

Mechanism of High Temperature Superconductivity

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ABSTRACT: Using the conception of nucleophil-electrophil reaction in organic chemistry, the mechanism of high temperature superconductivity is given. This mechanism unites seemingly antagonistic approaches of Anderson and Schrieffer, and includes the expectations of these both scientists.

The existence of a new mechanism of Cooper's pairs creation is confirmed, which Anderson has suggested. This mechanism is presented. In framework, the correctness of Anderson's conception of division of electron charge and spin is stated.

The Schrieffer's conception of existence of so called spin sacs - it means the regions, in which the superconducting electrons are concentrated, is corroborated.

The creation of holes in CuO shells and the existence of excitons is explained.

I

Mechanism of creation of Cooper's pairs.

1. Introduction

In this work the simple model, explaining the mechanism of high temperature superconductivity has been found, which unites the seemingly antagonistic models of P.W. Anderson [1,5] and of J.R. Schrieffer [6,10]. As the start point the popular in organic chemistry conception of nucleophil-electrophil reaction has been taken.

The Hellman-Feynman theorem has been used. It has assumed that between two atoms creating CuO shell exists the non zero density of probability of finding of electrons, just as

the non zero density of finding of electrons exists between two atoms creating chemical molecule or molecular crystal, and it is the function of spacial coordinates.

The shape of electron cloud connected with CuO shell has been the object of consideration. Two characteristic shapes of electron cloud have been analysed. It has been assumed, that in regions between Cu-O shells, the electron gas exists.

2. The nucleophil-electrophil reaction.

Let's consider an atom, called centre, at which there is an electric cloud.

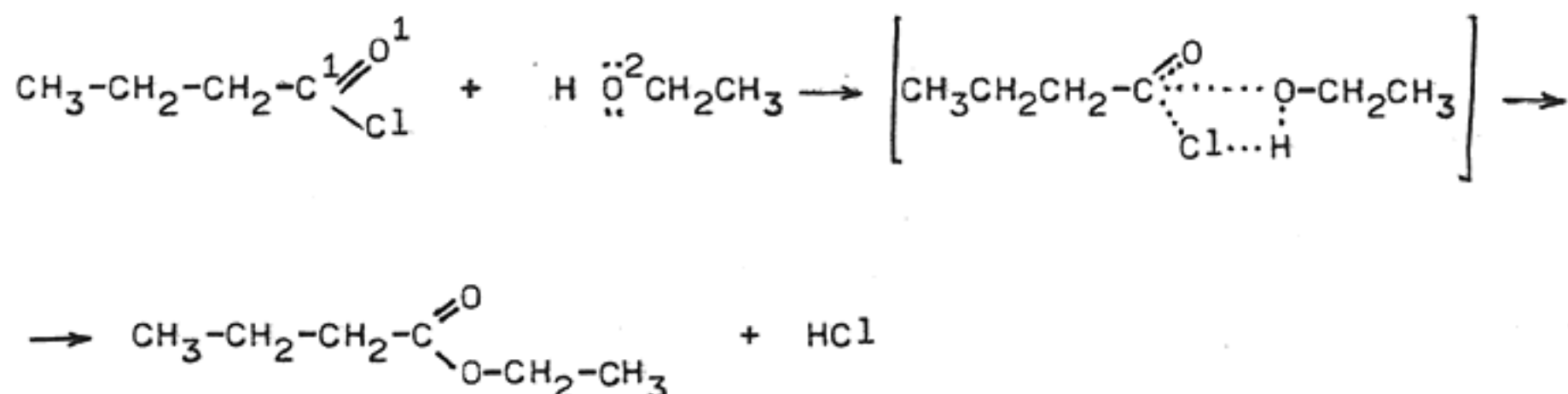
Let's analyse two centres such, that the density of electron charge at first centre (A) is less than the average density at neighbouring centres, and the density of electric cloud at second centre (B) is bigger than the average density at neighbouring centres.

Then the excess of electron density at centre B exists, which manifests tendency to attract positive charge. This centre is called nucleophil.

The deficiency of electron at centre A acts like effective positive charge which manifests tendency to attract negative charge. This centre is called electrophil.

The electric cloud is analysed naturally in the dense of Hellman-Feynman theorem.

Let's analyse this idea, using the example of esterification reaction:



There is a great deficit of electrons at carbon atom C¹ resulted by the existence of the two with this atom connected strongly electronegative atoms: oxygen O¹ and chlorine Cl. The deficiency of electrons at the carbon atom C¹ creates an

effective positive charge attracting negative charge which is concentrated in one of the two electron pairs at oxygen atom O^2 of alcohol molecule. The intermediate state originates and then the molecules of ester and of HCl are created.

3. The mechanism of Cooper's pairs creation in high temperature superconductivity.

In the high temperature conductivity, the CuO planes must play the main role. They are inseparably connected with the occurrence of the high temperature superconductivity. When they are not in a material, the high temperature superconductivity does not exist.

The nuclei of atoms in the CuO planes will be treated as positive charge inserted in the "sea" of negative charge. We will analyse only the negative charge of these planes and we assume, that it fills in a homogeneous way the flat, infinite plate with thickness b (see figure 1).

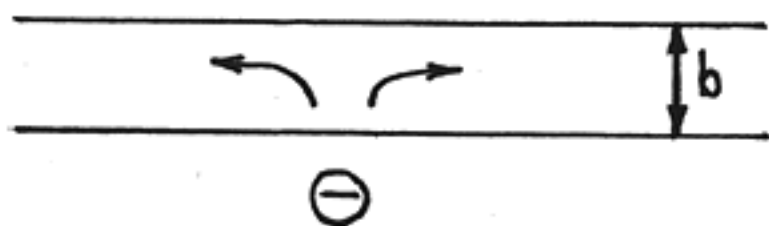


Figure 1

When the electron brings nearer to the plate, the repulsion of electrons in the plate occurs, and their translocation aside (see figure 1).

There is such a distribution of negative charge generated in the plate, that the electric field and electric potential, which are both created that way, can be described using the field (or potential) of the symmetrically put positive charge with absolute value, which is equal to the absolute value of negative charge coming to the plate (see figure 2).

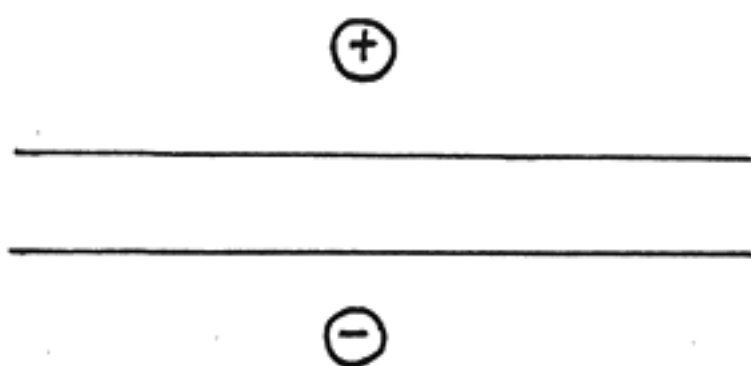


Figure 2

The regions with deficiency of negative charge, in comparison with other regions without deficit, behave, as if they had positive charge.

So we can write they have effective positive charge, which attracts

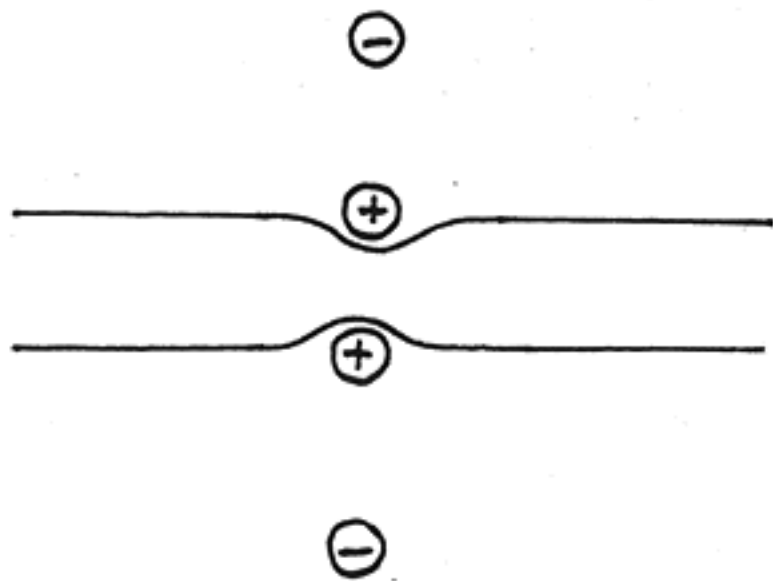


Figure 3.

This way Cooper's pair originates. It is possible because of existence of the negative charge of the plate. Let's imagine that a second negative charge (see figure 3) increases still more the binding effect of the plate, because two charges repel stronger the electrons in plate than one charge.

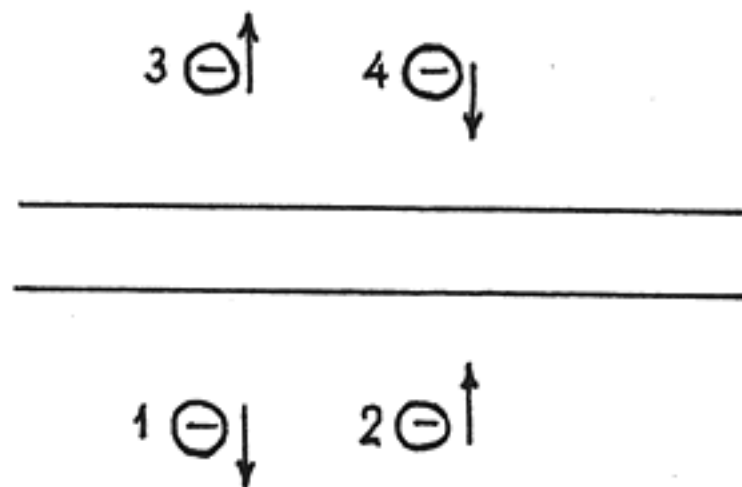


Figure 4

The electrons between plates create electron gas and Cooper's pairs.

Electron induces decreasing of electron density in plane opposite his position. If it finds the partner with opposite spin at the opposite side of the plate and creates with it Cooper's pair, the electron density of the plate between them as well as thickness of the plate in this place, are especially small. The positive feedback arises. This feedback increases power of bonding of Cooper's pair (electrons, because of interactions with other ones, are shoved to the regions of the plate, where negative charge is relatively small) and makes easier the tunneling, because of decreasing of the electron density

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the negative one.

So on the opposite side of the plate arises mirror effective positive charge, which attracts easily negative charge of electrons (see figures 2 and 3).

We obtain an electron pair.

Vis à vis each electron appears in the plate an effective positive charge (see figure 3).

We can say, that Cooper's pairs are created with both electrons at the same side of the plate. We have (figure 4) pairs: 1-3 and 2-4, but we can interpret them as pairs 1-2 and 3-4.

It is seen moreover (figure 3) that places with electron deficit in the plate, can be treated as holes, and the system of two electrons and two holes, as the system of two pairs of excitons [11].

and of plate's thickness between two electrons creating Cooper's pair.

This means, that partially only electrons can tunnel, which because of interaction with the plate, create Cooper's pair.

The electron gas exists between the plates, and part of electrons is adsorbed by the plane as Cooper's pairs. The electrons are in the electric field, created by this gas and by the plate. We will see in chapter II, that in this system the binding minimum of potential energy, exists.

The repulsion of electrons by the electron gas explains, why some electrons come up to the plate.

The bigger number of the plates is, and the closer they are placed - the superconducting effect is stronger, because then greater number of Cooper's pairs is created, and the way through the regions filled with electron gas is shorter. So the frequency of collisions of Cooper's pairs with electron gas, which lead to desintegration of Cooper's pair, is lower. Because of these facts, the increase of critical temperature occurs, when the distance between the plates decreases.

4. Possibilities and anticipations of the model

- a - The corroboration of Anderson's conception, who suggested, that electron can be treated as object with separated spin part and charge part.

Really, the charge is responsible for creation of the Cooper's pair of type 1-3 and 2-4 (see figure 4), and spin is responsible for creation of Cooper's pair of type 1-2 and 3-4.

- b - The corroboration of Schrieffer's conception of existence of the regions, in which Cooper's pairs are created. In case of more realistic distribution

of the electric negative charge in the plate (see figure 5), the regions containing Cooper's pairs are correlated with regions placed opposite to points, where the minimum thickness of the plate exists.

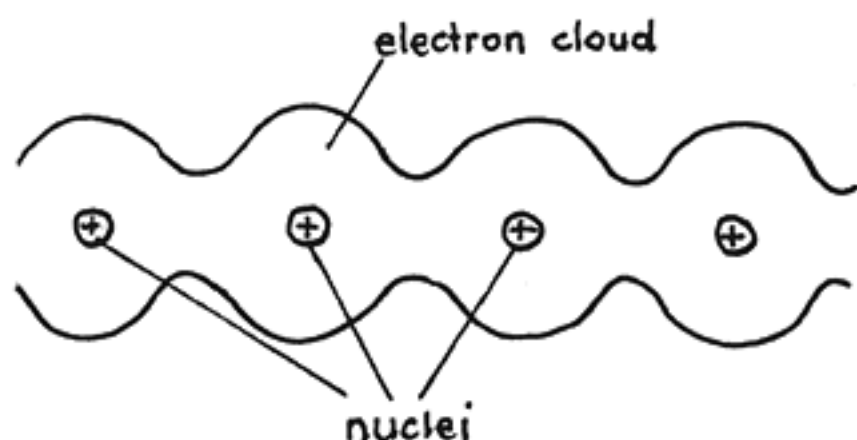


Figure 5

We will see in chapter III, that the bonding minimum of potential energy is correlated with these regions.

c - The explanation of the mechanism of creation of holes in CuO shell and creation of excitons in high temperature superconductors.

5. The flow of electric current in high temperature superconductor.

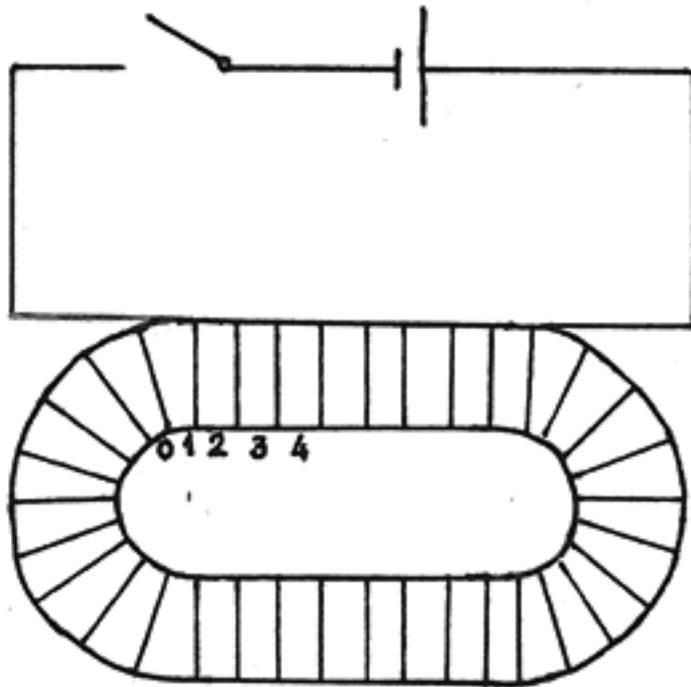


Figure 6

If we set a voltage to a superconductor, the part of electrons from space 1 will tunnel to space 2 through the plate separating these spaces, because the voltage makes the tunneling easier. The electrons between the plates create gas. If in the space 1 the number of electrons decreases, the negative pressure originates and the electrons flow from the circuit. In the space 2 the number of electrons increases, the overpressure originates, and with it the tendency of tunneling to the space 3, and so on.

If we eliminate the current, the electrons flow to the space 1 because of inertia; the overpressure creating the flow of electrons to the space 2 arises and the number of electrons is completed from the space 0. When we eliminate the current (and circuit) the system introduced into the superconducting state holds this state, because for arising of it, the Cooper's pairs are responsible, which can be destroyed only by high temperature and strong magnetic field.

The Cooper's pairs, for creation of which the plates are responsible, are far less supple for influence of temperature, than such Cooper's pairs, for creation of which the phonon mechanism is responsible.

The electron gas between plates holds the constant pressure. This means that it evidences the tendency of equation of pressures in neighbouring spaces. This tendency leads to retention of superconducting current after elimination of voltage.

This means, that increasing of concentration of electrons, also of these electrons creating Cooper's pairs, leads to increasing of frequency of collisions, which makes the tunneling through the plate easier for electrons with great kinetic energy.

The number of electrons with great kinetic energy increases with pressure.

The part of Cooper's pairs is desintegrated because of interaction with electron gas, but this lessening is completed by Cooper's pairs created at plates, as long as the critical temperature is not surpassed.

The CuO planes should lie as near as possible, and be identical, whereas the atoms of succeeding planes ought to lie on these same axes which run through them and are perpendicular to the planes. When the planes are placed in that way, the electron, for which the tunneling is most easy in the regions with the least thickness of plates (these regions are in the highest degree responsible for tunneling) and which creates the Cooper's pair, because after tunneling is bound with its partner at opposite side of the plate, is at once in the position opposite to the identical region with small thickness of plate. (see figure 7)

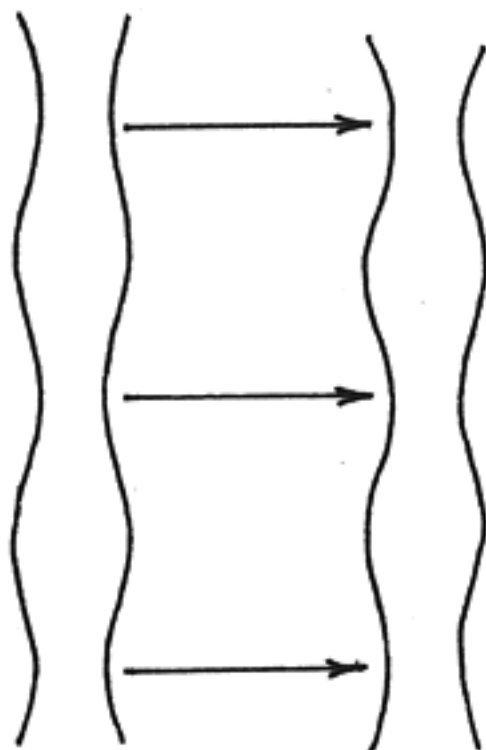


Figure 7

If the maxima of succeeding plates are moved (see figure 8), the electron creating Cooper's pair (after tunneling through the plate in the place with small thickness) meets the place of succeeding plate with great thickness.

In this situation the probability of tunneling decreases, or this electron has to enter the path of electron which has tunneled through the region of the great

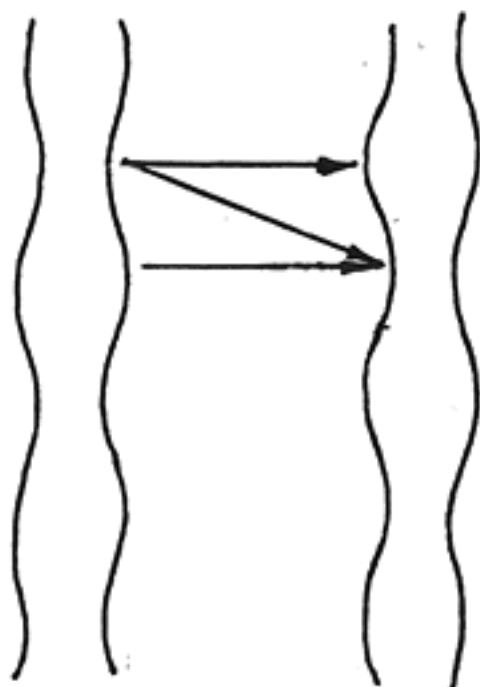


Figure 8

thickness of the plate and aims at the region with small thickness of the succeeding plate (see figure 8).

This is leading to interaction of electrons from two different Cooper's pairs, which can disrupt both pairs.

As a consequence of this, the decreasing of critical temperature occurs.

II

Model of an infinite, homogeneous plate

1. The role of potentials

Let's discuss quantitatively the problems described qualitatively in the previous chapter.

Let's assume, that electron charge of atomic shell creates the homogeneous electron plate. Let's assume moreover, that thicknesses of all plates and distances between plates are equal. The plates are naturally parallel and in our treatment infinite.

Let's designate the thickness of the electron plate as b and the distance between symmetry planes of nearest plates, as d (see figure 9).

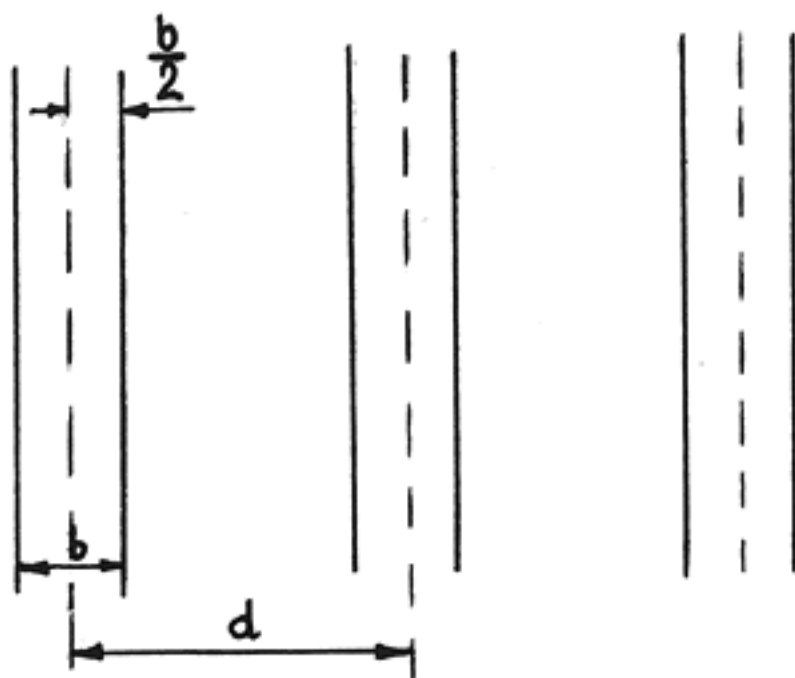


Figure 9

Because of the translational symmetry of the problem we will concentrate on analysis of one plate.

Because of the symmetry of problem we assume that distributions of electric charge, electric potential and electric field intensity are symmetrical at both sides of the plate.

We analyse the distribution of

charges and fields at distances smaller than $\frac{d}{2}$ from symmetry plane and omit the influences of fields created by other plates. We assume, that the density of negative charge is homogeneous in the plate and equal ρ_1 and its permittivity ϵ_1 , whereas between the plates there is the homogeneous electron gas with charge density ρ_2 and permittivity ϵ_2 . We omit the influence of positive charge inside plate.

If the potential energy has the binding minimum, the binding effect will occur, all the more when the regularly placed in the symmetry planes positive charge will be neglected.

Let's notice, that an influence of the positive charge on the tunnel effect shouldn't be important.

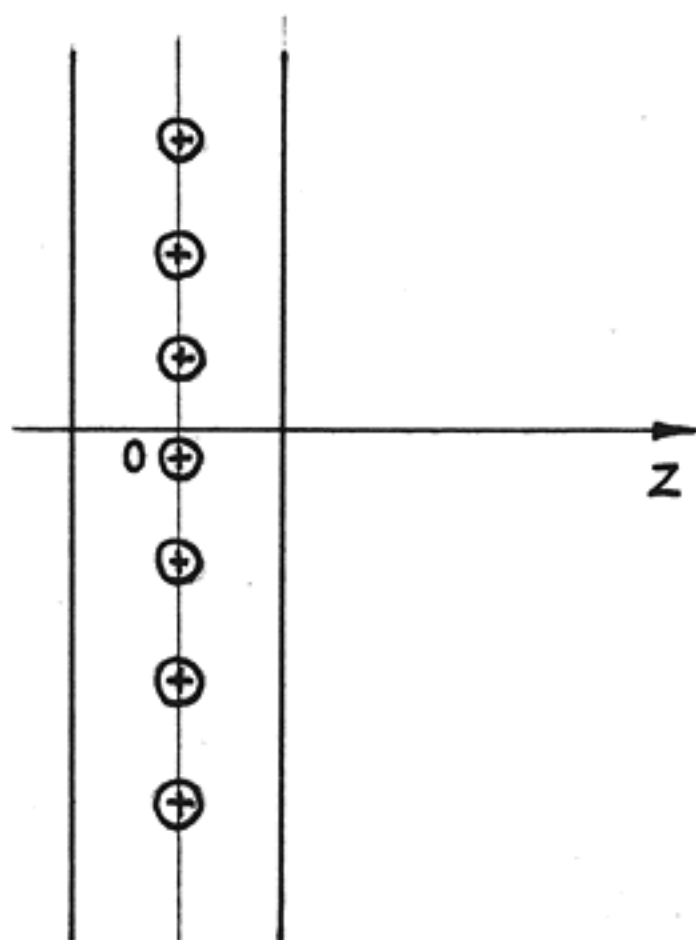


Figure 10

When $z > 0$ it makes easier the tunneling of electrons through the plate (see figure 10)

and when $z < 0$, then it makes it more difficult.

So the total influence of the positive charge ought to be omitted.

We will use the Hellman-Feynman theorem, which runs: the electric potential, which is created by the quantum distribution of charge, is such, as though in each point of space (x, y, z) and in each moment of time, the charge occurs, expressed by the formula:

$$q(x, y, z, t) = e \rho(x, y, z, t) \quad (1)$$

where: ρ - the density of probability of electron's position at the point x, y, z and in moment t .

e - elementary charge

Because of symmetry of problem and assumption of omitting the influences of neighbouring plates, we will analyse the situation in the space I $z \in \left(0, \frac{b}{2}\right)$ (see figure 10) and in the space II $z \in \left(\frac{b}{2}, \frac{d}{2}\right)$ (because we are interested in boundary pla-

ne $z = \frac{b}{2}$ (see figure 11) and in the points, which are distant less than $\frac{d}{2}$ from the plane).

We introduce the coordinate system such, that axes x, y are situated in the symmetry plane of plate and their directions reflect the rectangular symmetry of the plate, and axis z is perpendicular to symmetry plane of the plate, and ^{point} $z=0$ is situated on it.

So we have two spaces of homogeneous charge characterized by parameters suitably ρ_1, ϵ_1 and ρ_2, ϵ_2 (see figure 11).

Naturally $\rho_1 < 0$ and $\rho_2 < 0$ (because electron's charge is negative) and $\epsilon_1 > 0, \epsilon_2 > 0$. We assume, that after introduction of second charged plate in

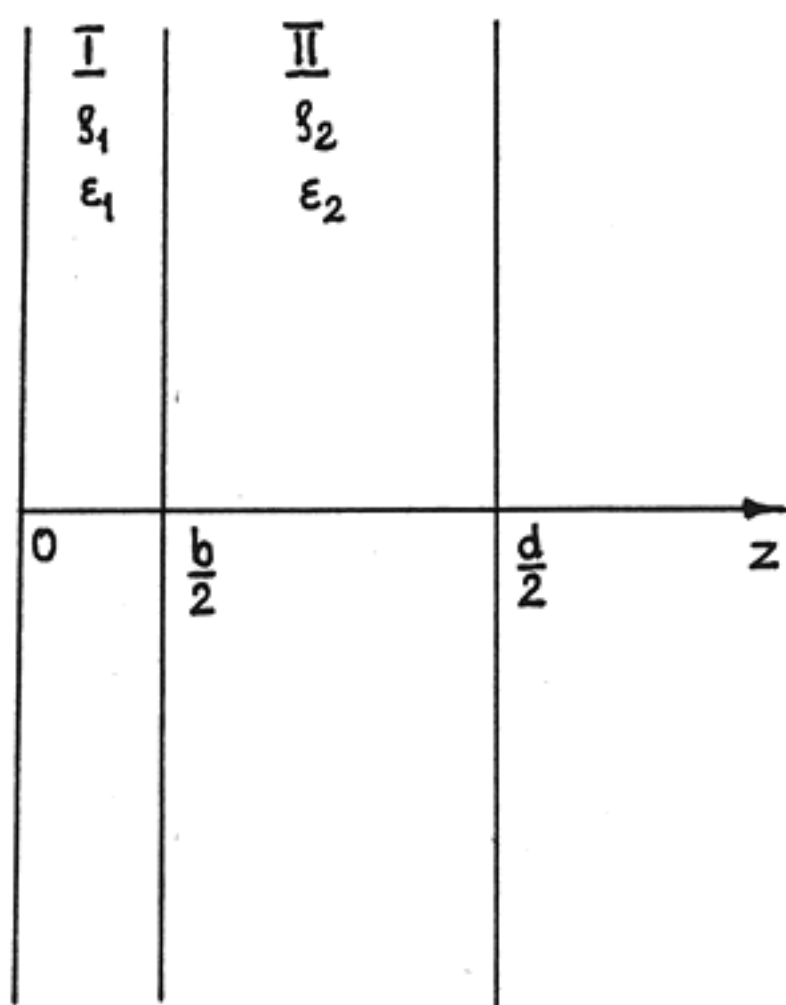


Figure 11

the space $z \in \left\langle \frac{b}{2}, \frac{d}{2} \right\rangle$ the translation of the electric charge in the plate $z \in \left\langle 0, \frac{b}{2} \right\rangle$ does not take place and vice versa. Because of it we can express the potential in space I as superposition of potential induced by plate I and by plate II. The similar situation is with electric potential in the space II induced by plate II in the space I and by the plate I in the space II. We will analyse situation when the space I is filled with charge with density ρ_1 , and the space II is empty ($\rho_2 = 0$, see figure 12)

and then we will repeat analogous analysis for space II when $\rho_2 \neq 0$ and $\rho_1 = 0$.

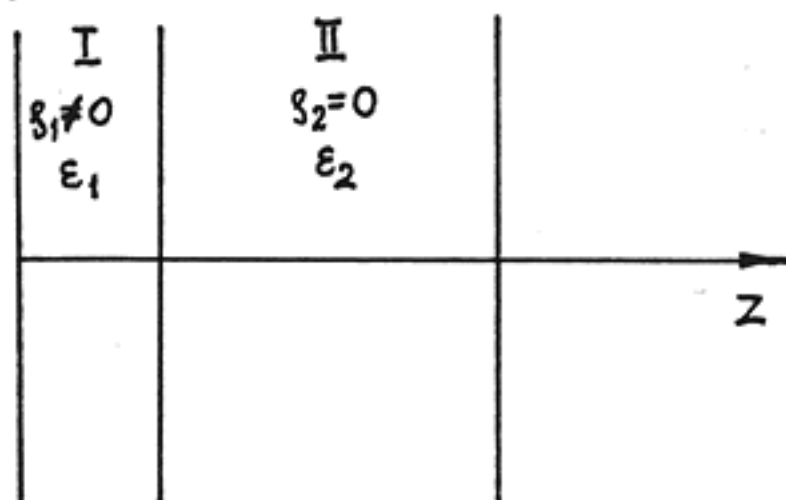


Figure 12

Because of the symmetry of problem, φ does not depend on x and y

We use Poisson's equation

$$\Delta \varphi = -\frac{\rho}{\epsilon}$$

in our situation

$$\frac{\partial^2 \varphi}{\partial z^2} = -\frac{\rho_1}{\epsilon_1}$$

so

$$\frac{\partial \varphi}{\partial z} = -\frac{\rho_1}{\epsilon_1} z + c_1$$

And in the space I

$$\varphi_I = -\frac{\rho_1}{2\epsilon_1} z^2 + c_1 z + c_2 \quad (2)$$

And in the space II

$$\varphi_{II} = c_3 z + c_4 \quad (3)$$

because $\rho = 0$ in this region.

Because of the symmetry, we obtain

$$\varphi_I = -\frac{\rho_1}{2\epsilon_1} z^2 \quad (4)$$

because the graph of function must be symmetrical in relation to the plane $z = 0$.

Moreover we use the freedom of choice of the potential constant and we assume, that $c_2 = 0$. The constants c_3 and c_4 are determined by boundary conditions.

$$\varphi_{II} = c_3 z + c_4 \quad (5)$$

The dependence (5) is correct, because when $z \rightarrow \infty$, the electric field induced by homogeneously charged plate is constant. The singularity does not occur.

c_3 and c_4 will be obtained by use of boundary conditions of continuity of potential function and its derivative at $z = \frac{b}{2}$

We have:

$$\frac{\partial \varphi_I}{\partial z} = -\frac{\rho_1}{\epsilon_1} z$$

$$\frac{\partial \varphi_{II}}{\partial z} = c_3$$

so:

$$c_3 = -\frac{\rho_1}{\epsilon_1} \frac{b}{2}$$

$$c_4 = \frac{\rho_1 b^2}{8 \epsilon_1}$$

And we obtain:

$$\varphi_I = -\frac{\rho_1}{2\epsilon_1} z^2 \quad z \in \left\langle 0, \frac{b}{2} \right\rangle \quad (4)$$

$$\varphi_{II} = -\frac{\rho_1 b}{2\epsilon_1} z + \frac{\rho_1 b^2}{8 \epsilon_1} \quad z \in \left\langle \frac{b}{2}, \frac{d}{2} \right\rangle \quad (6)$$

We take under consideration the situation when plate II is charged with density $\rho_2 \neq 0$ and its permittivity is equal ϵ_2 , and in space I $\rho_1 = 0$.

Then:

$$\chi_{II} = -\frac{\rho_2}{2\epsilon_2} z'^2 \quad ; \quad z' \in \left\langle \frac{b}{2}, \frac{d}{2} \right\rangle \quad (7)$$

$$\chi_I = -\frac{\rho_2 (d-b)}{2\epsilon_2} |z'| + \frac{\rho_2 (d-b)^2}{8\epsilon_2} \quad ; \quad z' \in \left\langle 0, \frac{b}{2} \right\rangle \quad (8)$$

We change ϵ_1 for ϵ_2 , ρ_1 for ρ_2 and notice, that $d-b$ plays the role of b .

There was the change of position of charge, so there is the change of type of function in the neighbouring spaces.

Naturally:

$$z + |z'| = \frac{d}{2} \quad |z'| = \frac{d}{2} - z \quad (\text{and } |z'|^2 = z'^2)$$

The dependences (7) and (8) have the shape:

$$\chi_{II} = -\frac{\beta_2}{2\epsilon_2} \left(\frac{d}{2} - z\right)^2 = -\frac{\beta_2}{8\epsilon_2} d^2 + \frac{\beta_2 d}{2\epsilon_2} z - \frac{\beta_2}{2\epsilon_2} z^2 \quad (9)$$

$$\chi_I = -\frac{\beta_2(d-b)d}{4\epsilon_2} + \frac{\beta_2(d-b)^2}{8\epsilon_2} + \frac{\beta_2(d-b)}{2\epsilon_2} z \quad (10)$$

We notice, that the signs of coefficients at z in linear functions (6) and (10), are opposite ($\beta < 0$). This is correct, because the linear function in the left and in the right side of plate, ought to be symmetrical.

The potential functions have the shape in spaces I and II:

$$\pi_I = \varphi_I + \chi_I \quad z \in \left\langle 0, \frac{b}{2} \right\rangle$$

$$\pi_{II} = \varphi_{II} + \chi_{II} \quad z \in \left\langle \frac{b}{2}, \frac{d}{2} \right\rangle$$

We know, that the boundary conditions are complied in case of φ_I, φ_{II} , and χ_I, χ_{II} so they are complied in case of π_I, π_{II} which are superpositions of φ and χ .

The functions φ, χ and π are positive (or equal zero) in the whole space, so they have the meaning of potential energy of electron (which minimum we want to obtain) because the potential energy in the electric field created by charges with the same sign is positive, and potential of the negative charge is negative.

The functions φ, χ, π are positive according to this convention of signs. This means, that they have the sense of potential energy, but they may be obtained from Poisson's equation because there was only multiplication of both sides of equation by the constant coefficient.

This argumentation can be supported by formulas. The electric potential is expressed by formula:

$$V = \sum_i \frac{q_i}{r_i}$$

and, if all signs are negative, then V is negative.

The potential energy is expressed by formula:

$$E = q \sum_i \frac{q_i}{r_i}$$

and, if the sign of q and of all q_i is the same, so the potential energy is positive.

We seek the minimum of the function:

$$\bar{\mathcal{J}}_I = -\frac{\beta_1}{2\epsilon_1} z^2 + \frac{\beta_2(d-b)}{2\epsilon_2} z - \frac{\beta_2(d-b)d}{4\epsilon_2} + \frac{\beta_2(d-b)^2}{8\epsilon_2}; \quad z \in \left\langle 0, \frac{b}{2} \right\rangle \quad [(13)]$$

$$\frac{\partial \bar{\mathcal{J}}_I}{\partial z} = 0 \Leftrightarrow -\frac{\beta_1}{\epsilon_1} z + \frac{\beta_2(d-b)}{2\epsilon_2} = 0; \quad -\frac{\beta_1}{\epsilon_1} > 0 \text{ because } \beta_1 < 0$$

So it is implicated, that the derivative is equal zero for:

$$z_1 = \frac{\beta_2}{2\beta_1} \frac{\epsilon_1}{\epsilon_2} (d-b) \quad (14)$$

$$\text{When } z > z_1 \quad \frac{\partial \bar{\mathcal{J}}_I}{\partial z} > 0$$

$$\text{When } z < z_1 \quad \frac{\partial \bar{\mathcal{J}}_I}{\partial z} < 0$$

So $\bar{\mathcal{J}}_I$ has the candidate for minimum at the point z_1 .

We look for the minimum of function

$$\bar{\mathcal{J}}_{II} = -\frac{\beta_2 z^2}{2\epsilon_2} + \left(-\frac{\beta_1 b}{2\epsilon_1} + \frac{\beta_2 d}{2\epsilon_2} \right) z + \frac{\beta_1 b^2}{8\epsilon_1} - \frac{\beta_2 d^2}{8\epsilon_2} ; \quad z \in \left\langle \frac{b}{2}, \frac{d}{2} \right\rangle \quad (14a)$$

(see (6), (9) and (12))

$$\frac{\partial \bar{\mathcal{J}}_{II}}{\partial z} = -\frac{\beta_1 b}{2\epsilon_1} + \frac{\beta_2 d}{2\epsilon_2} - \frac{\beta_2}{\epsilon_2} z$$

$$\frac{\partial \bar{\mathcal{J}}_{II}}{\partial z} = 0 \quad \text{when} \quad z_2 = \frac{d}{2} - \frac{\beta_1}{\beta_2} \frac{\epsilon_2}{\epsilon_1} \frac{b}{2} \quad (15)$$

$$\text{When } z > z_2 \quad \frac{\partial \bar{\mathcal{J}}_{II}}{\partial z} > 0$$

$$\text{When } z < z_2 \quad \frac{\partial \bar{\mathcal{J}}_{II}}{\partial z} < 0$$

so we have the next candidate for minimum at the point z_2 .

We have two candidates for minimum:

$$z_1 \in \left\langle 0, \frac{b}{2} \right\rangle ; \quad z_1 = \frac{\beta_2 \epsilon_1}{2\beta_1 \epsilon_2} (d-b)$$

$$z_2 \in \left\langle \frac{b}{2}, \frac{d}{2} \right\rangle ; \quad z_2 = \frac{d}{2} - \frac{\beta_1 \epsilon_2}{\beta_2 \epsilon_1} \frac{b}{2}$$

All depends now on relations between coefficients.

We have:

$$z_1 < \frac{b}{d} \quad \text{and} \quad \frac{\beta_2 \epsilon_1}{2\beta_1 \epsilon_2} (d-b) < b$$

So:

$$\frac{b}{d} = \frac{\frac{\rho_2 \epsilon_1}{\rho_1 \epsilon_2}}{1 + \frac{\rho_2 \epsilon_1}{\rho_1 \epsilon_2}} \quad (16)$$

$$\frac{b}{2} < z_2 < \frac{d}{2} \Rightarrow \begin{cases} \frac{d}{2} - \frac{\rho_1 \epsilon_2}{\rho_2 \epsilon_1} \frac{b}{2} < \frac{d}{2} \text{ is complied always} \\ \frac{d}{2} - \frac{\rho_1 \epsilon_2}{\rho_2 \epsilon_1} \frac{b}{2} > \frac{b}{2} \end{cases} \quad (17)$$

$$\frac{b}{d} \ll 1 \quad (18)$$

so b is small. If (17) is complied, we have minimum at z_2 .

If (17) is not complied, then $\frac{\rho_1 \epsilon_2}{\rho_2 \epsilon_1} \frac{b}{2}$ is great, and $\frac{\rho_1 \epsilon_2}{\rho_2 \epsilon_1}$ is

very great, and then $\frac{\rho_2 \epsilon_1}{\rho_1 \epsilon_2}$ is very small ,

and $\frac{b}{d} \approx \frac{\rho_2 \epsilon_1}{\rho_1 \epsilon_2}$ is very small, so (18) is complied.

When (16) is complied, (17) is not complied and vice versa.

So we have always one minimum and only one.

The analysed model implicates the existence of minimum of potential energy. We shall see in the next chapter, that more realistic distribution of charge implicates the existence of such minimum, too.

We have omitted the influence of positive charges. We can assume, that the positive charges of atomic cores are distributed homogeneously, and that at each point z_0 electron is attracted in the same way by the cores disposed in space $z < z_0$ and the cores disposed in space $z > z_0$.

The free charges can not exist in the state of equilibrium described by the minimum of potential energy, but we have here the electrons of atomic cores when $z \in \left(0, \frac{b}{2}\right)$ and the elec-

tron gas restrained in the space $z \in \left\langle \frac{b}{2}, \frac{d}{2} \right\rangle$.

2. The tunneling through the potential barrier.

The probability of the tunneling is expressed by the semi-classical formula:

$$P = \exp \left[- \int_{r_1}^{r_2} \chi(r) dr \right] \quad (19)$$

$$\chi(r) = \frac{1}{\hbar} \sqrt{2m [V(r) - E]} \quad (20)$$

$V(r)$ - potential barrier

E - energy of a tunneling particle (When E increases, $\chi(r)$ increases, and P increases, too. The higher the particle is in the energetic scale, the narrower the barrier is and the easier the tunneling.)

We assume, that the tunneling takes place in the space $z \in \left\langle -\frac{b}{2}, \frac{b}{2} \right\rangle$ so $V(r) = \overline{V}_I$ and it is symmetrical function.

$b < d$, b is small and in dependence (13) the terms depending linearly on b , dominate.

The dependence $\overline{V}(b)$ is approximately linear, because the term depending on b^2 gives very small contribution.

The third and fourth term of the dependence give the contributions

$$- \frac{\beta_2 db}{4\epsilon_2} \quad \text{and} \quad \frac{\beta_2 db}{4\epsilon_2} \quad \text{which countermand mutually.}$$

There is only the contribution of the second term equal

$$- \frac{\beta_2 bz}{2\epsilon_2} \sim -\beta_2 b$$

When b increases, the term increases, because $-\beta_2$ is positive. Then $V(r)$ increases, $\chi(r)$ increases and P decreases. (We remember, that the linear function changes the sign of linear coefficient for opposite when $z < z_0$, because $V(r)$ has to be even function).

It is implicated, that the thicker the plate is, the more difficult the tunneling is.

When the thickness of the plate changes, the tunneling is most intensive in the regions connected with the smallest thickness.

When ϵ_1 increases, $V(r)$ decreases, and P increases. When ϵ_1 increases, the outside electric field is more reduced, because the migration of electric carriers in the plate (in order to attain the induction of effective positive charge) is more intensive. The bigger the arising hollow is, so the smaller thickness is, and, as we know, the easier the tunneling is.

Let's discuss the dependence $P(d)$. Let's analyse the dependence $\overline{J}(d)$.

The terms containing d^2 dominate and give the contribution

$$\text{equal: } -\frac{g_2 d^2}{4\epsilon_2} + \frac{g_2 d^2}{8\epsilon_2} = -\frac{g_2 d^2}{8\epsilon_2} \quad (\text{see (13)})$$

When d increases, V increases, and P decreases. So it is the result consistent with the theoretical expectations [11] and with chapter I. The denser the plates are placed, the greater the intensity of Cooper's pairs creation is, and the bigger concentration of them is. Furthermore, the tunneling is easier in this case. So the model is conformable to literature data [11].

Let's notice, that we have calculated the potential barrier from classical electrodynamics. The probability of the tunneling has been obtained by us from semiclassical formula, and the tunnel effect is quantum phenomenon. Our semiclassical approximation foresees the existence of minimum and gives results conformable to the assumptions of model, and to literature.

III

Model of a sinusoidal plate.

Like in the previous chapter, we introduce the coordinate system such, that axes x, y are situated in the symmetry plane of the plate and their directions reflect the rectangular symmetry of the plate, and axis z is perpendicular to symmetry plane, and point $z=0$ is situated in this plane (see figure 13).

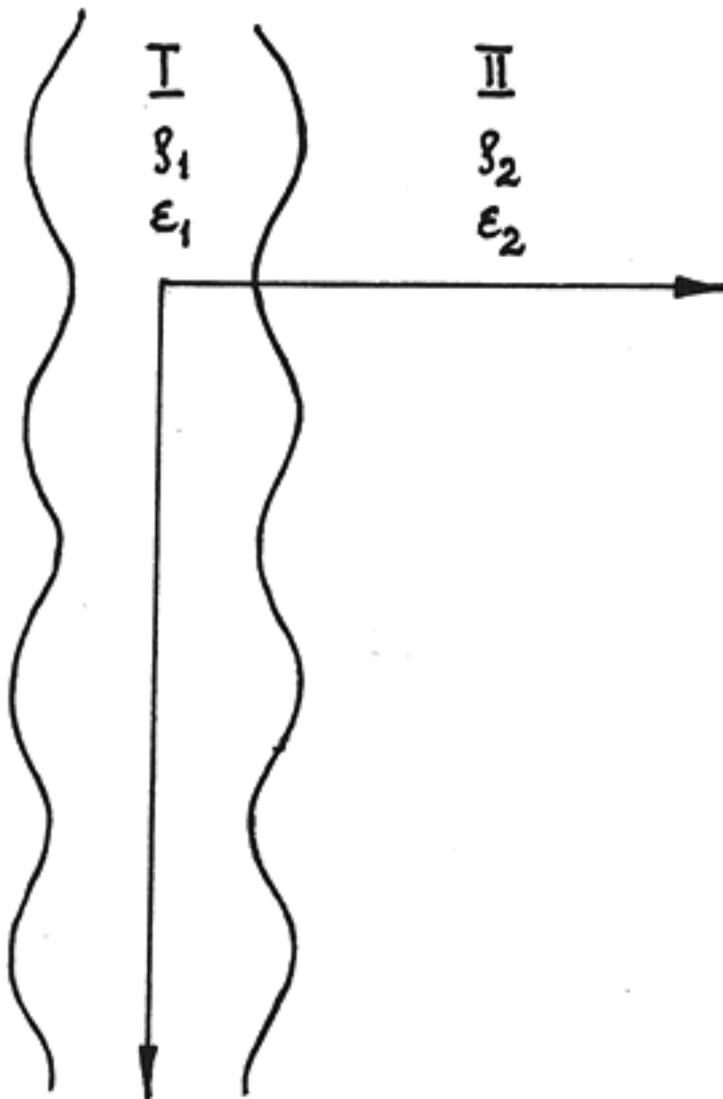


Figure 13

The line

$$z = z_0 + z_1 \sin \alpha x \sin \beta y ; |z_1| < z_0 \quad (20a)$$

divides the space into two regions:

- I filled homogeneously with charge with density ρ_1 (permittivity ϵ_1)
- II filled homogeneously with charge with density ρ_2 (electron gas), the permittivity equal ϵ_2 .

Using more realistic shape of electron cloud, we describe the contribution of the electric potential in the space.

The cloud between nuclei is thin, but in the direction perpendicular to the atomic plane which passes through nucleus, this cloud is thick.

Because of the symmetry of problem we will analyse one plate and one

neighbouring region. Moreover, we will describe only one side of the plate ($z > 0$), because the distribution of field at the opposite side of the plate is symmetrical.

We omit the influence of other plates too.

According to the convention of signs used in this work, and procedure employed in the previous chapter, the function, obtained from Poisson's equation, has the meaning of potential energy of electron. This energy is positive in the electric field of negative charges.

We will analyse separately the case when in the space I $\rho_1 \neq 0$ and in the space II $\rho_2 = 0$, and the case when in the space I $\rho_1 = 0$ and in the space II $\rho_2 \neq 0$.

We describe now the first from these cases. We expect that the solution of Poisson's equation will reflect the symmetry of problem.

So we look for the solution with the shape:

$$\psi(x, y, z) = \varphi(z) \sin \alpha x \sin \beta y + c \quad (21)$$

$$\text{where: } c > \max \varphi(z) \text{ for } z \in \langle 0, z_0 + z_1 \sin \alpha x \sin \beta y \rangle \quad (22)$$

This condition assures the positive value of function ψ in the analysed space I.

From Poisson's equation:

$$\Delta \psi = - \frac{\rho_1}{\epsilon_1}$$

We obtain:

$$\sin \alpha x \sin \beta y \left[\frac{\partial^2 \varphi(z)}{\partial z^2} - (\alpha^2 + \beta^2) \varphi(z) \right] = - \frac{\rho_1}{\epsilon_1}$$

The general solution:

$$\varphi_a(z) = A e^{-\sqrt{\alpha^2 + \beta^2} z} + B e^{\sqrt{\alpha^2 + \beta^2} z} \quad (23)$$

The particular solution:

$$\varphi_b = \frac{\rho_1}{\epsilon_1} \frac{1}{(\alpha^2 + \beta^2) \sin \alpha x \sin \beta y} \quad (24)$$

Taking under consideration (21), (23) and (24), we obtain:

$$\psi_I(x, y, z) = \left(A e^{-\sqrt{\alpha^2 + \beta^2} z} + B e^{\sqrt{\alpha^2 + \beta^2} z} \right) \sin \alpha x \sin \beta y + \frac{\rho_1}{\epsilon_1} \frac{1}{\alpha^2 + \beta^2} + c \quad (25)$$

It is the solution from the same class, as formula (21)

$$\text{and constant } C' = C + \frac{\beta_1}{\epsilon_1} \frac{1}{\alpha^2 + \beta^2}$$

Let's analyse the space II $(z_0 + z_1 \sin \alpha x \sin \beta y, \infty)$; $\beta_2 = 0$
and $\epsilon = \epsilon_2$.

We look for the solution with the shape:

$$\Psi_{II}(x, y, z) = \varphi(z) \sin \alpha x \sin \beta y + E$$

From Poisson's equation we obtain:

$$\sin \alpha x \sin \beta y \left[\frac{\partial^2 \varphi(z)}{\partial z^2} - (\alpha^2 + \beta^2) \varphi(z) \right] = 0$$

The general solution:

$$\varphi(z) = D e^{-\sqrt{\alpha^2 + \beta^2} z} \tag{26}$$

We have rejected the second term from the left side of dependence (23) because we don't want that: $-\text{grad } \Psi \rightarrow \infty$ (what means, that the intensity of electric field is infinite when $z \rightarrow \infty$) because it was finite in the case of the flat plate.

The particular solution does not occur, because of the shape of dependence (24) and because of the condition, that in this region $\beta = 0$.

Finally:

$$\Psi_{II}(x, y, z) = D e^{-\sqrt{\alpha^2 + \beta^2} z} \sin \alpha x \sin \beta y + E \tag{27}$$

We obtain the boundary condition:

$$\begin{aligned} & A e^{-\sqrt{\alpha^2 + \beta^2} z} \sin \alpha x \sin \beta y + B e^{\sqrt{\alpha^2 + \beta^2} z} \sin \alpha x \sin \beta y + \frac{\beta_1}{\epsilon_1} \frac{1}{(\alpha^2 + \beta^2)} + C = \\ & = D e^{-\sqrt{\alpha^2 + \beta^2} z} \sin \alpha x \sin \beta y + E \end{aligned}$$

for each x, y, z connected with the condition (20a).

So we have:

$$E = \frac{\rho_1}{\epsilon_1} \frac{1}{(\alpha^2 + \beta^2)} + C \quad (28)$$

$$A = 0$$

$$B = 0$$

And ultimately:

$$\Psi_{SII}(x, y, z) = A e^{-\sqrt{\alpha^2 + \beta^2} z} \sin \alpha x \sin \beta y + C + \frac{\rho_1}{\epsilon_1} \frac{1}{(\alpha^2 + \beta^2)} \quad (29)$$

Comparing (25) and (29), and taking under consideration (28) we state, that in the whole region $z \geq 0$, the function Ψ has the shape (29). Therefore the condition of equality of derivatives at the boundary surface is performed automatically.

Using the freedom of choice of C , we can put it so, that:

$$C > A + \frac{\rho_1}{\epsilon_1} \frac{1}{\alpha^2 + \beta^2} ; \rho_1 < 0$$

Let's take under consideration the space II.

$$\frac{d}{2} > z > z_0 + z_1 \sin \alpha x \sin \beta y$$

We assume, that $\rho_2 \neq 0$ and $\rho_1 = 0$.

The solution of Poisson's equation has in the whole space the shape:

$$\Psi_0(x, y, z') = F e^{-\sqrt{\alpha^2 + \beta^2} |z'|} \sin \alpha x \sin \beta y + G \quad (30)$$

$$\text{and } z + |z'| = \frac{d}{2}$$

$$G > |F|$$

The solution in the case $\rho_1 \neq 0$ and $\rho_2 \neq 0$ is the superposition of solutions (29) and (30), because the field created by two layers of charge is superposition of fields created by each layer analysed separately, with the assumption that an introduction of a neighbouring layer does not change the distribu-

tion of charge in each layer.

The coefficients A and F must have the same sign, because the function (30) arises from the function (29) by mirror reflection in relation to the plane $z = 0$, and by the translation equal $\frac{d}{2}$ (and possibly the multiplication by another positive coefficient and by addition of another constant).

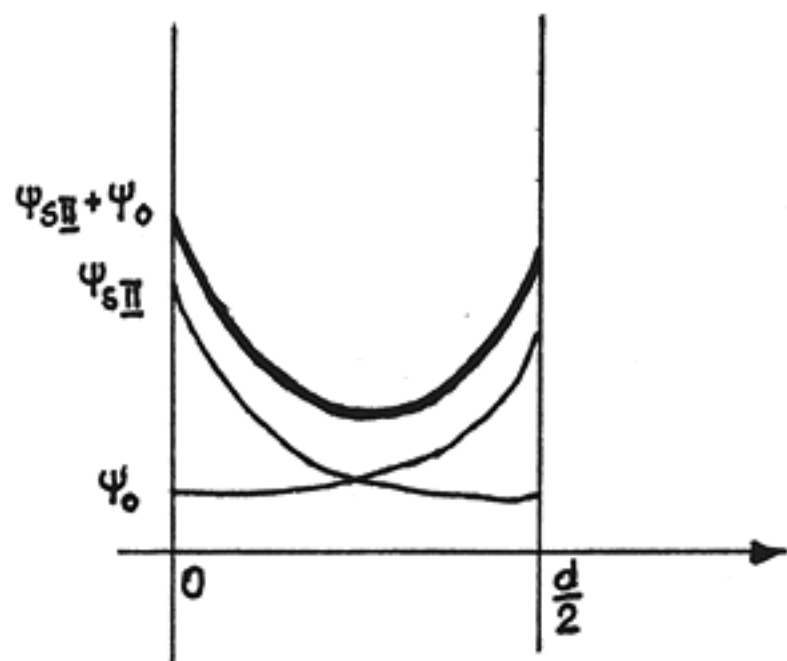


Figure 14

The superposition of functions ψ_{SII} and ψ_0 has for sure the extremum. (see figures 14 and 15)

If $A > 0$ and $B > 0$, then there is a minimum

If $A < 0$ and $F < 0$, then there is a maximum.

When $z_1 \rightarrow 0$ (see (20a)), the sinusoidal plate approaches the flat plate, and in this limiting case there is a minimum. (see previous chapter)

So we have in this case a minimum too, and $A > 0$, $F > 0$.

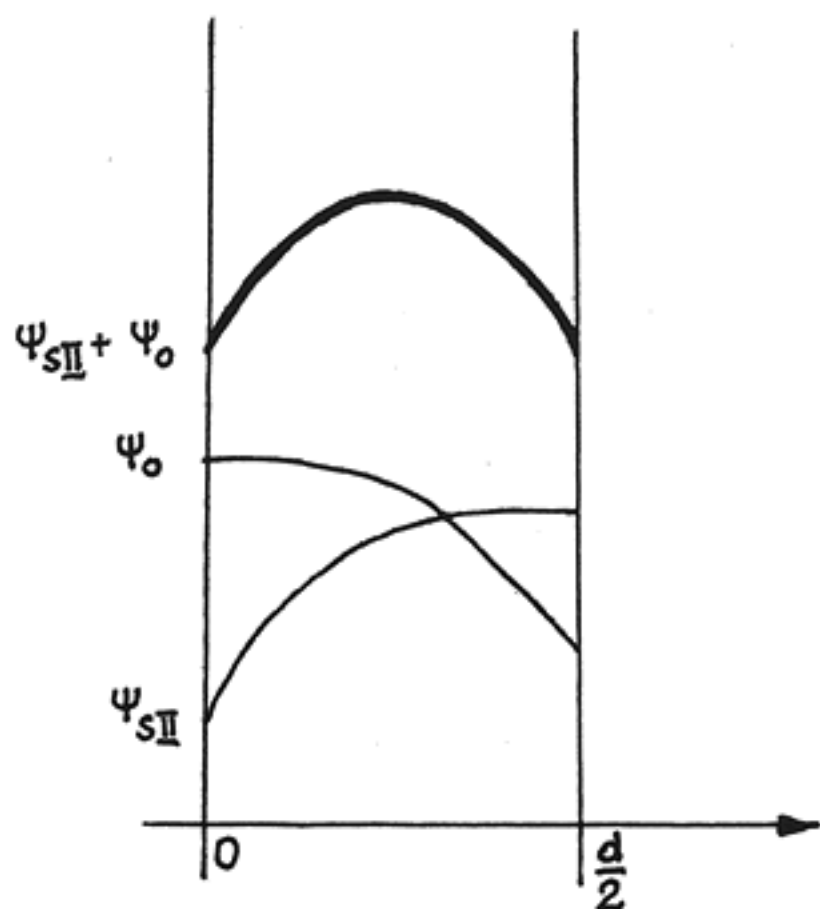


Figure 15

There is the minimum related to z , there are minima related to x and y , connected with minima of functions $\sin \alpha x$ and $\sin \beta y$. They lie opposite to the places with the smallest thickness of plate. There is a regular system of these minima at both sides of the plate, in which the concentration of Cooper's pairs is the greatest, and the possibility of tunneling (implicated by the smallest thickness of the plate) is the greatest, too. (see II 2)

It is very advantageous, that the minima of potential energy are correlated with the minima of thickness of the plate. Moreover,

when the minimum of potential energy exists for certain x, y , there is a minimum at the opposite side of the plate, too, and at these same x, y there are minima at each plates in the superconductor, because of translation symmetry.

When the superconducting current flows parallel to axis z from the minimum at one side of plate to the minimum at the other side of plate, then it tunnels through the plate and falls into the symmetrically laid minimum at the opposite side.

When the superconducting current flows parallel to axis x or y , it has to tunnel through the maxima of $\sin\alpha x$ and $\sin\beta y$, because the cooper's pairs are created in the positions correlated with minima of potential energy.

Let's discuss yet the dependence (29).

The condition $z_1 \rightarrow 0$ can be replaced by other condition: $\alpha \rightarrow 0$ and $\beta \rightarrow 0$ (see (20a)).

We have:

$$\lim_{\substack{\alpha \rightarrow 0 \\ \beta \rightarrow 0}} \sin\alpha x \sin\beta y = 0$$

$$\lim_{\substack{\alpha \rightarrow 0 \\ \beta \rightarrow 0}} A e^{-\sqrt{\alpha^2 + \beta^2} z} = A$$

$$\lim_{\substack{\alpha \rightarrow 0 \\ \beta \rightarrow 0}} \frac{\beta_1}{\epsilon_1} \frac{1}{(\alpha^2 + \beta^2)} = \infty$$

If the sinusoidal plate approaches the flat plate, the potential energy approaches infinity, and the oscillations are eliminated, so the potential energy has the same shape as in the case of the flat plate. Let's treat the function $\psi(\alpha, \beta)$ as the series of (z) .

We have:

$$\lim_{\substack{\alpha \rightarrow 0 \\ \beta \rightarrow 0}} \psi(\alpha, \beta) = \sum_{n=0}^{\infty} a_n z^n = a_0 + a_1 z$$

because we have put $a_n = 0$ for $n > 1$, because we want to obtain the limiting case of the plate (see (3)).

Then

$$\lim_{\substack{\alpha \rightarrow 0 \\ \beta \rightarrow 0}} \frac{\partial}{\partial z} \psi(\alpha, \beta) = a_1 \quad (31)$$

So the intensity of electric field approaches the constant in infinity.

When the sinusoidal plate approaches the flat plate, the oscillations don't occur, because the oscillating term disappears.

Let's calculate the intensity of electric field in the space $z \gg 0$.

We have:

$$\begin{aligned} \vec{E} = -\vec{\nabla} \psi = & -A e^{-\sqrt{\alpha^2 + \beta^2} z} \alpha \cos \alpha x \sin \beta y \vec{i}_x - A e^{-\sqrt{\alpha^2 + \beta^2} z} \beta \sin \alpha x \cos \beta y \vec{i}_y \\ & + A e^{-\sqrt{\alpha^2 + \beta^2} z} \sqrt{\alpha^2 + \beta^2} \sin \alpha x \sin \beta y \vec{i}_z + K \vec{i}_z \end{aligned} \quad (32)$$

Where $K = -a_1$ (see (31))

Because of freedom of choice, we can choose it so, that:

$$|a_1| > \sqrt{\alpha^2 + \beta^2} A$$

and the oscillations of sign of \vec{E}_z do not occur, which have no physical meaning.

Let's remember, that the condition $z_1 \rightarrow 0$ or equivalent $\alpha \rightarrow 0$ and $\beta \rightarrow 0$, describes the situation when $z \rightarrow \infty$, because the observer in infinity sees averaged folds of plate, and this plate is flat for him, and with thickness z_0 .

In infinity E_z approaches the constant different than zero, which must have been reflected in formula (32).

The oscillation of signs of components \vec{E}_x and \vec{E}_y are physically motivated.

They are correlated with oscillation of signs of functions $\sin \alpha x$ and $\sin \beta y$. These functions occur both in the dependence describing potential energy and in the dependences describing components \vec{E}_x and \vec{E}_y , and correspond with physical symmetry of problem.

IV

The binding character of existing minima.

We have to prove yet that appearing minimum is binding minimum, in order to the solution of problem would be complete.

For cancellation the consideration we analyse the case of flat plate.

The potential in the region of plate is expressed by the formula (13) and in the region of electron gas by the formula (14a).

It is seen that potential has the shape $V = ax^2 + bx + c$. We write the Schrödinger's equation with this potential

$$-\frac{\hbar^2}{2m} \Delta \psi + V\psi = E\psi$$

We mark

$$A =: -\frac{\hbar^2}{2m}$$

We write the wave function in the shape of series

$$\psi = \sum_{n=0}^{\infty} d_n x^n$$

and taking under consideration

$$\frac{\partial \psi}{\partial x} = \sum_{n=0}^{\infty} n d_n x^{n-1}$$

$$\frac{\partial^2 \psi}{\partial x^2} = \sum_{n=0}^{\infty} n(n-1) d_n x^{n-2}$$

the Schrödinger's equation obtains the shape

$$\begin{aligned} \sum_{n=0}^{\infty} a d_n x^{n+2} + \sum_{n=0}^{\infty} b d_n x^{n+1} + \sum_{n=0}^{\infty} (c-E) d_n x^n + \\ + \sum_{n=2}^{\infty} A n(n-1) d_n x^{n-2} = 0 \end{aligned}$$

We will obtain the information analysing the coefficients at the same degree of polynomial and equating them to zero.

The coefficient at x^{n+2} is equal

$$ad_n + bd_{n+1} + (c-E)d_{n+2} + A(n+4)(n+3)d_{n+3}$$

and at x^{n+1}

$$ad_{n-1} + bd_n + (c-E)d_{n+1} + A(n+3)(n+2)d_{n+3}$$

and at x^n

$$ad_{n-2} + bd_{n-1} + (c-E)d_n + A(n+2)(n+1)d_{n+2}$$

and at x^{n-1}

$$ad_{n-2} + bd_{n-2} + (c-E)d_{n-1} + A(n+1)n d_{n+1}$$

For certain n the series is discontinued.

It means that $d_n = 0$ and $d_{n+1} = 0$.

For $n=2$ $d_2=0$ and $d_{n-3} = d_{n-1} = 0$ as undefined.

So we have

$$ad_{n-2} + bd_{n-1} + (c-E)d_n = 0$$

$$ad_{n-3} + bd_{n-2} + (c-E)d_{n-1} = 0$$

and taking under consideration the previous facts, we obtain

$$ad_0 + bd_1 = 0$$

$$bd_0 + (c-E)d_1 = 0$$

It is the system of equations for d_0 and d_1 which has untrivial solution then and only then when its slater is equal zero.

So we have

$$-b^2 + a(c-E) = 0$$

so:

$$E = -\frac{b^2}{a} + c$$

(33)

$a > 0$ because $\beta < 0$.

Let's notice that

1) For obtaining the energy of the lowest quantum state we don't need to know any value d_j .

2) For $n=1$ we have only one equation

$$bd_1 = 0 \quad \text{so} \quad d_1 = 0$$

It means that wave function for $n=0$ is equal zero ($\psi=0$). We can't obtain in this situation any information.

The lowest quantum state is described by the quantum number $n=2$.

The equation (33) proves that minimum has binding character. Really, it is seen that:

$$E < \bar{\pi}_{I \max}$$

and

$$E < \bar{\pi}_{II \max}$$

Namely:

$$\bar{\pi}_{I \max} = \bar{\pi}_I(0)$$

$$\bar{\pi}_{II \max} = \bar{\pi}_{II}\left(\frac{d}{2}\right)$$

and

$$\bar{\pi}_I(0) = c$$

and $E_I = c - \frac{b^2}{a} < c$ because $a > 0$

and $E < E_{II}$ because there is the same parabola physically but only moved.

We may prove this second fact in another way yet.

We have to prove that $\bar{\pi}_{II}\left(\frac{d}{2}\right) > E_{II}$

or

$$\frac{\beta_2 d^2}{8\epsilon_2} + \frac{\beta_2 d^2 b}{2\epsilon_2} - \frac{\beta_1 b d}{4\epsilon_1} \geq \left(\frac{\beta_2}{2\epsilon_2} - \frac{\beta_1 b}{2\epsilon_1} \right)^2 / \frac{\beta_2}{2\epsilon_2}$$

The member $\left(\frac{\beta_1 b^2}{8\epsilon_1} - \frac{\beta_2 d^2}{2\epsilon_2} \right)$ was reduced at both sides.

and eventually the equivalent formula

$$\frac{1}{16} \frac{\beta_2^2 d^2}{\epsilon_2^2} - \frac{\beta_1^2 b^2}{4\epsilon_1^2} + \frac{3}{8} \frac{\beta_1 \beta_2 b d}{\epsilon_1 \epsilon_2} > 0$$

which is true for sure for certain parameters $\xi_1, \xi_2, \varepsilon_1, \varepsilon_2, b, d$, so minimum in this region has the binding character, too.

So we have proved that the lowest energetic level exists inside the potential well (and no over it) in the region $(0, \frac{d}{2})$, what is enough.

V

Recapitulation

In the chapters II and III we have corroborated quantitatively the expectations from the chapter I .

We have stated, that the minimum of potential energy occurs in case of two characteristic shapes of the electron cloud in the plates , and enables the creation of Cooper's pair , the tunneling towards the opposite side of the plate and binding with the partner from the Cooper's pair.

We have mathematically proved, that the intensivity of the superconducting current increases when the thickness of the plate decreases, and encreases when the distance between the plates decreases.

The compactness of the obtained results and their conformity to expectation evidences the correctness of simplifications, using of which is the normal procedure in the solution of the many body problems in the solid state physics.

The semiclassical description of the high temperature superconductivity based on Hellman-Feynman theorem and on classical electrodynamics creates great possibilities of description of various effects occuring in high temperature semiconductors.

So we have explained the mechanism of creation of Cooper's pair and mechanism of the flow of superconducting current through the CuO planes and regions between them.

The Anderson's conception of division of charge and spin of electron has been corroborated. We have stated, it is only a different treatment of mechanism of creation of Cooper's pairs, described in this work.

The Schrieffer's conception of creation of Cooper's pair in certain regions, has been confirmed, too. We have stated that these places are correlated with minimum of CuO thickness, which makes easier the tunneling.

On the ground of the presented conception, the necessity of parallelism of CuO planes, their translational symmetry, towards the axes perpendicular to them, and the necessity of minimum distance between them, have been recorded.

The conceptions of existence of holes in CuO layer has been confirmed, and the mechanism of creation of excitons has been explained.

The great role of electrostatic interactions in high temperature superconducting materials has been stated in [11] which is consistent with point presented in this work. In this treatment we have the repulsion of electrons by electron gas, the repulsion of electrons by electron plate in CuO planes, and the induction of effective positive charge in these plates and attraction of electrons by this charge.

We have explained, why only electrons creating Cooper's pair can tunnel, why the high temperature superconductivity and the critical temperature decrease when the distances between the plates increase.

The advantage of this work is the simplicity. The mathematical description is not complicated, but precise. The conformability to experimental facts occurs.

There is the permanent possibility of improvement of the results by introduction of more and more realistic distribution of electric charge.

The main advantage of this work is the unification of facts entered into composition of two seemingly antagonistic approaches of Anderson and Schrieffer.

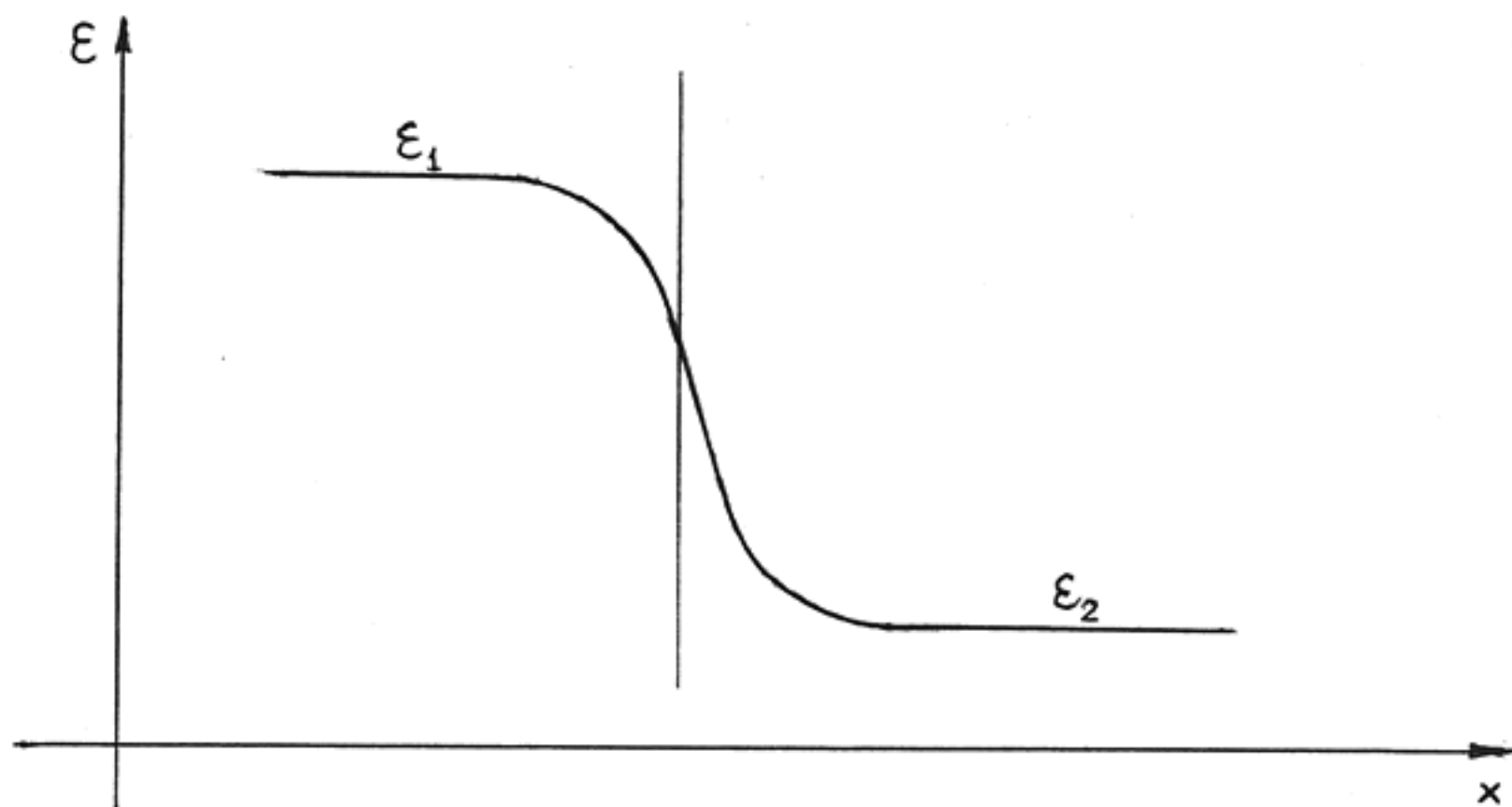
Both Anderson, who tells, that the new mechanism of creation of Cooper's pairs is needed, and Schrieffer, who tells that the small but important modification of BCS theory is necessary, are right. In this case the electron cloud in CuO layers mediates in creation of Cooper's pairs, and no crystal lattice.

The presented work confirms the old truth, that opposite theories are complementary and both contribute a great deal for understanding of the problem.

There is a necessity of making the analysis of boundary conditions: continuity of potential and its space derivative on the boundary of mediums. Generally other boundary conditions are used: continuity of perpendicular component of vector of induction and continuity of tangent component of vector of intensity of electric field.

But the tangent component of electric field in the case of plate, whose boundary is a plane, is equal zero from the symmetry of problem. So other boundary condition is necessary.

Next the condition of continuity of potential on the boundary of mediums is implicated by the fact that the situation is static. If the difference of potential exists on the boundary of mediums, the flow of current would appear, what is discrepant with the assumption.



Next the second boundary condition is implicated by the fact that on the boundary both mediums penetrate mutually and permittivity is locally continuous.

At the boundary we have:

$$D_{1\perp} = D_{2\perp}$$

$$\epsilon_1 \frac{\partial V_1}{\partial x} = \epsilon_2 \frac{\partial V_2}{\partial x}$$

and

$$\epsilon_1 \rightarrow \epsilon_2 \Rightarrow \frac{\partial V_1}{\partial x} = \frac{\partial V_2}{\partial x}$$

Appendix B

Two conventions are possible:

I g has the sign of charge: the negative sign in the case of electrons, and the Laplace equation contains potential φ multiplied by the charge - so potential energy.

II g is positive for all charges and isn't multiplied by the sign of charge.

The Laplace equation implicates then the potential φ which is not multiplied by e .

The convention I is used in this article.

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