low-temperature region the thermal conductivity should increase with increasing temperature like in normal metals. In the temperature-region between 0 and 30 K the thermal conductivity should increase linearly with temperature and then reach its constant maximum value. This temperature-region is mentioned explicit, because normal metals show a different behaviour: In normal metals at temperatures which are not too low the electrical and thermal resistivity is dominated by scattering of conduction-electrons at phonons, leading to the phenomenon of a maximum thermal conductivity in the just mentioned temperature-region.

In accordance to these considerations in many HTSC the thermal resistance is dominated by interaction (that means scattering) between EL and holes. In consequence, between 10 and 30 K the heat conduction **does not** decrease with increasing temperature.

Meanwhile this prediction is confirmed. Up to 30 K the heat-conductivity of HTSC is increasing steep. At higher temperatures it is nearly independent of temperature. (This does not work in the SC-state, naturally.)

From the formula of heat-conduction in two dimensions by movable charge-carriers:

$$K_h = \frac{\pi^2 n k_b^2 T}{3m_h v_F} \cdot l \quad \text{and with } l = \frac{1}{\frac{Z.d.Gs.}{meter} \cdot n_{th} \sigma_0} \text{ results}$$

$$K_{Lö} = \frac{\pi^2 n k_b^2 T}{3m_{lo} v_F} \cdot \frac{v_F^4}{2 \cdot 10^5 n_{th} \cdot Z.d.Gs./meter} \cdot \text{shieldingfactor} .$$

$$\text{With } v_F = 2,9 \cdot 10^{-4} \cdot \sqrt{\frac{N}{A}} \quad \text{results} \quad K_{Lö} = 33,6 \cdot 10^{-45} \cdot \left(\frac{N}{A}\right)^{2,5} \frac{W}{mK} \cdot \text{shieldingfactor} .$$

$$= \frac{\pi^2 n k_b^2 T}{3m_h v_F} \cdot \frac{v_F^4}{2 \cdot 10^5 n_{th} \cdot Z.d.Gs.} \text{ and } v_F = 2,9 \cdot 10^{-4} \cdot \sqrt{\frac{N}{A}}$$

$$\text{results } K_h = 3,36 \cdot 10^{-46} \cdot \left(\frac{N}{A}\right)^{-2,5} . \quad (21)$$

Table 14. Thermal conduction coefficient in various HTSC

Substance	N/A [$10^{18} m^{-2}$]	$(N/A)^{+2,5}$ [$10^{+45} m^2$]	$K_{Lö}$ [W/mK] calc., without shielding	$K_{Lö}$ [W/mK] calc., with shielding	$K_{Lö}$ [W/mK] experimental value
LSCO, x = 0,17	1,19	1,55	0,5	2,5	4,5 ¹⁵
LSCO, x = 0,2	1,4	2,3	0,8	3	Circa 3 ⁵³
YBCO6,3					1,9 ⁵⁴
YBCO6,53					2,3 ⁵⁴
YBCO6,7	1,36	2,2	0,7	3	5,0 ⁵⁴ ; 2,5 ⁵⁵
YBCO6,77	1,83	4,5	1,5	4	2,9 ⁵⁴
YBCO6,9	2,7	12	4,0	8,0	8,0 ⁵³ ; 2,5 ⁵⁴ ; 3,5 ⁵⁶ ; 4,0 ⁵⁷ ;

On heat-conduction also exists convergence between theory and experiment, if it is considered, that the experimental values show a big variation and the phonons are also contributing to the heat-conduction.

For $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8-y}$ the thermal-conduction-coefficient also has a small temperature-dependence⁵⁸.

9.2 Wiedemann-Franz-law⁵⁹ and Lorenz-number

The theoretical relation between heat-conduction and electrical conductivity is:

$$L_0 = \frac{K_{Lö}}{\sigma T} = 3,36 \cdot 10^{-46} \left(\frac{N}{A} \right)^{2,5} \cdot 7,35 \cdot 10^{37} \cdot \left(\frac{N}{A} \right)^{-2,5} W\Omega K^{-2} = 2,47 \cdot 10^{-8} W\Omega K^{-2}.$$

For $\text{YBa}_2\text{Cu}_3\text{O}_{6,9}$ was measured: $L_0 = 10,5 \cdot 10^{-8} W\Omega K^{-2}$ ⁽⁵³⁾. bzw. $5 \cdot 10^{-8} W\Omega K^{-2}$ ⁽⁴⁶⁾.

It is characteristic, that these measured quantities do not depend on temperature, corresponding to the represented theory. Unfortunately for other HTSC no values are available. Oddly the value of the Lorenz-number is the double as in conventional metals.

Answering why is possible not yet. Also the values of L_0 only show a small dependence of temperature, what is predicted by theory also.

9.3 Result

In conventional metals between 10 and 30 K no solid Lorenz-number is received. But a so-called “Lorenz-relation”, starting decreasing with increasing temperature, than reaching a minimum and then increasing again⁶⁰. **This conclusion is very important:**

It **proves** that in the HTSC` s electrical resistance and thermal resistance (of the holes) are created by processes with the same effectiveness **at every temperature**. By that both types of collision processes are of the same effectiveness, an elastically or nearby elastically scattering is necessarily. In HTSC` s the thermal and the electrical resistance are coming about by elastically scattering. That is established by obeying the Wiedemann-Franz-law at all temperatures. From this reason, inelastically scattering can be excluded. Therefore the scattering of holes comes about by elastically scattering processes with a collision cross-section σ_0 or a frequency increasing linearly with temperature. Scattering of conduction-electrons (in HTSC almost holes) always is inelastically and by that as an explanation it isn` t useful. Attempting to explain this result by dynamical elastic scattering of holes at bosons, the density of this bosons also has to increase at the lowest temperatures linearly with the temperatures. (In HTSC the resistance is increasing linearly with T at the lowest temperatures.) That is possible only, if the characteristic exciting-energy of this bosons is going to zero. That is sizeable unrealistic, but thinkable. But if the excitement-energy is in the near of zero, the matrix-element of the hole-boson-coupling goes to zero. And with a coupling-constant near zero the electrical resistance also is going to zero, at every temperature.

The extra-ordinary temperature-dependence of resistivity cannot be explained by an interaction with bosons. Then the only explanation is the elastic interaction with fermions.

The number or the collision cross-section σ_0 of these fermions also has to increase linearly with the temperature. The one and only fermions in HTSC with these presuppositions are the thermal excited Cu-3d-EL. It is significant, that these types of electrical and thermal resistivity and the anomalies in the WF-law exist only in the HTSC's. Indeed, in the heavy-fermion –superconductors the resistivity at low temperatures increases (nearly) with the temperature, but it is proved, that this scattering is inelastic⁶¹.

In principle a scattering of holes at ordered areas in the crystal is possible. But then the ordering in the crystal must increase with temperature, what is in contradiction to the second main theorem of thermodynamic. It only rests the solution, that the holes are scattered at the thermal excited Cu-3d-EL.

This does not prove the coming about of superconductivity by interactions between holes and Cu-3d-EL, but it is obvious.

X) Conclusion

10.1 It was demonstrated in **sections VI) to IX)**, that electrical resistance and heat resistance in HTSC are created by interaction between mobile holes and localized Cu-3d-electrons. High-temperature-superconductivity is explained by a closely related mechanism. Furthermore the mechanism presented in this abstract also can explain all the other experimental results qualitatively and quantitatively. This theory of HTSC is closed, quantified and able to explain the phenomena connected with the cuprate-based superconductivity.

The relations presented here, between experimental verified metal-parameters and the superconductivity, are totally more quantitative than all, which was offered till now by the theory of superconductivity.

Apart from that this theory is unusually, there is no doubt on her correctness.

It should be remarked for completeness, that this mechanism is also appreciable to electron-doped HTSC's. But it is true, that the interaction between negative loaded Cu-3- $d_{x^2-y^2}$ -EL and conduction-electrons is weaker than with positive loaded holes, leading to lower critical temperatures.

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Diagrams: see extra-files