Calculation of the Superconductivity Gap of Metal from Its Parameters in Normal State

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A previously considered model interpreted a superconductor as an electron gas immersed in a medium with the dielectric constant $\varepsilon$ and a certain elasticity, which could be determined by measured sonic speed in the metal. The obtained expression of effective electron-electron interaction (EEI) potential unambiguously implied that, contrary to the suggestions of BCS theory, it is its long-wave limit which is responsible for the emergence of bound two-electron states and, consequently, for gap formation in one-electron spectrum of the metal. However, the existence of singularities in the EEI potential expression continued to pose a problem, which did not allow a calculation of the gap value for specific superconducting materials, first of all, for metals belonging to periodic table (PT). In the present work, I suggest taking into account matrix elements traditionally attributed to electron scattering in EEI effective potential calculations. For superconductors that has been made on the basis of a semiconductor material by implanting electro-active defects into it, this inclusion results in the appearance of an uncertainty of electron momentum $\delta p \sim l^{-1}$, where $l$ is the electron free path. When considering pure PT metals, Hamiltonian terms relating to creation and annihilation of phonons should be taken into account, which also produces an uncertainty of electron momentum. This uncertainty results in a regularization of EEI potential expression and, therefore, in a possibility of examination of physical properties of specific superconductors. Results of calculation of superconductivity gap value for a range of simple metals (Al, Zn, Pb, Sn) confirm the consistency of the developed approach.

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I. INTRODUCTION

According to the opinion expressed by the most part of the scientific community, the present-day situation of the superconductivity theory can hardly be called satisfactory. Indeed, while the BCS theory [1] provides a qualitative explanation of phenomena observed in superconductors, it is unable to produce reliable predictions of their quantitative parameters. At the same time, it is implicitly suggested that the BCS theory contains no contradictions in its description of the 'conventional' superconductivity; problems are only believed to appear in connection with the description of high-temperature superconductivity.

That is why recent studies mostly concern high-temperature superconductors alone [2, 3]. All these studies include the BCS theory considered as an extreme case; they only differ in mechanisms producing the attraction between electrons. Therefore, these models do not essentially change the microscopic picture of the phenomenon.

According to the concept of the so called BCS-BEC crossover [4], the phase transition in the BCS theory shares many features with the Bose-Einstein condensation (BEC) phenomenon, which, eventually, allowed connecting it with the Ginzburg-Landau theory [5]. Currently, attempts are being made at providing a more precise description of superconductors within the framework of this concept. These models also incorporate the BCS model for an extreme case.

It should be noted that, in 1980-90s, superconductivity theories unrelated to the BCS theory have been put forward. Most of these models contradict experimental data even at the level of the qualitative description. By the present date, the interest towards such models has seen a substantial decrease.

The superconductor model to be described in the present paper does not contain the BCS model as an extreme case either, and has nothing in common with the BEC phenomenon. Nevertheless, the model under development can already claim, at least, a semi-quantitative agreement with the experiment. Its present-day status is described in Sections 2 and 3. This approach has been discussed in detail in a number of publications [6, 7]; therefore, here we restrict ourselves to a shortest possible description, only indicating its initial differences with currently universally acknowledged concepts.

The goal of the present study is a calculation of the superconducting gap in the framework of the proposed model in order to compare it with the analogous calculation results of the BCS theory. The study is performed on simple metals belonging to PT.

Fitting parameters obtained out of the quantitative calculation have the order of magnitude corresponding to that predicted by the theory. This agreement makes the approach under consideration look more attractive than the BCS theory.
II. RENORMALIZATION PROCEDURE FOR METALS

A procedure of renormalization for a system comprised of electrons and phonons correctly taking into account the singular nature of matrix elements of electron-phonon interaction (EPI) in the long-wave limit has been performed previously [6]. The Hamiltonian of a monatomic metal electron system, as obtained from the renormalization, has the following form:

\[ H = H_0 + H_{ee} \]  

(1)

where

\[ H_0 = \sum_{\sigma, p} t_p c_{\sigma, p}^+ c_{\sigma, p}, \]  

(2)

\[ H_{ee} = \Omega^{-1} \sum_{\sigma, p, \nu, k} \sum_q U_{q}^{p, k} c_{\sigma, p + q}^+ c_{\nu, k - q}^+ c_{\nu, k} c_{\sigma, p}, \]  

(3)

\[ U_{q}^{p, k} = \frac{2\pi e^2}{\varepsilon q^2} + \delta U_{q}^{p, k}, \]  

(4)

\[ \delta U_{q}^{p, k} = \frac{\pi z e^2 K_F^2}{3\varepsilon m M} \left[ \frac{1}{(t_p q - t_p)^2 - S_1^2 q^2} + \frac{1}{(t_k - t_k q - t_p)^2 - S_1^2 q^2} \right], \]  

(5)

c and \( c \) are creation and annihilation operators, respectively, of conductivity band electrons; \( \sigma \) and \( \nu \) electron spin indexes; \( z \) is the number of conductivity electrons per atom; \( m \) is the electron mass; \( t_p = \frac{e^2}{2m} \); \( M \) is the ion mass; \( S_1 \) is a parameter related to the observed sonic speed of the longitudinal polarization \( S \) as \( S_1^2 = S^2 - \frac{z K_F^2}{6 m M} \); \( K_F \) is Fermi vector; \( \Omega = L \times L \times L \); \( L \) is the crystal dimension, and \( \varepsilon \) is the statical long-wave limit of the metal dielectric function caused by interband transitions.

The above expression for the initial potential of EEI substantially differs from other known results, first of all because \( \delta U \sim q^2 \) at \( q \to 0 \). Evidently, this result cannot be obtained within the framework of Fröhlich model [8] as this model lacks a consistent accounting for screening effects when calculating the EPI Hamiltonian terms. This circumstance has long been known [9]; now it is worthwhile to note here that it is the Fröhlich model that makes a basis for Eliashberg equations, which the majority of authors [10] consider to represent the most integral superconductor description in BCS theory.

The expression (4) obtained for the initial EEI excludes the formation of bound two-electron states in the system at this stage of problem examination. Indeed, the Coulomb term is significantly larger than \( \delta U \), since \( \delta U \to 0 \) at \( M \to \infty \). As a formation of bound two-electron states of the Hamiltonian (1) appears to be impossible, any ‘bosonization’ of the system is completely out of question. That is why the models involving BEC to clarify the superconductivity phenomenon seem to be insufficiently substantiated.

III. EXCITATION SPECTRA IN MULTI-PARTICLE SYSTEMS

Let us assume by definition that the Hamiltonian \( \tilde{H} \), defined as:

\[ \tilde{H} = \sum_{\sigma, p} t_p c_{\sigma, p}^+ c_{\sigma, p} + \Omega^{-1} \sum_{\sigma, p, \nu, k} \sum_q \tilde{U}_{q}^{p, k} c_{\sigma, p + q}^+ c_{\nu, k - q}^+ c_{\nu, k} c_{\sigma, p}, \]  

(6)

has the same two-electron excitation spectrum as the initial Hamiltonian (1) accounting for multi-particle effects. Thus, in fact, we rigorously define the notion of the EEI effective potential \( \tilde{U}_{q}^{p, k} \) involved in the right-hand side of Eq. (6).

We start the procedure of definition of \( \tilde{U}_{q}^{p, k} \) by considering the following transformation:

\[ C_{\sigma, p}^+ = c_{\sigma, p}^+ + \sum_{\nu, k, q} \tilde{U}_{q}^{p, k} c_{\nu, k - q}^+ c_{\nu, k} c_{\sigma, p}, \]  

(7)
where

\[ \theta_{p,q}^{\sigma} = \frac{1}{2} \left( \delta_{k-p}^{q} - \delta_{k}^{q} \right) + c_{p,q}^{\sigma}, \]

\[ \theta_{p,k}^{\sigma} = -\delta_{q}^{0} + \chi_{p,q}^{\sigma}, \]  

(8)

\[ \chi_{0,q}^{p,k} \text{ and } \chi_{1,q}^{p,k} \text{ are expressed in terms of wave functions (WFs) of stationary two-particle states } \langle \psi_{0}^{p,k} \rangle = \sum_{q} \chi_{0,q}^{p,k} \left( c_{\uparrow,p+q}^{+} c_{\downarrow,k-q}^{+} - c_{\downarrow,p+q}^{+} c_{\uparrow,k-q}^{+} \right) \text{ and } \langle S_{0}^{p,k} \rangle = \sum_{q} \chi_{1,q}^{p,k} \left( c_{\uparrow,p}^{+} c_{\downarrow,k}^{+} + c_{\downarrow,p}^{+} c_{\uparrow,k}^{+} \right) \left| 0 \right\rangle \text{ in the following way:} \]

\[ \tilde{H} \langle S_{1}^{p,k} \rangle = \left( t_{p} + t_{k} + \delta E_{1}^{p,k} \right) \langle \psi_{1}^{p,k} \rangle, \]

\[ \tilde{H} \langle \psi_{0}^{p,k} \rangle = \left( t_{p} + t_{k} + \delta E_{0}^{p,k} \right) \langle \psi_{0}^{p,k} \rangle, \]  

(9)

It is easy to demonstrate that the transformation (7) reduces the Hamiltonian \( \tilde{H} \) to the diagonal form in the two-particle state space:

\[ \tilde{H} = \sum_{\sigma,k} t_{k} C_{\sigma,k} C_{\sigma,k} + \frac{1}{2} \sum_{\sigma,p \neq k} \delta E_{1}^{p,k} C_{\sigma,p}^{+} C_{\sigma,k} C_{\sigma,k} + \frac{1}{4} \sum_{\sigma,p \neq k} \delta E_{0}^{p,k} \left( C_{\uparrow,p}^{+} C_{\downarrow,k}^{+} + C_{\downarrow,p}^{+} C_{\uparrow,k}^{+} \right) \left( C_{\downarrow,k} C_{\uparrow,p} + C_{\uparrow,k} C_{\downarrow,p} \right) \]

\[ + \sum_{p} \delta E_{0}^{p,k} C_{\downarrow,p}^{+} C_{\downarrow,k}^{+} C_{\downarrow,k} C_{\downarrow,p} + \frac{1}{4} \sum_{p \neq k} \delta E_{0}^{p,k} \left( C_{\downarrow,p}^{+} C_{\downarrow,k}^{+} - C_{\downarrow,p}^{+} C_{\downarrow,k}^{+} \right) \left( C_{\downarrow,k} C_{\downarrow,p} - C_{\downarrow,k} C_{\downarrow,p} \right). \]  

(10)

Taking into account multi-particle effects in electron gas is performed in the random phase approximation (RPA) as follows. Consider the inverse transformation of (7):

\[ c_{\sigma,p}^{+} = C_{\sigma,p}^{+} + \sum_{\nu,k,q} \theta_{\sigma-k,q}^{p+q} C_{\sigma,p}^{+} C_{\sigma,k} C_{\sigma,k}^{+} C_{\sigma,p}^{+}, \]

\[ c_{\sigma,p} = C_{\sigma,p} + \sum_{\nu,k,q} \theta_{\sigma-k,q}^{p+q} C_{\sigma,p} C_{\sigma,k} C_{\sigma,k}^{+} C_{\sigma,p}^{+}. \]  

(11)

Then express the initial Hamiltonian (1) in terms of operators \( C^{+} \) and \( C \) using the transformations (11). In this form, the Hamiltonian comprises terms of the structure \( C^{+} C^{+} C^{+} C \), which, in the RPA, can be reduced to the form of \( \langle C^{+} C \rangle C^{+} C^{+} C \). These terms define additional potentials \( D_{q}^{p,k} \), which can be included in the equation for effective potentials \( U_{q}^{p,k} \):

\[ U_{q}^{p,k} = U_{q}^{p,k} + D_{q}^{p,k}. \]  

(12)

Eqs. (9) and (12) form a self-consistent system for \( U_{q}^{p,k} \) definition.

It is important to note that, in the framework of the proposed approach, it is the Hamiltonian (10) which is related to the initial Hamiltonian (1) by the unitary transformation (7), and the introduction of the Hamiltonian (6) into the theory is of an auxiliary nature and is used to calculate the parameters \( \delta E_{1}^{p,k} \) and \( \theta_{p,q}^{\sigma} \). We should specify more explicitly in which sense we name the transformation (7) unitary, since the anti-commutators \( [C^{+}, C]_{+} \) and \([C, C]_{+} \) differ from standard fermion commutation relations in the presence of terms \( c^{+} c^{+} c^{+} c^{+} \) and \( c^{+} c^{+} c^{+} c^{+} \), respectively [3]. It is, however, easy to demonstrate that, in two-electron state space, a transition from \( \psi_{0}^{p,k} \) states to \( \psi_{1}^{p,k} \) states does not alter the WFs scalar products; therefore, the transformation (7) for this case should be considered to be unitary.

Then, the right-hand sides of Eqs. (6,7,11) can be considered as two first terms of the series with the number of terms equal to the number of particles in the system. These series are composed while determining the multi-particle excitation spectrum using the same procedure as invoked above for the calculation of a two-electron excitation spectrum. Of course, the transformation (7) completed with the terms of the corresponding series is unitary for all states, in which the number of particles is less than or equal to the number of particles in the system.

Using the RPA for the examination of an excitation spectrum allows for an introduction the Hartree-Fock method for calculating of one-electron energies into the above calculation routine. From this point of view, the proposed approach is essentially a generalization of the Hartree-Fock approximation for a multi-particle spectrum calculation.

Previously [3], the above mentioned self-consistent system for the potential (4) have been formulated and solved using the perturbation theory for solution of eigenvalue problems (9). It should also be noted that considering the
Coulomb EEI alone (see Appendix A) within the framework of the proposed scheme is well consistent with the modern idea of the effective EEI in a degenerate plasma. This fact confirms the consistency of the proposed approach for treatment of multi-particle problems with interaction.

Combining (A5) with previously obtained results yields the following equation:

\[ \tilde{U}^{p,k}_q = 2\pi e^2 \frac{\varepsilon q^2}{(\varepsilon q^2 + \lambda^2)^2} - 4 \left( \frac{zm}{3M} \right)^2 \frac{2K_p}{\varepsilon q^2} \left( q^2 - \chi^2 \right), \]

where \( \chi = 4m^2 \left( S^2 - \frac{2K_p^2}{3mM} \right) \). In this form, the equation for \( \tilde{U}^{p,k}_q \) is valid in two limits: \( M \to \infty \) and \( q \to 0 \).

It ensues from Eq. (13) that an attraction between electrons is present in the long-wave limit. Now according to Eliashberg equations, Cooper pair formation is mainly due to short-wave phonons with a wave vector \( q \approx 2K_p \). Evidently, the authors of the theory were guided by the erroneous hypothesis of absence of electrons attraction in the long-wave limit, which had been suggested based on the plasma model analysis performed back in 1950’s.

If Eqs. (9) do not allow the appearance of bound states, then \( \delta E^{p,k}_i \sim \Omega^{-1} \), and the theory describes a normal metal. Appearance of bound states with the binding energy \( \delta E^{p,k} \) for unbound states of electron pairs, the Hamiltonian (10) for a superconductor can be written as

\[ H = \sum_{\sigma,\mathbf{k}} \varepsilon_{\mathbf{k}} C^+_{\sigma,\mathbf{k}} C_{\sigma,\mathbf{k}} - \sum_{\mathbf{k}} E_0 C^+_{\uparrow,\mathbf{k}} C^+_{\downarrow,\mathbf{k}} C_{\downarrow,\mathbf{k}} C_{\uparrow,\mathbf{k}} - \frac{1}{4} \sum_{\mathbf{k}} E_0 \left( C^+_{\uparrow,\mathbf{p}} C^+_{\downarrow,\mathbf{p}} - C^+_{\downarrow,\mathbf{p}} C^+_{\uparrow,\mathbf{p}} \right) \left( C_{\downarrow,\mathbf{p}} C_{\uparrow,\mathbf{p}} - C_{\uparrow,\mathbf{p}} C_{\downarrow,\mathbf{p}} \right) \left\{ \mathbf{p} \neq \mathbf{q} : |\mathbf{p}_\alpha - \mathbf{k}_\alpha| \leq 2\pi/L, \alpha = x, y, z \right\} \]

It is easily seen that the ground state \( |\Phi_0\rangle \) of the Hamiltonian (14) coincides with the well-known expression for a non-interacting Fermi gas:

\[ |\Phi_0\rangle = \prod_{\mathbf{p} < K_F} C^+_{\uparrow,\mathbf{p}} C^+_{\downarrow,\mathbf{p}} |0\rangle. \]

Therefore, from the point of view of the new theory, there is no ground for suggesting a possibility of formation of BEC, although the theory does discuss wave functions of bound states of electron pairs. Hence, the Ginsburg-Landau theory also lacks microscopic grounds. Nevertheless, we take it as evident that main predictions of the Ginsburg-Landau theory are reproduced within the framework of the proposed theory; therefore, the absence of BEC in the system in question is not to be worried about.

Along with the ground state \( |\Phi_0\rangle \), also the one-electron and one-hole excitations are the stationary states of Hamiltonian (14). This allows to calculate the arising energy gap value \( 2\Delta_0 \) in the one-electron spectrum of the ground state. If there exists only one bound solution with a zero spin and a fixed pair momentum, the value of \( \Delta_0 \) is calculated as:

\[ \Delta_0 = 7E_b. \]

IV. REGULARIZATION OF EEI EFFECTIVE POTENTIAL

The expression (13) is evidently inapplicable for calculation of superconductive properties of metals due to the presence of singularities at \( q = 0 \) and \( q = \sqrt{\chi} \). On the other hand, we have not up to now taken into account the Hamiltonian terms usually related to scattering processes, which can result in an uncertainty of electron momentum and, consequently, in a removal of singularities even in the initial EEI potential \( U^{p,k}_q \).

Let us begin with the simplest case of a metal that has been made on the basis of a semiconductor material by implanting electro-active defects into it. Evidently, in this case, the abovementioned momentum uncertainty is \( \delta p \sim l^{-1} \), where \( l \) is the free path of electrons as determined by the scattering on lattice defects.

In the case of pure PT metals, the following considerations should be taken into account. The renormalization procedure for metals used only longitudinal phonons with a distinctly expressed singularity of the EPI potential in the long-wave limit. However, due to various reasons, the EPI terms remaining in the Hamiltonian after this renormalization have a weak non-analyticity in the said limit for acoustic phonons. Neglecting relativistic effects these terms have the following form:

\[ H_{ep} = \sum_{\sigma,\mathbf{p}} \sum_{m,q,g} \sqrt{\omega_{m,q}} e^{\mathbf{p},\mathbf{q},\mathbf{g}} \left( c^+_{\sigma,\mathbf{p}-\mathbf{q}-\mathbf{g}} c^+_{\sigma,\mathbf{m},\mathbf{q}} b^+_{\sigma,\mathbf{m},\mathbf{q}} + H.c. \right), \]
where $\omega_{m,q}$ is the phonon frequency; $b_{m,q}^+$ and $b_{m,q}$ are phonon creation and annihilation operators, respectively, including the case of transversal polarization, $m$ and $q$ are the phonon mode index and phonon quasi-momentum, respectively, and $\mathbf{g}$ is the reciprocal lattice vector. As to $F_{m,q}^p$, it is a piecewise regular function with respect to variations of the arguments $p$ and $q$.

Taking into account the term $H_{sp}$ radically alters the WFs of stationary one-electron states due to the possibility of spontaneous creation of phonons from electrons, since Fermi speed is much greater than the sonic speed. Therefore, from the point of view of calculation of the effective EEI, the phonon system acts as a reservoir that electrons can exchange momentum with, which can be accounted for by a regularization of EEI potential expressions.

Let us try to determine the arising momentum uncertainty from the consideration of the temperature dependence of the specific resistance $\rho$ at temperatures $T \gg \theta_D$, where $\theta_D$ is Debye temperature. Then, according to the Fermi’s Golden Rule, the following relation is valid for electron-phonon transition frequency $\nu_T$ of an electron of momentum $p$:

$$\nu_T \sim T \sum_{m,g} \int (q + g)^2 \left| F_{m,q}^p \right|^2 \delta \left( t_p - t_{p-q-g} - \omega_{m,q} \right) dq,$$

(18)

which takes into account that in this case, the transitions are induced by phonons with a distribution function approximately equal to $T/\omega_{m,q}$.

Of course, what we are interested in is the spontaneous transition frequency $\nu_0$. It can be expressed as:

$$\nu_0 \sim \sum_{m,g} \int (q + g)^2 \left| \sqrt{\omega_{m,q}} F_{m,q}^p \right|^2 \delta \left( t_p - t_{p-q-g} - \omega_{m,q} \right) dq,$$

(19)

Comparison of Eqs. (18) and (19) yields:

$$\frac{\nu_0}{\nu_T/T} = \bar{\omega},$$

(20)

where

$$\bar{\omega} = \frac{\sum_{m,g} \int (q + g)^2 \omega_{m,q} \left| F_{m,q}^p \right|^2 \delta \left( t_p - t_{p-q-g} - \omega_{m,q} \right) dq}{\sum_{m,q} \int \left( q + g \right)^2 \left| F_{m,q}^p \right|^2 \delta \left( t_p - t_{p-q-g} - \omega_{m,q} \right) dq}.$$

(21)

It is important to note that the following relationships are strictly fulfilled for $\bar{\omega}$:

$$0 < \bar{\omega} < \omega_{\max},$$

(22)

where $\omega_{\max}$ is the maximum frequency of the phonon spectrum.

On the other hand, the Hamiltonian (17) is in certain cases the main cause of energy dissipation in electron tunneling between superconductors. That is why a correct numerical processing of the current-voltage characteristics (CVC) in the region where the tunnel junction (TJ) behaves itself similarly to resistance yields a more precise evaluation of the parameter $\bar{\omega}$ than the relationship (22).

The $\nu_T/T$ value can be roughly evaluated from Drude formula for specific resistance $\rho$ at high temperatures:

$$\nu_T/T = \frac{\Omega_{pl}^2 \rho^\prime}{4\pi},$$

(23)

where $\Omega_{pl}$ is plasma frequency determined in optical studies of metals in the infrared (IR) range, $\rho^\prime$ is the derivative of the specific electric resistance over temperature, for which, evidently, $\rho^\prime \approx \rho/T$. Considering that the free path of a single electron in the system is calculated as $l = \langle V_F \rangle / \nu_0$, where $\langle V_F \rangle$ is an average electron velocity over the Fermi surface, the definitive expression for the sought uncertainty $\delta p$ of a stationary single-electron state is:

$$\delta p = \frac{\Omega_{pl}^2 \rho^\prime \bar{\omega}}{4\pi \langle V_F \rangle}.$$

(24)

In the further study, taking into account that for the metals considered in the present paper $\chi < 0$, we use the following regularized expression of the EEI effective potential (cf. Eq. (13)):

$$U_{q}^{pk} = 2\pi e^2 \frac{\varepsilon q^2}{(\varepsilon q^2 + \chi^2)} - 4 \left( \frac{zm}{3M} \right) - 4 \left( \varepsilon q^2 + \delta p^2 \right) \left( \frac{K_F^2}{q^2 + \sqrt{\chi^2 + \delta p^2}} \right)^2.$$

(25)

This version of regularization allows to obtain an analytical expression for the EEI potential in a coordinate representation, which simplifies the calculation procedure.
V. SUPERCONDUCTIVITY GAP CALCULATIONS FOR PT METALS

Equation (25) is suitable for calculating the superconductivity gap. From the technical point of view, the task can be reduced to determining the energy of bound states of pairs for a potential that is spherically symmetrical in the coordinate representation, whose Fourier transform was defined in Eq. (25).

Considering the validity of the relationship \( \lambda \gg \delta \rho \), it can easily be concluded that in the coordinate representation the first term of the right-hand side of Eq. (25), which describes a screened Coulomb repulsion of electrons, has a form of a delta-shaped function as compared with the second term. Therefore, its existence can be accounted for virtually without affecting the precision of the calculation by introducing the boundary condition of a delta-shaped function as compared with the second term. Therefore, its existence can be virtually discounted without affecting the precision of the calculation by introducing the boundary condition of a delta-shaped function as compared with the second term. Thus, its existence can be accounted for virtually without affecting the precision of the calculation by introducing the boundary condition of a delta-shaped function as compared with the second term.

Having solved Eq. (26) we evaluated the appearing superconductivity gap using Eq. (16) or its generalized form

\[
E_0 = \frac{\gamma_{opt}}{2 \gamma_{el}} V_0^0 S_F^0,
\]

and

\[
S_F/S_F = \gamma_{el} S_F^0 V_F^0.
\]

where \( V_F^0 \) and \( S_F^0 \) are Fermi velocity and Fermi surface area as calculated based on the metal valence, similarly to \( \Omega_0 \). On the other hand, considering the ratio of density of states at Fermi level over its value calculated for an ideal electron gas of the same concentration, we obtain:

\[
\langle V_F \rangle S_F = \frac{\gamma_{opt}}{2} V_F^0 S_F^0,
\]

which provides a solution of the problem as stated.

The only ill-defined parameter of the calculation is the value of \( \bar{\omega} \), which is only limited by the relationships (22). That is why the proposed version of the calculation used this value as fitting parameter. In other terms, the parameter \( \bar{\omega} \) used in the definition of \( \delta \rho \) was chosen such as to make the resulting width of the superconductivity gap coincide with its experimentally known values.

Table I lists both initial parameters \( (z, \gamma_{opt}, \gamma_{el}, \varepsilon, \Delta_0) \) and the calculated values of the parameter \( \bar{\omega} \) for Al, Zn, Pb, and Sn. An analysis of the ratio \( \bar{\omega}/\theta_D \), as provided in the same table indicates that fitting parameters \( \bar{\omega} \) have the same order of magnitude as the Debye temperature \( \theta_D \) in full accord with Eq. (21). It should be noted here that the initial data of the calculations had a fairly wide variation range: \( (M^{(pb)}/M^{(ai)})^2 \approx 60 \), \( \rho^{(pb)}/\rho^{(ai)} \approx 7 \), \( \Delta_0^{(pb)}/\Delta_0^{(z)} \approx 9 \), \( \varepsilon^{(Sn)}/\varepsilon^{(pb)} \approx 4.5 \), \( \theta_D^{(al)}/\theta_D^{(pb)} \approx 4 \). In view of this fact, a physicist would normally consider accidental coincidences out of question, and acknowledge the proposed theory.

This circumstance suggests that a discussion on the approximations introduced within the framework of the approach under development, involving experts in both theoretical physics and mathematics, would be quite useful.

Figs. 1-4 illustrate the calculation results for the considered metals.
TABLE I: The initial and calculated parameters of some simple PT metals. The values of $\rho'$ are given for the temperature $T = 291$ K.

| Metal | $z$ | $10^3\rho'$, Ohm $\cdot$ cm/K | $10^{-5}S$, cm/sec | $\gamma_{opt}$ [14] | $\gamma_{el}$ | $\varepsilon$ [15, 16, 17] | $\Delta_0$, K | $\bar{\omega}$, K | $\theta_D$, K | $\bar{\omega}/\theta_D$ |
|-------|----|------------------|------------------|-----------------|-------------|-----------------|-------------|----------------|--------------|----------------|
| Al    | 3  | 12.2             | 6.4              | 1.25            | 1.48        | 26              | 1.97        | 382            | 394          | 0.97          |
| Zn    | 2  | 22.6             | 4.17             | 0.51            | 0.85        | 30              | 1.75        | 264            | 234          | 1.13          |
| Pb    | 4  | 89.4             | 2.16             | 1.11            | 1.97        | 10              | 15.55       | 28             | 94.5         | 0.30          |
| Sn    | 4  | 50.9             | 3.32             | 1.12            | 1.29        | 45              | 6.25        | 48             | 170          | 0.28          |

FIG. 1: Calculated potential $V(r)$ (lower semiplane) and WF $\psi(r)$ (upper semiplane) for bound state in Al. Values of $V$ are given in degrees Kelvin, $r$ is in Angstroms and $\psi$ in arbitrary units.

FIG. 2: Calculated potential $V(r)$ (lower semiplane) and WF $\psi(r)$ (upper semiplane) for bound state in Zn. Values of $V$ are given in degrees Kelvin, $r$ is in Angstroms and $\psi$ in arbitrary units.

FIG. 3: Calculated potential $V(r)$ (lower semiplane) and WFs $\psi(r)$ (left-hand sides of the curves are in the upper semiplane) for two bound states in Pb. Values of $V$ are given in degrees Kelvin, $r$ is in Angstroms and $\psi$ in arbitrary units.
VI. CONCLUSIONS

The following circumstance attracts attention. The data on the superconductivity gap for the considered metals contradict the natural consequences of the BCS theory. Indeed, according to this theory, the higher is the value of \( \theta_D \) the larger should be \( \Delta_0 \); now comparing, e.g., the Table 1 data for Al and Zn with those for Pb and Sn does not confirm this prediction. In this situation, a study of beryllium, for which \( \theta_D = 1000 \text{ K} \), and the transition temperature \( T_c = 0.03 \text{ K} \), would be of an incontestable interest.

In the framework of the BCS theory, such deviations from its predictions are compensated by considering the value of the so-called Coulomb pseudopotential \( \mu^* \), which is used as a fitting parameter [10]. This is due to impossibility of a satisfactorily precise evaluation of \( \mu^* \) without a comparison with the data on transition temperature or superconductivity gap.

On the other hand, as specified above, the value of \( \bar{\omega} \) can be estimated within the framework of the new theory after a correct processing of the CVC of TJ; therefore, a final version of superconductivity gap calculation for PT metals can be totally free of fitting parameters. From this point of view, the proposed theory appears to be more advantageous than the BCS theory.

We may note as a conclusion that a calculation of the gap value for superconductors produced from semiconductors can be performed without determining the parameter \( \bar{\omega} \) at all. Indeed, assuming that the frequency of electron transitions induced by a scattering on an ionized impurity is substantially higher that the frequency of EPI-caused spontaneous transitions, the value of \( \delta p \) can be estimated, e.g., based on Hall mobility data. In this case, considering the superconductors obtained from semiconductors could provide the most convincing evidence in favor of our theory.

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APPENDIX A: CALCULATION OF THE EFFECTIVE EEI POTENTIAL IN THE CASE OF COULOMB INTERACTION

Self-consistency equations for the effective EEI potential simplified based on the approximate evaluation of integrals within Fermi sphere [7] for this case can be expressed in the form of:

\[
\begin{align*}
\tilde{U}_{p,q}^{0} & = \frac{2\pi e^2}{\epsilon \pi^2 q^2} \int_{\epsilon \pi q}^{\epsilon \pi q} \tilde{U}_{p,q}^{0} + \frac{e^2 m}{\epsilon \pi^2 q^2} \int \left( \frac{pq}{q} \right) U_{q}^{0} + q \right) \tilde{U}_{p,q}^{0} \nonumber \\
- \frac{e^2 m}{\epsilon \pi^2 q^2} I \left( \frac{ka}{q} - q \right) U_{q}^{0,k} & + \frac{e^2 m}{\epsilon \pi^2 q^2} I \left( \frac{ka}{q} + q \right) U_{k,-q}^{0,k} \\
+ \frac{e^2 m}{\epsilon \pi^2 q^2} I \left( \frac{ka}{q} \right) U_{q}^{0,p+q} & - \frac{e^2 m}{\epsilon \pi^2 q^2} I \left( \frac{pq}{q} + q \right) U_{p+q}^{0} \\
- \frac{e^2 m}{\epsilon \pi^2 q^2} I \left( \frac{ka}{q} - q \right) U_{k}^{0,k-q} & + \frac{e^2 m}{\epsilon \pi^2 q^2} I \left( \frac{ka}{q} - q \right) U_{k,-q}^{0,k-1}.
\end{align*}
\] (A1)
where \( I(x) = \pi \left( K_F^2 - x^2 \right) \ln \left| \frac{K_F^2 - x^2}{K_F^2 + x^2} \right| - 2\pi K_F x \) and the following relationships are satisfied:

\[
\begin{align*}
\hat{U}_{q,k}^{p} &= \hat{U}_{q,-p}, \\
\hat{U}_{q,k}^{p} &= \hat{U}_{q,p-k}, \\
\hat{U}_{q,k} &= \hat{U}_{q,-k}.
\end{align*}
\]  

(A2)

It follows immediately that:

\[
\hat{U}_{q,0} = \frac{2\pi e^2}{\varepsilon q^2 + \lambda^2},
\]  

(A3)

where \( \lambda^2 = 4e^2 m K_F / \pi \).

Henceforth, we restrict ourselves to the case \( p, k \approx K_F \), i.e. that of electron interaction in the vicinity of Fermi surface. Then, considering that \( \varepsilon K_F^2 \gg \lambda^2 \), the equation for \( \hat{U}_{q,0} \) can be simplified omitting a series of terms \( \sim \frac{e^2 \varepsilon K_F^2}{\lambda^2} \).

As a result, it becomes as follows:

\[
\left[ 1 - \frac{m e^2}{\varepsilon q^2} I\left( \frac{pq}{q^2} + \frac{q}{2} \right) \right] \hat{U}_{q,0} = \frac{2\pi e^2}{\varepsilon q^2} + \frac{m e^2}{2\pi q^2} I(q) \hat{U}_{q,0}.
\]  

(A4)

Now take into account that the value \( \langle I'(\frac{pq}{q^2} + \frac{q}{2}) \rangle \) averaged over the angles between the vectors \( p \) and \( q \) is approximately equal to \( -4\pi K_F \) at \( q \to 0 \). Then, simple calculation yields:

\[
\hat{U}_{q,k}^{p} = 2\pi e^2 \frac{\varepsilon q^2}{(\varepsilon q^2 + \lambda^2)^2},
\]  

(A5)

which, on the whole, agrees with the present-day concept of the EEI effective potential, as \( \hat{U}_{q,k}^{p} \sim e^2 / \lambda^2 \) at \( q \sim \lambda / \sqrt{\varepsilon} \).

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