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Electron–Phonon Interaction in Cylindrical Nanostructures

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The superconductivity properties of cylinder with nano cross-section are investigated. In the nearest neighbours approximation, electron Hamiltonian of cylinder decays onto two independent Hamiltonians. One corresponds to electrons which propagate along chains parallel to the axis of cylinder. Second correspond to electrons moving in discs. The electron–phonon interaction Hamiltonians are found and superconductive properties were examined in the frames of BCS approach. It was shown that superconductive temperature in chains is several Kelvins, while in discs it can be higher for two orders of magnitude. It is also shown that magnetic field produced by electron currents in discs is of the order of thousand Tesla, i.e., extremely high.

Keywords: Nano Cross-Section, BCS Approach, Critical Superconductive Temperature, Magnetic Field Produced by Disc Currents.

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1. INTRODUCTION

Cylindrical nanostructures have very intensive production nowadays.[1–3] The most popular are carbon cylinders.[4–5] In these cylinders do not appear electrical currents. The goals of our analysis are metallic cylindrical structures and their superconductive properties.

In cylindrical nanostructres the cross-section is of nano order, while their linear dimension can be of nano order or infinite.

We ad hoc exclude nanocylinders of nano length since the electron waves propagating along short line (short height) are standing waves whose currents are equal to zero (see for example Ref. [6]). If the height of cylindrical structure is macroscopic the electron state are plane waves and then the current propagating along height is different from zero. The superconductive properties of these electrons will be shortly exposed.

Besides the currents propagating in cylindrical axis direction we have cyclic currents which propagate in discs. We shall consider cylinders with nano radius of disc. It is important to note that cyclic invariance in discs[7] gives the possibility to expand electron wave functions over specific linear waves, similar to one dimensional plane waves.

2. ELECTRON–PHONON INTERACTION IN CYLINDRICAL STRUCTURES

Concerning behaviour of electrons in discs it is important to know that all physical characteristics of discs must be cyclically invariant.

The last means that in discs is valid cyclicity condition

$$\Psi_m = \Psi_{m+M+1} \tag{1}$$

where $M+1$ is number of atoms in disc. For our further analysis the cyclicity invariance of plane waves is very important.

For plane wave e^{ikm}, on the basis of formula (1), we obtain $e^{ikm} = e^{ik(m+M+1)}$, wherefrom it follows that $e^{ik(M+1)} = 1$, i.e.,

$$k = \frac{2\pi\lambda}{M+1}; \quad \lambda = 0, \pm 1, \pm 2, \ldots \tag{2}$$

This value of k allows the most simple representation of Kronecker symbol[8]

$$\sum_{m=0}^{M} e^{\pm i2\pi m(k-k')} = (M+1)\delta_{k,k'} \tag{3}$$

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or

$$\sum_{k=0}^{M} e^{\pm i(2\pi/(M+1))k(m-m')} = (M+1)\delta_{m,m'} \tag{4}$$

The formulae (3) and (4) allow us to expand the physical characteristics of disc over plane waves.

Generally speaking we can write the Hamiltonian of electron subsystem of the cylinder (it was pointed out that we shall analyze the disc of infinite length) in the following form:

$$\begin{aligned} H = \sum_{n}\sum_{m=0}^{M}[&(W_{n,m;n+1,m} + W_{n,m;n-1,m} + W_{n,m;n,m+1} \\ &+ W_{n,m;n,m-1})F^{+}_{n,m}F_{n,m} - F^{+}_{n,m}(W_{n,m;n+1,m}F_{n+1,m} \\ &+ W_{n,m;n-1,m}F_{n-1,m} + W_{n,m;n,m+1}F_{n,m+1} \\ &+ W_{n,m;n,m-1}F_{n,m-1})] \end{aligned} \tag{5}$$

The quoted Hamiltonian (5) is simplified Hubbard Hamiltonian[9, 10] taken in the nearest neighbours approximation. Operator $F^{+}_{n,m}$ create m-th electron of n-th disc.

We assume that the lattice constant of the chains normal to discs is a while the lattice constant in the discs is b and it is the length of the chord connecting in the nearest neighbours discs. In the nearest neighbours approximation a and b are minimal distances between atoms. The length $\sqrt{a^2+b^2}$ is higher than a and b, and therefore the atoms and these distances are not within the frames of the nearest neighbour approximation. Consequently, in the nearest neighbours approximation empty cylinder is the set of two independent subsystems.

One of them makes identical infinite chains parallel with z axis of cylinder, i.e., parallel with its height. The second subsystem makes discs with circular currents.

On the basis of upper reasoning we shall analyze the simplified electronic Hamiltonian H_h, which is given by:

$$H_h = \sum_{n}[2X\alpha^{+}_{n}\alpha_n - X\alpha^{+}_{n}(\alpha_{n+1} + \alpha_{n-1})] \tag{6}$$

and the Hamiltonian of disc electrons

$$H_c = \sum_{m=1}^{M}[2Y\beta^{+}_{m}\beta_m - Y\beta^{+}_{m}(\beta_{m+1} + \beta_{m-1})] \tag{7}$$

Operators α^{+}_{n} create electrons in the chain parallel with the cylinder axis and operators β^{+}_{n} create electrons in discs.

Introduction of two electron Hamiltonian cylinder requires introduction of two corresponding Hamiltonians of mechanical oscillations. Those are:

$$H_{ph} = \frac{1}{2M}\sum_{n} p^2_{hn} + \frac{C_h}{4}\sum_{n}[(\xi_{n+1} - \xi_n)^2 + (\xi_{n-1} - \xi_n)^2] \tag{8}$$

and

$$H_{pc} = \frac{1}{2M}\sum_{m=0}^{M} p^2_{cn} + \frac{C_c}{4}\sum_{n}[(\xi_{n+1} - \xi_n)^2 + (\xi_{n-1} - \xi_n)^2] \tag{9}$$

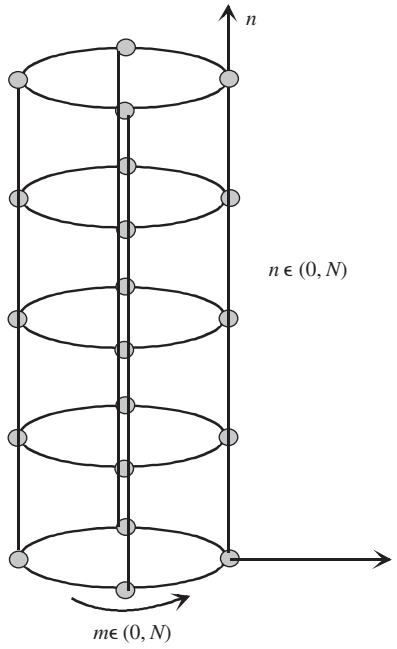

Fig. 1. Distribution of electrons in nano cylinder of infinite length.

The formula (8) represents mechanical oscillations in chains parallel with z axis while (9) represents phonons in discs.

We shall first define Hamiltonian of electron–phonon interaction in infinite chains.

In the frozen crystal the distance between atoms at positions n and n' is the modulus $|n'-n|a$. Since the atoms are on line parallel to z-axis for positions of atoms will not be used vector notations. In heated chain $na \to na + \xi(na)$ and $n'a \to n'a + \xi(n'a)$. Here must be pointed out that displacements ξ have not to be parallel to z-axis, so that, strictly speaking, for values ξ must be used vector notation. Assuming, approximately, that displacements change only inter-distance between atoms we omitted vector notation for ξ.[11]

On the basis of the upper explanations we can write the distance

$$\begin{aligned} d_{n',n} &= (n'-n)a + \xi(n') - \xi(n) \\ &= (n'-n)a + \xi[n + (n'-n)] - \xi(n) \end{aligned} \tag{10}$$

For the nearest neighbours the displacement $\xi[n+(n'-n)]$ can be expanded as follows:

$$\xi[n+(n'-n)] = \xi(n+1) \approx \xi(n) + \frac{\partial\xi(n)}{\partial n} = \xi + \frac{\partial\xi}{\partial n} \tag{11}$$

Using this formula and formula (10) written for the nearest neighbours we have the distance d for the nearest neighbours

$$d_{n+1,n} = a + \frac{\partial\xi}{\partial n} \tag{12}$$

This formula is valid for $n' > n$. For $n' < n$ is

$$d_{n-1,n} = -a - \frac{\partial \xi}{\partial n} \tag{13}$$

In both cases the modulus of distance is given by

$$|d| = a + \frac{\partial \xi}{\partial n} \tag{14}$$

The interaction between the nearest neighbours of heated crystal

$$\tilde{X}(a) = X\left(a + \frac{\partial \xi}{\partial n}\right) \approx X + \frac{\partial \xi}{\partial n}\frac{\partial \xi}{\partial a} \tag{15}$$

The electronic Hamiltonian of frozen chain is given by the formula (6). For heated chain in formula (6) X has to be substituted with $\tilde{X}$ from (15). In such a way the Hamiltonian of heated chain is sum of Hamiltonian (6) and the Hamiltonian

$$H_{ep} = \frac{\partial X}{\partial a}\sum_n \frac{\partial \xi}{\partial n}[2\alpha_n^+\alpha_n - \alpha_n^+(\alpha_{n+1} + \alpha_{n-1})] \tag{16}$$

which represents interaction between electrons and phonons.

The Hamiltonians (6), (8) and (16) have to be written in momentum representation. By means of formulas

$$\alpha_n = \frac{1}{\sqrt{N}}\sum_k \alpha_k e^{ikan} \tag{17}$$

and

$$\xi_n = \frac{1}{\sqrt{N}}\sum_q \sqrt{\frac{\hbar}{2M\omega_q}}\left(b_q e^{iqan} + b_q^+ e^{-iqan}\right) \tag{18}$$

where b_q and b_q^+ are Bose operators creating and annihilating phonons, we obtain

$$H_{he} = \sum_k E_{kh}\alpha_k^+\alpha_k \tag{19}$$

where

$$E_{kh} = 4X\sin^2\frac{ak}{2}; \quad ak = \frac{2\pi\nu}{M+1}, \quad \nu = 0, 1, 2, \ldots \tag{20}$$

and

$$H_{ph} = \sum_q \varepsilon_{qh}\left(b_q^+ b_q + \frac{1}{2}\right) \tag{21}$$

where

$$\varepsilon_{qh} = \hbar\omega_{qh} = 2\sqrt{\frac{C_h}{M}}\sin\frac{aq}{2} \tag{22}$$

The Hamiltonian of the electron–phonon interaction is:

$$H_{eph} = \frac{i}{\sqrt{N}}\sum_{k,q}\frac{\partial X}{\partial a}\sqrt{\frac{8\hbar}{M\omega_{k-q}}}a(k-q) \times \sin^2\frac{aq}{2}\left(\alpha_k^+\alpha_q b_{k-q} - \alpha_q^+\alpha_k b_{k-q}^+\right) \tag{23}$$

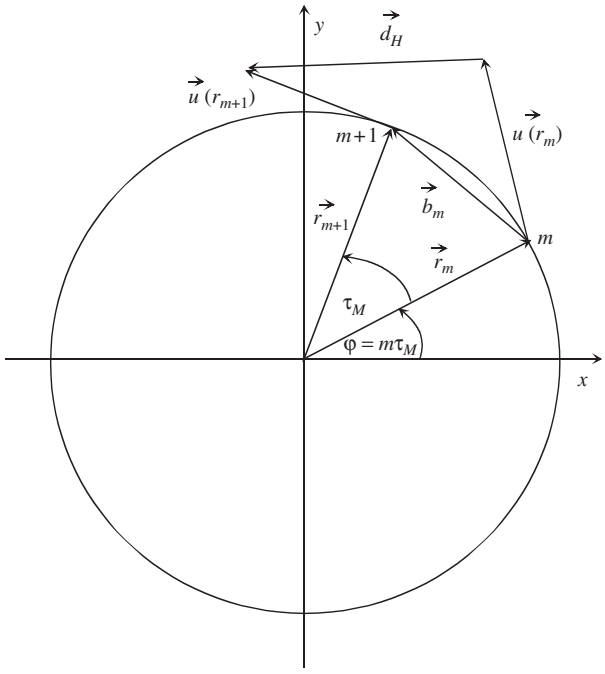

Fig. 2. Distances between neighbours atoms in frozen and heated crystal.

Now we shall look for the Hamiltonian of electron–phonon interaction in discs. The atoms in disc are located at the vertices of regular polygon. The distance between the nearest neighbours is a modulus of chord vector $\vec{b}_m$. The said is presented on Figure 2.

In the frozen crystal radius vectors $\vec{r}_m$ and $\vec{r}_{m+1}$ of atoms at the positions m and $m+1$ respectively are given by:

$$\begin{aligned}\vec{r}_m &= \vec{i}R\cos\tau_M + \vec{j}R\sin\tau_M \\ &= \vec{i}R\cos m\tau_M + \vec{j}R\sin m\tau_M \\ \vec{r}_{m+1} &= \vec{i}R\cos\tau_M + \vec{j}R\sin\tau_M \\ &= \vec{i}R\cos(m+1)\tau_M + \vec{j}R\sin(m+1)\tau_M\end{aligned} \tag{24}$$

where R is radius of disc and τ_M is central angle given by

$$\tau_M = \frac{2\pi}{M+1} \tag{25}$$

The chord vector $\vec{b}_m$ is:

$$\begin{aligned}\vec{b}_m &= \vec{r}_{m+1} - \vec{r}_m \\ &= 2R\sin\frac{\tau_M}{2}\left[-\vec{i}\sin\left(m+\frac{1}{2}\right)\tau_M + \vec{j}\cos\left(m+\frac{1}{2}\right)\tau_M\right] \\ &= \vec{i}b_{mx} + \vec{j}b_{my}\end{aligned} \tag{26}$$

where

$$\begin{aligned}b_{mx} &= -b_M\sin\left(m+\frac{1}{2}\right)\tau_M \\ b_{my} &= b_M\cos\left(m+\frac{1}{2}\right)\tau_M\end{aligned} \tag{27}$$

The value b_M is intensity of chord vector $\vec{b}_m$. It is given by:

$$b_m = |\vec{b}_m| = 2R \sin \frac{\tau_M}{2} \tag{28}$$

and the interaction between frozen atoms m and $m+1$ is the function of b_M:

$$Y_F \equiv Y = Y(b_M) \tag{29}$$

In heated crystal $\vec{r}_m \to \vec{r}_m + \vec{\xi}(\vec{r}_m)$ and $\vec{r}_{m+1} \to \vec{r}_{m+1} + \vec{\xi}(\vec{r}_{m+1})$. It means that the distance between atoms m and $m+1$ in heated crystal is given as

$$|\vec{d}_H| = |\vec{r}_{m+1} - \vec{r}_m + \vec{\xi}(\vec{r}_{m+1}) - \vec{\xi}(\vec{r}_m)| \tag{30}$$

The value $|\vec{d}_H|$ can be calculated by means of cosine theorem applied to the triangle on Figure 3, i.e., it is given by:

$$|\vec{d}_H| = \sqrt{|\vec{r}_{m+1} - \vec{r}_m|^2 + |\vec{\xi}(\vec{r}_{m+1}) - \vec{\xi}(\vec{r}_m)|^2 - 2(\vec{r}_{m+1} - \vec{r}_m) \cdot (\vec{\xi}(\vec{r}_{m+1}) - \vec{\xi}(\vec{r}_m))} \tag{31}$$

Since $|\vec{\xi}|^2 \ll |\vec{b}_M|^2$ second term in square root can be neglected. So we obtain

$$|\vec{d}_H| = \sqrt{b_M^2 - 2\{b_{mx}[\xi_x(\vec{r}_{m+1}) - \xi_x(\vec{r}_m)] + b_{my}[\xi_y(\vec{r}_{m+1}) - \xi_y(\vec{r}_m)]\}} \tag{32}$$

Now can be found approximate expressions for components $\xi_s(\vec{r}_{m+1})$, where $s = x, y$.

We can write

$$\vec{\xi}(\vec{r}_{m+1}) = \vec{\xi}(\vec{r}_m + \vec{b}_m) \tag{33}$$

and consequently

$$\xi_s(\vec{r}_{m+1}) = \xi_s(\vec{r}_m + \vec{b}_m) \approx \xi_s(x_{m+1}, y_{m+1}) \approx \xi_s(x_m, y_m) + b_{mx}\frac{\partial \xi_s}{\partial x} + b_{my}\frac{\partial \xi_s}{\partial y} \tag{34}$$

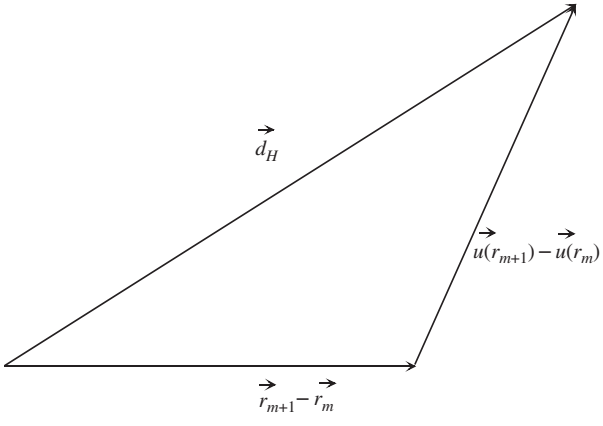

Fig. 3. Distance between neighbour atoms in heated crystal.

On the basis of the formulas (24) radius vectors and displacements are expressed in polar coordinates R and τ_M. It means that in formula (34) me must go over from Descartes coordinates to the polar ones.

$$\begin{aligned} x &= \rho\cos\varphi \quad y = \rho\sin\varphi \\ \frac{\partial}{\partial x} &= \cos\varphi\frac{\partial}{\partial \rho} - \frac{\sin\varphi}{\rho}\frac{\partial}{\partial \varphi} \\ \frac{\partial}{\partial y} &= \sin\varphi\frac{\partial}{\partial \rho} + \frac{\cos\varphi}{\rho}\frac{\partial}{\partial \varphi} \end{aligned} \tag{35}$$

In the considered case $R = \rho = \text{const}$, i.e., $\partial/\partial\rho \to \partial/\partial R = 0$, while $\varphi = \tau_M$.

It means (see formulae (27)) that (34) goes over to

$$\begin{aligned} \xi_s(\vec{r}_{m+1}) &= \xi_s(\vec{r}_m) + \frac{b_M}{R\tau_M}\left[\sin m\tau_M \sin\left(m+\frac{1}{2}\right)\tau_M \right. \\ &\left. + \cos m\tau_M \cos\left(m+\frac{1}{2}\right)\tau_M\right]\frac{\partial \xi_s}{\partial m} \\ &= \frac{\partial \xi_s}{\partial m}\frac{b_M}{R\tau_M}\cos\frac{\tau_M}{2} = \xi_s(\vec{r}_m) + \frac{\sin\tau_M}{\tau_M}\frac{\partial \xi_s}{\partial m} \end{aligned} \tag{36}$$

After substitution (27) and (36) into (32) we obtain

$$|\vec{d}_H| = \sqrt{b_m^2 + 2b_m\frac{\sin\tau_M}{\tau_M}\left[\frac{\partial \xi_x}{\partial m}\sin\left(m+\frac{1}{2}\right)\tau_M - \frac{\partial \xi_y}{\partial m}\cos\left(m+\frac{1}{2}\right)\tau_M\right]}$$

and this after expanding of square root into series becomes:

$$\begin{aligned} |\vec{d}_H| = b_m + \frac{\sin\tau_M}{\tau_M}\left[\frac{\partial \xi_x}{\partial m}\sin\left(m+\frac{1}{2}\right)\tau_M \right. \\ \left. - \frac{\partial \xi_y}{\partial m}\cos\left(m+\frac{1}{2}\right)\tau_M\right] \end{aligned} \tag{37}$$

In the last formula we shall use the following simplification

$$\xi_x = \xi_y = \frac{\xi}{\sqrt{2}}; \quad \xi = |\vec{\xi}| \tag{38}$$

The formula (38) goes over to

$$|\vec{d}_H| = b_m + \theta_m\frac{\sin\tau_M}{\tau_M}\frac{\partial \xi}{\partial m} \tag{39}$$

where

$$\theta_m = \frac{\sin\left(m+\frac{1}{2}\right)\tau_M - \cos\left(m+\frac{1}{2}\right)\tau_M}{\sqrt{2}} \tag{40}$$

Further analysis of electron–phonon interaction in disc and analysis of superconductivity effect connected with the formula (39) can be done, but it is very complicated, since it leads to momentum non-conservation in discs. This is not strange since cyclic invariance not obligely ensures

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translational invariance. Besides some qualitatively new effects can appear. All mentioned requires special investigation and therefore it will be subject of our future works. Here we introduce additional simplification substituting function θ_m by square root from average of its square, i.e.,

$$\theta_m \approx \sqrt{\frac{1}{M+1}\sum_{m=0}^{M}\theta_m^2} = \frac{1}{\sqrt{2}} \tag{41}$$

After this approximation the inter-atomic distance of heated crystal becomes:

$$|\vec{d}_H| = b_M + \frac{1}{\sqrt{2}}\frac{\sin\tau_M}{\tau_M}\frac{\partial\xi}{\partial m} \tag{42}$$

The Hamiltonian of heated disc is given by:

$$H_{eH} = \sum_{m=1}^{M}[2\tilde{Y}\beta_m^+\beta_m - \tilde{Y}\beta_m^+(\beta_{m+1}+\beta_{m-1})] \tag{43}$$

where

$$\tilde{Y} = Y\left(b_m + \frac{1}{\sqrt{2}}\frac{\sin\tau_M}{\tau_M}\frac{\partial\xi}{\partial m}\right) \approx Y(b_m) + \frac{1}{\sqrt{2}}\frac{\sin\tau_M}{\tau_M}\frac{\partial\xi}{\partial m}\frac{\partial Y}{\partial b_M} \tag{44}$$

After substitution (44) into (43) we obtain

$$H_{cH} = H_c + H_{ep} \tag{45}$$

where H_c is given by the formula (7) and

$$H_{ep} = \frac{1}{\sqrt{2}}\frac{\partial Y}{\partial b_m}\frac{\sin\tau_M}{\tau_M}\sum_{m=0}^{M}\frac{\partial\xi}{\partial m}[2\beta_m^+\beta_m - \beta_m^+(\beta_{m+1}+\beta_{m-1})] \tag{46}$$

The total Hamiltonian of disc has to be written in momentum representation.

Using Fourier transformation

$$\beta_m = \frac{1}{\sqrt{M+1}}\sum_{\mu=0}^{M} e^{(2\pi\mu/(M+1))m}\beta_\mu \tag{47}$$

we reduce Hamiltonian of electron subsystem of disc into

$$H_{ec} = \sum_{\mu=0}^{M} E_{\mu c}\beta_\mu^+\beta_\mu \tag{48}$$

where

$$E_{\mu c} = 4Y\sin^2\frac{\pi\mu}{M+1} \tag{49}$$

By means of the transformation for displacements

$$\xi_m = \sum_{\lambda=0}^{M}\sqrt{\frac{\hbar}{2M(M+1)\omega_\lambda}}\left(b_\lambda e^{i(2\pi\lambda/(M+1))m} + b_\lambda^+ e^{-i(2\pi\lambda/(M+1))m}\right) \tag{50}$$

we obtain the phonon Hamiltonian of disc

$$H_{pc} = \sum_{\lambda=0}^{M} E_{\lambda c}\left(b_\lambda^+ b_\lambda + \frac{1}{2}\right) \tag{51}$$

where

$$E_{\lambda c} = 2\hbar\sqrt{\frac{C_c}{M}}\sin\frac{\pi\lambda}{M+1} \tag{52}$$

Taking into account transformations (47) and (50) we obtain the expression for Hamiltonian of electron–phonon interaction in disc:

$$H_{epc} = 2i\frac{\partial Y}{\partial b_m}\sin\tau_M\sqrt{\frac{\hbar}{M(M+1)}}\sum_{\mu,\nu=0}^{M}\frac{\mu-\nu}{\sqrt{\omega_{\mu-\nu}}} \times \sin^2\frac{\tau_M\nu}{2}(\beta_\mu^+\beta_\nu b_{\mu-\nu} - \beta_\nu^+\beta_\mu b_{\mu-\nu}^+) \tag{53}$$

Using the formulae (19), (21) and (23) we shall analyze superconductive properties of electrons propagating along chains which are parallel with the height of cylinder. The formulae (48), (51) and (53) will be used in analysis of superconductive properties of electrons in discs.

In both cases will be used BCS approach[12–13] and Bogolyubov's unitary transformations[11, 14] from electron operators to operators of Cooper's pairs.

3. BCS APPROACH IN STUDY OF CYLINDER

BCS approach is well known in analysis of superconductivity properties. We shall quote here only basic steps of this approach. Derivations will be reduced to minimum since they can be found even in textbooks.[16–18]

The main idea of BCS approach is that electron–phonon interaction in narrow layer enveloping Fermi surface leads to attractive electron–electron interaction which bind electrons in pairs (Cooper's pairs).[19–20] These pairs form condensate near Fermi surface which causes superfluid moving of pairs.[9]

The main steps in BCS approach are unitary transformation of Hamiltonian containing electrons, phonons and their interaction which leads to the Hamiltonian with attractive electron–electron interaction. The following step is Bogolyubov's transformation from electrons to pairs. These transformations give energy spectrum of pairs. This spectrum contains constant superconductive gap whose magnitude defines critical conductive temperature.

The described procedure will be applied to the Hamiltonian in definite chains parallel to the axis of cylinder. This Hamiltonian was found in previous section but for clearness we shall repeat its form:

$$H_h = H_{eh} + H_{ph} + H_{eph} \tag{54}$$

where electronic Hamiltonian is given by:

$$H_{eh}(k) = \sum_k E_{kh}\alpha_k^+\alpha_k \tag{55}$$

The electron energy is as follows:

$$E_{kh} = 4X\sin^2\frac{ak}{2} \tag{56}$$

The phonon Hamiltonian is given by:

$$H_{ph}(q) = \sum_q \varepsilon_{qh}\left(b_q^+ b_q + \frac{1}{2}\right) \tag{57}$$

where phonon energies are:

$$\varepsilon_{qh} = \hbar\omega_{qh} = 2\sqrt{\frac{C_h}{M}}\sin\frac{aq}{2} \tag{58}$$

$$H_{eph} = \frac{1}{\sqrt{N}}\sum_{k,q}(J_{k,q}\alpha_k^+\alpha_q b_{k-q} + J_{k,q}^*\alpha_q^+\alpha_k b_{k-q}^+) \tag{59}$$

where

$$J_{k,q} = i\frac{\partial X}{\partial a}\sqrt{\frac{8\hbar}{M\omega_{k-q}}}a(k-q)\sin^2\frac{aq}{2} \tag{60}$$

Before Frölich's unitary transformations of Hamiltonian (54),[22,23] Hamiltonian of electron's subsystem must be written in chemical potential representation, i.e., we must take that $E_{eh} \to E_{eh} - \mu_0$, where μ_0 is chemical potential. It will be taken as maximal value of E_{eh} of boundary of the first Brillouin zone, i.e.,

$$\mu_0 = (E_{eh})_{\max} = 4X \tag{61}$$

Besides, electron Hamiltonian is used in quadratic approximation for sine function. It means that in further Hamiltonian of electron subsystem will be written in the form:

$$E_{eh}(k) = Xa^2(k^2 - k_F^2) \equiv \rho_k \tag{62}$$

where

$$k_F = \frac{2}{a} \tag{63}$$

Frölich's transformation is transition from Hamiltonian (54) to the equivalent Hamiltonian taken in approximation

$$H_h = e^{\hat{S}}H_h e^{-\hat{S}} \approx H_h + [\hat{S}, H_h] \tag{64}$$

where $\hat{S}$ is antihermitian operator $\hat{S} = -\hat{S}^+$. Operator $\hat{S}$ can be represented as $\hat{S} = \hat{P} - \hat{P}^+$, so that (64) can be written as

$$H_h = H_h + [\hat{P}, H_h] + [\hat{P}^+, H_h] \tag{65}$$

The operator $\hat{P}$ has to be chosen in such a form to cancel all third order terms from (65). The obtained result has to be averaged over phonon vacuum.

The final result of this described procedure is electron Hamiltonian with attractive electron–electron interaction:

$$H = \sum_k Xa^2(k^2 - k_F^2)\alpha_k^+\alpha_k - \frac{1}{N}\sum_{k,q}\frac{2|J_{k-q}|^2}{E_{eh}(q) - E_h(k) + \varepsilon_{ph}(k-q)}\alpha_k^+\alpha_q^+\alpha_q\alpha_k \tag{66}$$

Electron–electron interaction will be estimated by taking average value of the function figuring in the second term of formula (66). Averaging will be made over k and q. Besides, taking into account that active electrons have momenta close to k_F, we shall take that $E_{eh}(q) - E_h(k) \approx 0$. It means that we have to find the average of the function:

$$W(k,q) = 8\frac{1}{C_h}\left(\frac{\partial X}{\partial a}\right)^2\frac{a^2(k-q)^2}{\sin^2(a(k-q)/2)}\sin^4\frac{aq}{2} \tag{67}$$

Introducing new variable $a(k-q) = \gamma$, $\gamma \in (-2k_F, 2k_F)$ and $aq = p$, $p \in (-k_F, k_F)$ we obtain for average value:

$$\langle W\rangle = \frac{1}{8k_F}\int_{-2k_F}^{2k_f} d\gamma \int_{-k_F}^{k_f} 8\frac{1}{C_h}\left(\frac{\partial X}{\partial a}\right)^2\frac{\gamma^2}{\sin^2(\gamma/2)}\sin^4\frac{p}{2}\,dp = \frac{16a^4k_F^4}{5}\frac{1}{C_h}\left(\frac{\partial X}{\partial a}\right)^2 \tag{68}$$

Taking into account (68) we can write Hamiltonian (66) in the form

$$H = \sum_k Xa^2(k^2 - k_F^2)\alpha_k^+\alpha_k - \frac{1}{N}\langle W\rangle\sum_{k,q}\alpha_k^+\alpha_q^+\alpha_q\alpha_k \tag{69}$$

This Hamiltonian given in BCS theory was unitary transformed by Bogolyubov. The Bogolyubov transformations connecting electron operators α with pairs operators η are the following:

$$\begin{gathered}\alpha_k = u(\vec{k})\eta_{1k} + v(\vec{k})\eta_{2k}^+; \quad \alpha_k^+ = u(\vec{k})\eta_{1k}^+ + v(\vec{k})\eta_{2k} \\ \alpha_{-k} = u_k\eta_{2k} - v_k\eta_{1k}^+; \quad \alpha_{-k}^+ = u_k\eta_{2k}^+ - v_k\eta_{1k} \\ u^2 + v^2 = 1\end{gathered} \tag{70}$$

The transformation functions are given by:

$$\begin{gathered}u_k^2 = \tfrac{1}{2}\left(1 + \frac{\rho_k}{\sqrt{\Delta_k^2 + \rho_k^2}}\right); \quad v_k^2 = \frac{1}{2}\left(1 - \frac{\rho_k}{\sqrt{\Delta_k^2 + \rho_k^2}}\right) \\ u_k v_k = \frac{1}{2}\frac{\Delta_k}{\sqrt{\Delta_k^2 + \rho_k^2}}\end{gathered} \tag{71}$$

The energy of Cooper's pairs is given by:

$$E = \sqrt{\Delta_k^2 + \rho_k^2} \tag{72}$$

The gap Δ_k is determined by the formula

$$\Delta_k = \frac{1}{2}\frac{\langle W\rangle}{N}\sum_q\frac{\Delta_q}{\sqrt{\Delta_q^2 + \rho_q^2}} \tag{73}$$

The usual approach for finding Δ_k is based on the approximation that Δ_k does not depend on wave vector. From sum we go over to the integral from $k_F - k_G$ to $k_F + k_G$, where $k_F \ll k_G$. It allows approximation:

$$k^2 - k_F^2 = (k + k_F)(k - k_F) \approx 2k_F(k - k_F) \tag{74}$$

The above assumptions and approximations translate (73) into

$$1 = \frac{a\langle W\rangle}{4\pi}\int_{k_F-k_G}^{k_F+k_G}\frac{dk}{\sqrt{\Delta^2+4X^2a^4k_F^2(k-k_F)^2}} \tag{75}$$

After substitution $2Xa^2k_F(k-k_F)=Z$ integral can be easily solved as well as the Eq. (75).

The superconductive gap is given by the following expression:

$$\Delta = \frac{2Xa^2k_Fk_G}{\sinh\left[\frac{5}{4}\frac{XC_h}{(ak_F)^3}\left(\frac{\partial X}{\partial a}\right)^{-2}\right]} \tag{76}$$

If we assume that ion–ion interaction is of Coulomb type than formula (76) gives gap of the order $10k_B$. In other words, along chain parallel to z axis, can be expected superconductivity up to 10 K.

The BCS approach which shortly was described at the beginning of this section will be now applied to the Hamiltonian of discs. Disc Hamiltonian was found at the previous section and it is of the form:

$$H_c = H_{ec} + H_{pc} + H_{epc} \tag{77}$$

The Hamiltonian of electron subsystem is given by:

$$H_{ec} = \sum_{\mu=0}^{M} E_{\mu c}\beta_\mu^+\beta_\mu \tag{78}$$

where

$$E_{ec}(\mu) = 4Y\sin^2\frac{\pi\mu}{M+1} \tag{79}$$

The Hamiltonian of phonon subsystem is given by:

$$H_{pc} = \sum_{\lambda=0}^{M} E_{\lambda c}\left(b_\lambda^+b_\lambda+\frac{1}{2}\right) \tag{80}$$

where

$$E_{pc}(\lambda) = 2\hbar\sqrt{\frac{C_c}{M}}\sin\frac{\pi\lambda}{M+1} \tag{81}$$

The Hamiltonian of electron–phonon interaction is:

$$H_{epc} = \frac{1}{\sqrt{M+1}}\sum_{\mu,\nu=0}^{M}(D_{\mu,\nu}\beta_\mu^+\beta_\nu b_{\mu-\nu}+D_{\mu,\nu}^*\beta_\nu^+\beta_\mu b_{\mu-\nu}^+) \tag{82}$$

where

$$D_{\mu,\nu} = 2i\frac{\partial Y}{\partial b_M}\sin\tau_M\sqrt{\frac{\hbar}{M}}\frac{\mu-\nu}{\sqrt{\omega_{\mu-\nu}}}\sin^2\frac{\tau_M\nu}{2} \tag{83}$$

Before going over to equivalent Hamiltonian by means of Frölich transformation we shall determine energy of electrons in chemical potential representation.[24] It means that we shall take:

$$E_{ec}(\mu)\to E_{ec}(\mu)-\mu_0 = 4Y\sin^2\frac{\tau_M\mu}{2}-4Y \tag{84}$$

The chemical potential denoted with μ_0 is equal to $4Y$. In the BCS approach electron energy is used in quadratic approximation, i.e., in (84) has to be taken $\sin^2(\tau_M\mu/2)\approx(\tau_M^2\mu^2/4)=\pi^2\mu^2/(M+1)^2$. In this approximation chemical potential is given by:

$$\mu_0 = 4Y\frac{\pi^2\mu_F^2}{(M+1)^2} = 4Y \tag{85}$$

wherefrom it follows that:

$$\mu_F^2 = \frac{(M+1)^2}{\pi^2} \tag{86}$$

On the basis of the quoted formulas we finally have

$$\tilde{E}_{ec}(\mu) = 4Y\frac{\pi^2}{(M+1)^2}(\mu^2-\mu_F^2) = Y\tau_M^2(\mu^2-\mu_F^2) \tag{87}$$

From the Hamiltonian H_c, given by the formula (77) we go over to the equivalent Hamiltonian

$$H_{eq} = e^{\hat{S}}H_ce^{-\hat{S}} = H_c+[\hat{S},H_c] \tag{88}$$

where $\hat{S}$ is antihermitian operator

$$\hat{S}^+ = -\hat{S} \tag{89}$$

If we take that

$$\hat{S} = \hat{P}-\hat{P}^+ \tag{90}$$

the formula (88) becomes:

$$H_{eq} = H_c+[\hat{P},H_c]+[\hat{P},H_c]^+ \tag{91}$$

Operator $\hat{P}$ will be taken in the form:

$$\hat{P} = \sum_{\mu,\nu=0}^{M}\Psi_{\mu,\nu}\beta_\mu^+\beta_\nu b_{\mu-\nu} \tag{92}$$

The function $\Psi_{\mu,\nu}$ has to be determined so that from (91) disappear third order forms of operators. Besides, (88) has to be averaged over phonon vacuum.

The result of this procedure is Hamiltonian with attractive electron–electron interactions in the narrow domains about Fermi momentum $p_F=\hbar k_F$.

This Hamiltonian is of the form:

$$\begin{aligned}H &= \sum_{\mu=0}^{M}\tilde{E}_{ec}(\mu)\beta_\mu^+\beta_\mu \\ &\quad -\frac{2}{M+1}\sum_{\mu,\nu}^{M}\frac{|D_{\mu,\nu}|^2}{\tilde{E}_{ec}(\nu)-\tilde{E}_{ec}(\mu)+E_{pc}(\mu-\nu)}\beta_\mu^+\beta_\nu(\beta_\mu^+\beta_\nu)^+ \\ &= \sum_{\mu=0}^{M}\tilde{E}_{ec}(\mu)\beta_\mu^+\beta_\mu \\ &\quad -\frac{2}{M+1}\sum_{\mu,\nu}^{M}\frac{|D_{\mu,\nu}|^2}{\tilde{E}_{ec}(\nu)-\tilde{E}_{ec}(\mu)+E_{pc}(\mu-\nu)}|\beta_\mu^+\beta_\nu|^2\end{aligned} \tag{93}$$

From this formula is clear that near boundary of Fermi domain, where $\tilde{E}_{ec}(\nu)-\tilde{E}_{ec}(\mu)\approx 0$, the electron–electron interaction (i.e., second term in (93)) is really attractive.

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Further analysis containing Bogolyubov's transformation from electron operators to Cooper pairs operators will be omitted since it was exposed in the first part of this section. The crucial difference of the usual analysis which includes calculations in continual variables, appears in the formula defining gap. In considered case variables are discrete and they belong to the set which has ten elements, maximally. It means that in considered case of disc is senseless introducing of narrow momentum layer enveloping Fermi boundary. Instead of narrow layer we shall take Fermi boundary only ($\mu = \mu_F$). It means that standard formula defining the gap:

$$\Delta_q = \frac{1}{2}\frac{\langle W\rangle}{N}\sum_q \frac{\Delta_q}{\sqrt{\Delta_q^2+\rho_q^2}} \tag{94}$$

where $q \in (q_F - q_G, q_F + q_G)$ with $q_G \ll q_F$, in the case of disc, where $\tilde{E}_{ec}(\mu) \to \tilde{E}_{ec}(\mu_F)$, will be substituted with:

$$\Delta = \frac{1}{M+1}\left\langle \frac{|D_{\mu,\nu}|^2}{E_{pc}(\mu-\nu)}\right\rangle \tag{95}$$

where

$$\left\langle \frac{|D_{\mu,\nu}|^2}{E_{pc}(\mu-\nu)}\right\rangle = \frac{1}{(M+1)^2}\sum_{\alpha,\beta=0}^{M}\frac{|D_{\alpha,\beta}|^2}{E_{pc}(\alpha-\beta)} = \frac{1}{C_c}f(M)\left(\frac{\partial Y}{\partial b_m}\right)^2\sin^2\tau_M \tag{96}$$

The function $f(M)$ appearing in (99) is given by:

$$f(M) = \frac{1}{(M+1)^2}\sum_{\alpha=0}^{M}\sum_{\beta=0}^{M}\frac{(\alpha-\beta)^2}{\sin^2(\tau_M/2)(\alpha-\beta)}\sin^4\frac{\tau_M\beta}{2} \tag{97}$$

Substituting (96) into (95) we obtain the following formula for gap:

$$\Delta = \frac{f(M)}{M+1}\frac{1}{C_c}\left(\frac{\partial Y}{\partial b_M}\right)^2\sin^2\frac{2\pi}{M+1} \tag{98}$$

Assuming ion–ion interaction of Coulomb's type we can write

$$\left(\frac{\partial Y}{\partial b_M}\right)^2 = \frac{Z^2(9\cdot 10^9)^2(1.6\cdot 10^{-19})^4}{b_M^4}\left(\frac{\mathrm{J}}{\mathrm{m}}\right)^2 \tag{99}$$

where Z is valency.

The Hook's constant is given by

$$C_c = \frac{1.67\cdot 10^{-27}Av_0^2\cdot 10^6}{b_M^2}\frac{\mathrm{J}}{\mathrm{m}^2} \tag{100}$$

where $1.67\cdot 10^{-27}\cdot A$ is atomic mass and $v_0\cdot 10^3$ is velocity of sound.

The gap Δ will be presented as $\Delta = k_B T_\Delta$ J, where $k_B = 1.38\cdot 10^{-23}$ J/K is Boltzmann's constant and T_Δ is absolute temperature of superconductivity.

Combining (99)–(100) and $\Delta = k_B T_\Delta$ we obtain the following formula:

$$b_M^2 = 2.3\cdot 10^{-12}\frac{Z^2 f(M)}{Av_0^2 T_\Delta}\sin^2\frac{2\pi}{M+1} \tag{101}$$

It is seen from the last formula that superconductive critical temperature T_Δ is inverse proportional to the square of disc lattice constant.

As an example we consider lead disc, where $Z = 4$, $A = 207$, and $v_0 = 3$. The superconductivity temperature T_Δ is taken to be $T_\Delta = 100$ K. The value $f(M)$ was calculated by the formula (97) for three atoms in disc and it was found that $f(2) = 0.697$. These date, inserted into (101) give the following result:

$$b_M = 1 \text{ nm} \tag{102}$$

As it can be seen from formula (102) in lead disc containing three atoms and having lattice constant $b_M = 1$ nm, the superconductive propagation of charges can be expected up to 100 K.

The energy spectrum of Cooper pair's is given by[14]

$$E = \sqrt{\Delta^2 + [Y\tau_M^2 b_M^2(k^2 - k_F^2)]^2}; \quad k = \frac{\mu}{b_M} \tag{103}$$

Superconductivity can be considered as superfluidity of pairs in narrow layer enveloping Fermi boundary. The condition of superfluidity has given by Landau[15] and this condition is the existence of positive minimum of phase velocity $c_f = E_k/k$.

Dividing (103) with $k - k_F$ we obtain phase velocity in the form:

$$c_f = \frac{E}{k-k_F} = \sqrt{\frac{\Delta^2}{(k-k_F)^2} + [Y\tau_M^2 b_M^2(k+k_F)]^2} = \sqrt{\frac{\Delta^2}{(k-k_F)^2} + [Y\tau_M^2 b_M^2(k-k_F+2k_F)]^2} \tag{104}$$

Differentiating (104) with respect to $k - k_F$ we obtain:

$$\frac{dc_f}{d(k-k_F)} = \frac{(Y\tau_M^2 b_M^2)^2(k-k_F)^3 + 2k_F(Y\tau_M^2 b_M^2)^2(k-k_F)^2 - \Delta^2}{(k-k_F)^2\sqrt{\frac{\Delta^2}{(k-k_F)^2} + [Y\tau_M^2 b_M^2(k-k_F+2k_F)]^2}} \tag{105}$$

The phase velocity has extremum if the numerator in (105) is equal to zero. Since the numerator equated with zero is cubic algebraic equation minimum one of roots of the equation is real. This real value can be found numerically. Substituting this value in (104) we obtain positive minimal value for c_f. It means that pairs move without friction, in other words—superconductivitely.

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It is well known that superconductors produce very high magnetic fields. In the considered case it can be tested by equating magnetic force to centrifugal mechanical force

$$eBv = \frac{m^* v^2}{R} \tag{106}$$

In this formula m^* is the effective mass of electrons, which can be found from formula (87). The expression for effective mass is given by:

$$m^* = \frac{\hbar^2}{2Yb_M^2} \tag{107}$$

The velocity v is probability current of electrons:

$$j = \frac{\hbar}{2m^* i}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right) \tag{108}$$

In the case of disc $\Psi \to |\Phi\rangle = \sum_{m=0}^{M} \frac{1}{\sqrt{M+1}} \times e^{i(mb_M)(\tau_M/b_M)}\beta_m^+|0\rangle$ and $\partial/\partial x \to \partial/\partial(mb_M)$ so that formula (108) goes over to

$$j = v = \frac{\hbar \tau_M}{m^* b_M} = \frac{4\pi b_M Y}{(M+1)\hbar} \tag{109}$$

The radius of the circle can be found from (28). It is given by:

$$R = \frac{b_M}{2\sin(\tau_M/2)} \tag{110}$$

Putting (107), (109) and (110) into (106) we obtain

$$B = \frac{4\pi\hbar}{e} \frac{\sin(\pi/(M+1))}{(M+1)b_M^2} \tag{111}$$

In this formula will be used data obtained for lead with three atoms in disc, i.e., $b_M = 10^{-9}$ m and $M = 2$. It leads to value $B = 2400$ T, which is really very high.

4. CONCLUSION

The results of analysis superconductive properties of metallic discs whose cross-section is of nano order can be summarized as follows:

(1) In the nearest neighbours' approximation electrons in disc are splitted into two independent subsystems, i.e., to electrons moving in the direction of cylinder height, and to electrons moving on periphery of disc circles.

(2) Electron–phonon interaction is defined as the function of modulus of inter-atomic distance. To this fact often is not paid full attention.

(3) It is shown that electrons which move in the direction parallel with cylinder axis can have gap which corresponds to critical superconductive temperature of few Kelvins.

(4) For electrons moving in discs critical temperature has sharp dependence on chord length which connects neighbour atoms. This dependence is of the type $T_c \sim b_M^{-2}$.

(5) The main practical advantage of cylinders is the fact that the cyclic currents in disc produce very high magnetic fields which are of the order of thousand Tesla and more. Since the magnitude of magnetic field is proportional to reciprocal number of atoms in discs, it can be concluded that high magnetic fields are typical nano effect.

This work is built on a set of simplification. We quote the main of them.

In the nearest neighbours approximation electron system of cylinder goes over to two independent systems: electrons moving in z direction and circular electrons in discs. In such picture it is clear that electrons from chains can transit into disc and vice versa. Since such transitions occur in one point, the interaction of exchanging electrons is of delta function type. It is well known that scattering length on delta potential is equal to zero,[25] we can conclude that it is impossible to differ, wherefrom are electrons in that point.

The system of three atoms make rather cluster than disc. However in theory of protein solitons clusters containing three atoms are substituted with Scott's disc[26] and this approximation gave realistic picture of behaviour of the system. The same we expect here.

Our estimation of magnetic field is made in full idealization: the contributions of electron spin were not taken into account, the orbital momentum of electrons were not introduced into calculations etc.

All quoted decreases magnitude of magnetic field obtained here, we are of opinion that this decrease can reduce the field for order of magnitude.

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