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TI-Bipolaron Coaxial Cable: A Path to Room Temperature Superconductivity Without Extreme Pressures

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TI-Bipolaron Coaxial Cable: A Path to Room Temperature Superconductivity Without Extreme Pressure

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ТИ-биполяронный коаксиальный кабель: путь к комнатной сверхпроводимости без сверхдавлений

Классический поиск комнатной сверхпроводимости в гидридах зашел в тупик из-за необходимости применения экстремальных давлений в миллионы атмосфер, что делает их практическое использование в электронике невозможным. В отличие от этого подхода, трансляционно-инвариантная (ТИ) биполяронная теория предлагает решение, реализуемое методами современной наноинженерии. Данная работа переводит квантовомеханическую модель в конкретные геометрические и материаловедческие параметры трехслойной коаксиальной гетероструктуры. Мы демонстрируем, что пространственное разделение носителей позволяет достичь критической температуры $T_c \approx 300$ К при нормальном давлении.

Ключевые слова: биполяронная масса, бозе-конденсат, YBCO, двойной слой,модель локальных пар

Viktor Dmitrievich Lakhno

TI-Bipolaron Coaxial Cable: A Path to Room Temperature Superconductivity Without Extreme Pressure

The classical search for room temperature superconductivity in hydrides has reached a dead end due to the need for extreme pressures of millions of atmospheres, making their practical use in electronics impossible. In contrast, translation-invariant (TI) bipolaron theory offers a solution that can be implemented using modern nanoengineering methods. This work translates the quantum mechanical model into specific geometric and materials science parameters for a three-layer coaxial heterostructure. We demonstrate that spatial carrier separation allows a critical temperature of $T_c \approx 300$ K to be achieved at ambient pressure.

Key words: bipolaron mass, bose-condensate, YBCO, double layer, preformed pairs model

1. Introduction: The crisis of the high-pressure method and the relevance of the TI-alternative

Modern condensed matter physics is in a deep methodological crisis regarding high-temperature superconductivity (HTS). A historic breakthrough in the synthesis of superconducting hydrides (such as H_3S, LaH_{10}, Lu-H-N) made it possible to get very close to room transition temperatures (T_c). However, this success is strictly limited by the concept of ultrahigh pressures – the structures are stable only in diamond anvils under compression to millions of atmospheres (150 to 250 GPa) [1]-[6].

To date, the global scientific agenda is virtually devoid of alternative, physically sound proposals for creating room-temperature superconductors at normal (atmospheric) pressure. Attempts to empirically search for bulk materials beyond hydrides have led to metastable phases that cannot be independently verified. A fundamental impasse arises: room-temperature superconductivity has been physically proven, but is technologically dead, since devices based on it cannot be integrated into real industry.

This work suggests a way out of this impasse by shifting the focus from macroscopic mechanical compression to nanoscale quantum compression of a Bose gas. It is widely believed among experts on superconductivity that the very large mass of a bipolaron is an obstacle to the realization of the bipolaron mechanism of superconductivity. For this reason, the Bose-Einstein condensate of such bipolarons will have a very low condensation temperature. This is indeed true for small-radius bipolarons (SRP), for which the effective mass increases exponentially with increasing electron-phonon coupling constant. For large-radius bipolarons with broken symmetry (Landau-Pekar polarons), the mass does not grow exponentially, but according to a power law with increasing coupling constants; however, it still turns out to be too large for sufficiently large coupling constants. Attempts to adjust the parameters of the SRP theory so that the SRP is light (i.e., delocalized over several nodes) bring the model of light SRP closer to the case of LRP, for which, as noted above, the mass remains too large. This "curse of mass" is completely eliminated by the theory of translationally invariant (TI) polarons and bipolarons. In this theory, superconductivity is caused by excited states of bipolarons, which describe the states of current carriers delocalized throughout the crystal volume even with an infinite mass of a polaron or bipolaron in the ground state. The expression for the temperature of the Bose-Einstein condensate of TI-bipolarons [7] uses not the effective mass of the bipolaron, but the usual band mass of the current carrier (Appendix 1). The main problem in the realization of high-temperature room-temperature superconductors based on the bipolaron mechanism in this case is the low concentration of TI bipolarons, whose concentration in high-temperature superconductors is several percent of the total number of current carriers [7]. Overcoming this problem is the purpose of this paper.

Based on the translation-invariant (TI) bipolaron theory, we have developed an architecture of a coaxial nanocable capable of generating room temperature T_c at

normal pressure due to the forces of electrostatic displacement of unpaired quasiparticles and the creation of an increased concentration of bipolarons in the cable.

2. Geometry of a coaxial nanocable

Instead of isotropic chemical doping, which is destructive for the HTSC crystal lattice, the TI-bipolaron concept dictates the spatial separation of charge generation bands and their superconducting conductivity band. Below is a diagram of the cross-section of a coaxial nanocable, where the conducting layers initially contain a mixture of TI-polarons and TI-bipolarons, but are separated by a functional dielectric barrier.

Geometric parameters for epitaxial synthesis:

- **Inner cable (Central core, radius R_{core}):** it is made of an absolutely pure, ideal monocrystalline HTSC material (for example, optimally doped $YBa_2Cu_3O_{7-x}$ cuprate). The core radius should be commensurate with the coherence length of the TI-bipolaron gas (ξ_{bp}). In the case of a realistic electron-phonon coupling constant (EPI α = 3) the radius is R_{core} ≈2.0 nm (the total diameter is D_{in} ≈ 4nm).
- **Buffer nanolayer (Thickness d_{buf}):** An epitaxial dielectric with a thickness of $d_{buf} \approx 1.$ нм (3 atomic layers) prevents the mutual diffusion of heavy ions and isolates the core from the parasitic Coulomb fields of stationary shell defects.
- **Outer cable (Concentric shell, layer thickness t_{shell}):** The same basic cuprate low-oxygen-doped material (for example $YBa_2Cu_3O_6$), containing deep electron-neutral impurity centers. The layer thickness is chosen on the order of the Debye screening length of a superconductor with impurities: $t_{shell} \approx 1.5$ nm. For a fixed core radius of $R_{core} = 2$ nm the outer radius of the entire structure will be $R_{out} \approx 4.5$ nm, which corresponds to equal volumes of the shell and the core $V_{shell}/V_{core} = 1$
- The figure shows a schematic representation of the cable.

3. The physics of selective charge separation and the energy window

According to [7], [8], both free individual TI polarons (holes) and their paired states, TI bipolarons, can coexist in a doped matrix. The key to solving the problem is their fundamentally different interaction with defects.

In the framework of the TI theory, the coupling energies of a free TI-bipolaron (E_{bp}) an individual TI-polaron (E_p) are given by the EPI constant α. Based on weighted experimental data for cuprates, we take the coupling constant as $\alpha = 3$.

Let us substitute this value into the basic equations:

1. The coupling energy of a free strong-coupling TI-bipolaron:

$$|E_{bp}| = 0.44 \cdot \alpha^2 \omega_0 \approx 0.134 \text{ eV}$$

2. The coupling energy of an individual TI polaron:

$$|E_p| = 0.126 \cdot \alpha^2 \omega_0 \approx 0.0383 \text{ eV}$$

3. The energy window of selectivity:

$$E_{aff} < |E_{bp}| - 2|E_p| = 0.19 \cdot \alpha^2 \omega_0 \approx 0.0574 \text{ eV}$$

Note that the $\omega_0 = 33{,}8$ meV optical phonon frequency used in the optimal doping phase ($YBa_2Cu_3O_{6,92\text{-}6,95}$, $T_c = 92 - 93{,}5$ K) falls within the peak range of the intraplane oscillations of oxygen atoms O(2), O(3) in conducting CuO_2 layers. Such oscillations represent in-phase or out-of-phase displacements of oxygen atoms along the crystallographic axes of the ab plane. This optical mode is strongly related to the in-palane hole gas by the electron-phonon interaction. Upon transition to the superconducting state, it experiences an anomalous softening and profile asymmetry (Fano mode) precisely in the region of 33-34 meV.

In order for the outer shell of the cable to function as a selective filter, the gain energy of a free T-bipolaron compared to two polarons localized on impurity centers must be smaller than E_{aff} , but still positive.

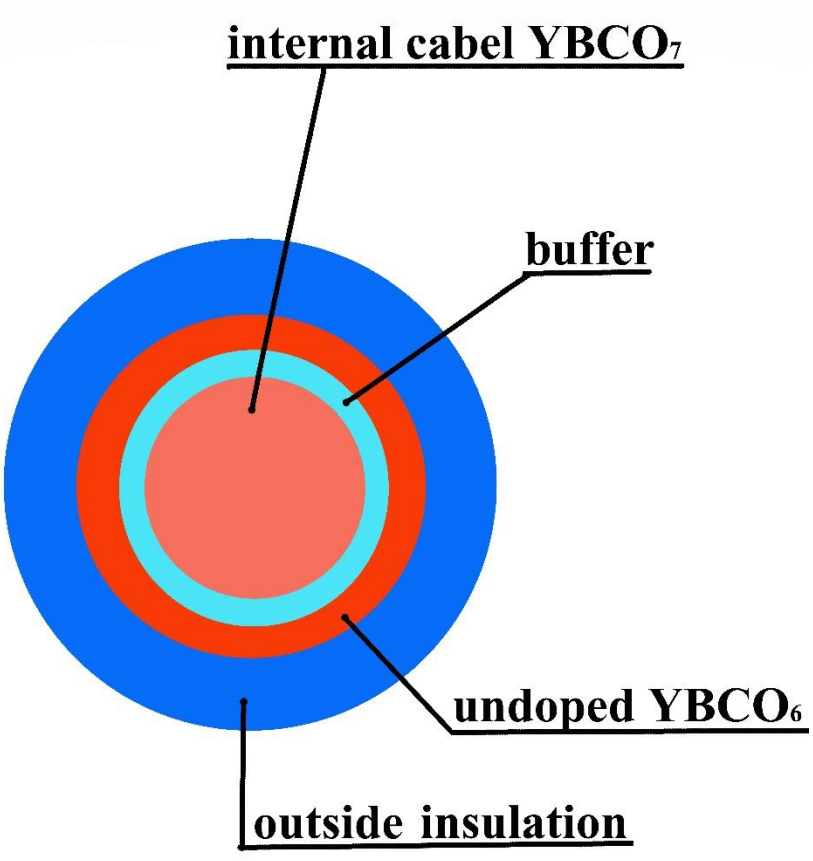

Fig.°1 Superconducting cable

In this case, mobile bipolarons will form in the outer cable, which will then migrate to the inner cable to neutralize the excess negative charge formed in it after the holes migrate to the outer cable. In [7], it was proposed to use magnetic impurities for this purpose, which interact differently with TI polarons having spin and TI bipolarons that have no spin. As shown in [8], ordinary non-magnetic impurities can also be used to create a room-temperature superconductor. An example of such an impurity is the substitution of lanthanum for barium: La^{3+} instead of Ba^{2+} at low doping levels (see Appendix 2).

For a bipolaron with a high binding energy (0.134 eV), the Coulomb repulsion from the doubly positive charge of the impurity complex and its own large deformation radius make capture energetically disadvantageous. The bipolaron has too high binding energy to localize in such a shallow polarization well and is not captured by this defect. Another classic example of a defect with a similar behavior is an **isolated interstitial oxygen vacancy** in the interplane space under weak stoichiometry violation. Selective capture, in which individual polarons are localized on impurities, while bipolarons remain free, radically changes the transport properties of YBCO in the normal (non-superconducting) state [9].

4. Estimation of the increase in the critical temperature T_c

As shown in [10], the existence of bipolaron superconductivity requires the presence of a clearly defined Fermi surface. Therefore, the increase to room temperature must occur while maintaining the Fermi surface.

Let us set the concentration of unpaired carriers (Fermi gas) in the core equal to $n_h = 10^{21}$ cm^{-3}, and the initial concentration of T-bipolarons equal to $n_{bp}^{init} = 10^{19}$ cm^{-3}. These are typical values used in the TI bipolaron theory of superconductivity. We limit the volume of free hole "pumping" from the core to 10% ($\Delta n_h = 10^{20}$ cm^{-3}), in order to ensure the connectivity and topology of the Fermi surface in the inner part of the wire.

Since the traps in the shell bind individual holes, in order to preserve the overall electroneutrality, free T-bipolarons (each carrying a charge of 2*e*) are displaced by Coulomb forces into the inner core. The number of injected bosons is:

$$\Delta n_{bp} = \frac{\Delta n_h}{2} = 5 \cdot 10^{19} cm^{-3}$$

For this, the impurity concentration in the outer cable must be equal to Δn_h. when the volumes of the outer and inner cables are equal. (The maximum volume concentration of lanthanum La in the YBCO structure is $2.88 \cdot 10^{21} cm^{-3}$ when barium is replaced and up to $8.6 \cdot 10^{21} cm^{-3}$ when yttrium is completely replaced).

The final density of T-bipolarons in the inner core increases by exactly 6 times:

$$n_{final} = n_{bp}^{init} + \Delta n_{bp} = 6 \cdot 10^{19} cm^{-3} = 6 \cdot 10^{25} m^{-3}$$

In the TI bipolaron theory, the critical temperature of Bose condensation is proportional to $\left(n_{bp}\right)^{2/3}$. For this reason, the increase factor due to the 6-fold compression of the Bose gas is equal to $6^{2/3} \approx 3.30$. If the initial pure cuprate had a nitrogen temperature $T_c^{init} \approx 91$ K (the standard for YBCO), then the new critical core temperature will be:

$$T_c^{final} = 91\text{K} \cdot 3.30 = 300.3\text{K}$$

We obtain room-temperature superconductivity (~27°C) while maintaining 90% of the Fermi surface.

5. Discussion

We have considered the possibility of creating a room temperature conductive cable with extremely small (nanometer) dimensions. Such a nanometer cable would have an ultra-high critical current density and an ultra-high critical magnetic field. Although creating such a cable with current nanotechnology is possible, it would present significant technical challenges. To overcome these challenges, the task could be scaled up, for example by increasing its dimensions by two orders of magnitude (while maintaining a 12 nm buffer).

Increasing the size of the core and outer cable by 100 times will completely transfer the system to a macroscopic scale.

With this scaling, the geometry will take the following parameters:

Core radius: 2.5 μm.

Buffer thickness: 12nm (remains nanoscale).

Internal radius of the outer cable: 2.512 μm.

The outer radius of the entire system is 6.25 μm (the outer cable thickness is 3.74 μm). This will lead to the following consequences. A double layer will form on the buffer between the bipolaron gas of the outer cable and the polaron-bipolaron gas of the inner cable. The electric field intensity of the double layer will be determined by the equality of the electrochemical potentials of the outer and inner cables (approximately $E_F = eE\varepsilon d_{buf}$, where ε is the dielectric constant of the buffer, which for a buffer material such as SrTiO3 is of the order of 300) and for the Fermi energy of optimally doped YBCO ($E_F \approx 0.37$eV) will be $10^2 \div 10^3$ V/cm in order of magnitude. An increase in the buffer size in the micron-sized version by an order of magnitude compared to the nanowire will, on the one hand, reliably block the diffusion of impurities into the inner cable in such a field, while, on the other hand, it will significantly impede the transition of bipolarons to the inner cable. Polaron tunneling can be accelerated by applying a strong electric field or a laser pulse.

We leave the discussion of these technical problems until the experimental confirmation of the fundamental question of achieving room temperature T_c in this way.

Appendix 1. Why the superconducting transition temperature is determined by the band mass and not the bipolaron mass

In the translationally invariant bipolaronic theory of superconductivity, the diagonal elements of the density matrix correspond to the density of TI bipolarons. Accordingly, the off-diagonal elements of the density matrix are key parameters for understanding the long-range order and determine the degree of coherence between different quantum states [8]. In the case of a Bose gas under consideration, its state is described by plane wave functions of particles with momentum k: $\varphi_k(R_i) = e^{ikR_i}/\sqrt{V}\varphi$, where R_i are the coordinates of the i-the particle, and V is the volume of the system.

The general form of a single-particle density matrix is determined by the expression:

$$g(R_1, R_2) = \sum_k n_k \varphi_k^*(R_1)\varphi_k(R_2), \quad \text{(A1)}$$

where $n_k = \{exp[(E_k - \mu)/T] - 1\}^{-1}$ is the Bose distribution function of particles. Separating the contribution of the condensate with k=0 from the temperature component, we can rewrite this expression as:

$$g(R_1, R_2) = \frac{N_0}{V} + \frac{1}{(2\pi\hbar)^3}\int d^3k \frac{exp[ik(R_1 - R_2)/\hbar]}{exp[(E_k - \mu)/T] - 1}, \quad \text{(A2)}$$

where N_0 is the number of particles in the Bose condensate. The energy of the TI bipolaron E_k, participating in (A2), according to [7]-[8], has the form:

$$E_k = \left[\Delta_k + E_{bp} + k^2/2M\right], k > 0, \quad \text{(A3)}$$

where E_{bp} is the energy of the ground state of the bipolaron, $\Delta_k = \omega_k$, where ω_k is the phonon frequency, which has the meaning of the size of the superconducting gap:

$$\Delta_k = \omega_0, \quad \text{(A4)}$$

- for an s-type gap and an optical phonon whose frequency ω_0 does not depend on k, and:

$$\Delta_k = \omega_0 + \Delta_0\left|\cos k_x a - cosk_y a\right|, \quad \text{(A5)}$$

- for a gap of the s+d type, where M=2m, m is the effective mass of an electron (hole). From (A1) it follows that the diagonal components of the density matrix $g(R_1, R_2)$ are equal to $g(0) = N/V$ and describe the particle number density in an ideal gas of TI bipolarons with $N = N_0 + N'$:

$$N = \sum_k n_k \ , \tag{A6}$$

$$N_0 = 1/(e^{(E_{bp}-\mu)/T} - 1), \qquad N' = \sum_{k\neq 0} 1/(e^{(E_k-\mu)/T} - 1),$$

where N_0 is the number of particles in the bipolaron ground state, N' is the number of particles in higher states, $\mu = E_{bp}$, where E_{bp} is the energy of the ground state of the TI bipolaron. The equality $\mu = E_{bp}$ corresponds to an infinitely large density of states of the Bose condensate near the gap $\Delta_k = \omega_0$ in the spectrum of TI bipolarons. Having replaced the summation in the expression for N' in (A6) with integration over the quasi-continuous spectrum (A3), we obtain from (A6) an equation for determining the critical temperature of Bose condensation of TI bipolarons with T_c:

$$T_c(\omega_0) = \left(F_{1/2}(0)/F_{3/2}(\omega_0/T_c)\right)^{2/3} T_c(0), \tag{A7}$$

$$T_c(0) = 3{,}31\hbar^2 n^{2/3}/M, \qquad F_{3/2}(x) = \frac{2}{\sqrt{\pi}}\int_0^\infty \frac{t^{1/2}dt}{e^{t+x}-1},$$

where $n = N/V$ is the concentration of TI bipolarons. It is important that (A7) includes M=2m and not the heavy mass of the bipolaron. This eliminates the problem of low condensation temperature, which arises both in the theories of superconductivity of small-radius polarons and large-radius polarons, where expression A7) includes the heavy mass of the bipolaron [7]-[8].

In the case of an *s*+*d*- type gap (A5) the first term on the right-hand side of (A5) corresponds to the contribution of the *s*-type wave, and the second term to the contribution of the *d*-type wave. From (A5), the following condition follows, when the main contribution to the integral (A2) is given by the values $k \approx \sqrt{2MT}$ and $ka \ll 1$. In this case, from (A2) and (A5), we obtain: $\Delta_0\left|cosk_x a - cosk_y a\right|/T \cong \Delta_0 Ma^2/\hbar^2 \ll 1$. Thus, for $\omega_0 \geq \Delta_0 Ma^2T/\hbar^2$ the main contribution to the integral will be given by the *s*-type wave. In this case, the results obtained above for the case of an *s*-type condensate will remain unchanged. For example, in the case of YBCO, the value of ω_0/Δ_0 is ≈ 0.15 [11], [12] and the s-approximation condition in this case is satisfied with high accuracy.

Appendix 2. How selective impurity works

It should be noted that Mott and Alekxandrov proposed increasing the bipolaron concentration in HTSC YBCO by heterovalently substituting Ba^{2+} with La^{3+} [13]-[15]. In the classical YBCO matrix, holes are the main charge carriers in CuO_2 planes. Replacing divalent barium (Ba^{2+}) with trivalent lanthanum (La^{3+}) introduces an excess positive ion charge into the system. To compensate for this local excess charge, the electrons move into the conductive CuO_2 planes. This leads to partial suppression (compensation) of free holes in the planes. Free (delocalized) holes in cuprates are reluctant to form small-radius bipolarons due to strong interelectron Coulomb

repulsion. When La^{3+} ions are introduced, the additional positive charge of La^{3+} acts as a local Coulomb center of attraction for the holes remaining in the planes. This localizes the hole charge carriers in space as small-radius polarons. The reason why the positive charge of La^{3+} attracts holes, according to Mott and Alexandrov, is that La^{3+} has a smaller ion radius and, consequently, a higher charge density than Ba^{2+}. This leads to a displacement of oxygen ions (O^{2-}) towards it. The strong distortion of the medium caused by them creates a polarization well and the displaced oxygen ions shield the lanthanum potential with "overcompensation". As a result, for holes located in neighboring CuO_2 planes, this local region of lattice deformation acts as an effective potential well (trap).

Although this method successfully increases the concentration and stability of bipolarons, in practice, significant substitution of Ba^{2+} for La^{3+} often leads to a decrease in the macroscopic temperature T_c. This is because excessive hole localization makes bipolarons too heavy, since their mass m* becomes so large that it lowers their Bose condensation temperature $(T_c \propto 1/m^*)$.

In the case of TI-bipolarons, the problem of heavy mass is eliminated, since the expression for the T_c of their Bose condensate involves not the heavy mass of the bipolaron, but the ordinary band mass of paired holes. In the approach we are considering, the replacement of Ba^{2+} with La^{3+} occurs in the outer cable and does not lead to deformation of the ionic lattice of the inner cable.

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