**Invited Research Article**

**Possible Fano resonance for high-$T_c$ multi-gap superconductivity in p-Terphenyl doped by K at the Lifshitz transition**

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**Abstract** – Recent experiments have reported the emergence of high-temperature superconductivity with critical temperature $T_c$ between 43 K and 123 K in a potassium-doped aromatic hydrocarbon para-Terphenyl or p-Terphenyl. This achievement provides the record for the highest $T_c$ in an organic superconductor overcoming the previous record of $T_c = 38$ K in $C_{60}$ fulleride. Here we propose that the driving mechanism is the quantum resonance between superconducting gaps near a Lifshitz transition which belongs to the class of Fano resonances called shape resonances. For the case of p-Terphenyl our numerical solutions of the multigap equation shows that high $T_c$ is driven by tuning the chemical potential by K doping and it appears only in a narrow energy range near a Lifshitz transition. At the maximum critical temperature, $T_c = 123$ K, the condensate in the appearing new small Fermi surface pocket is in the BCS-BEC crossover while the $T_c$ drops below 0.3 K where it is in the BEC regime. Finally, we predict the experimental results which can support or falsify our proposed mechanism: a) the variation of the isotope coefficient as a function of the critical temperature and b) the variation of the gaps and their ratios $2\Delta/T_c$ as a function of $T_c$.

**Introduction.** – Recently high-temperature superconductivity with $T_c$ in the range of 43–123 K has been reported following different growth procedures in a potassium-doped aromatic hydrocarbon p-Terphenyl [1–3]. The superconducting crystalline phase is expected to be $K_3C_{18}H_{14}$. Superconducting pairing with a large 15 meV gap opening at about 60 K was confirmed on a K-doped surface of a p-Terphenyl single crystal [4]. Para-Terphenyl, a linear molecule made of a chain of 3 benzene rings, and its derivatives are aromatic biological molecules present in edible mushrooms [5]. Pharmaceutical research is in progress for their use as immunosuppressive, anti-inflammatory and anti-tumor agents, and it also has technological applications as laser dye, sunscreen lotion and in photon detectors. If these results will be confirmed, K$_x$ p-Terphenyl provides today the record for the highest critical temperature in carbon-based materials and larger than in many cuprates oxides and in many iron-based superconductors. The search for macroscopic quantum coherence at high temperature in organics and organometallics has been a long standing search for the holy grail of room temperature...
superconductors. Superconductivity in graphite intercalation compounds has been an active topic for several decades, but $T_c$ ranges only up to $11.5 \text{ K}$ for CaC$_6$ [6]. The highest critical temperature $T_c = 38 \text{ K}$ in doped fullerides $A_2$C$_{60}$ ($A = K, Rb, Cs$) has been found in Cs$_3$C$_{60}$ with A15 structure by application of 7 Kbar hydrostatic pressure [7]. This system provides a complex phase of condensed matter where structural polymorphism controls both magnetic and superconducting properties [8] and shows a fluctuating microscopic heterogeneity made of the coexistence of both localized Jahn-Teller active and itinerant electrons [9]. Recently the material research for high-temperature superconductors was oriented toward metal-intercalated aromatic hydrocarbons by the discovery of superconductivity with $T_c = 18 \text{ K}$ by doping potassium into picene (C$_{22}$H$_{14}$) [10,11]. Picene is a hydrocarbon molecule made of five benzene rings condensed in an armchair manner. Looking for high $T_c$ in alkali-metals or alkali-earth-metals–doped polycyclic-aromatic-hydrocarbons (PAHs), the previous record $T_c = 33 \text{ K}$ was held by in K$_x$ 1,2:8,9-dibenzo[18]cyclopentaene (C$_{30}$H$_{18}$) [12]. The recent indications for $T_c = 123 \text{ K}$ in p-Terphenyl open a new roadmap for the search of higher critical temperatures in the large family of doped metal-organic compounds, with the hope to overcome the highest superconducting critical temperature known so far, $T_c = 203 \text{ K}$ in pressurized H$_3$S [13,14]. There is today high interest on understanding both the quantum mechanism beyond the emergence of $T_c = 123 \text{ K}$ in p-Terphenyl and the relation between the nanostructure and quantum functionality in organics. This is needed to develop novel quantum plasitcs materials, taking advantage that conducting polymers can be prepared in a large variety of polymeric heterostructures at atomic limit [15–17] and possess the combination of easy processability, light weight, and durability. Using density functional theory and Eliashberg’s theory of superconductivity in the single band approximation the superconducting critical temperature has been predicted to be in the range $3 < T_c < 8 \text{ K}$ in K$_3$ picene [18] and around 6.2 K in K$_2$C$_6$H$_6$, moreover, it was argued that all hydrocarbons should show $T_c$ in the search of higher critical temperatures of benzene [20–22]. Therefore unconventional pairing mechanisms were invoked for high $T_c$ in doped p-Terphenyl: a) the Bose-Einstein Condensation (BEC) of preformed bipolarons [1–3]; b) the Resonating Valence Bond (RVB) theory in a scenario with two coexisting doped Mott insulators [23] c) the so-called $s_{+/-}$--pairing mechanism mediated by a repulsive interaction in a scenario with two strongly correlated bands forming two similar Fermi surfaces connected by a nesting vector [24].

Here we propose the mechanism for $T_c$ amplification driven by Fano resonances [25,26] in a multigap superconductor between different gaps occurring where the chemical potential is tuned at an electronic topological Lifshitz transition [27]. In this regime the configuration interaction between the pairing scattering channels in the $(n-1)$-th bands with high Fermi energy $E_F(n-1)$ in the BCS approximation and the $n$-th pairing scattering channel in the new appearing $n$-th small Fermi surface with a low Fermi energy $E_F(n)$ can give a resonance in the superconducting gaps, called shape resonance [28,29] like in nuclear physics and molecular physics [30] or a Feshbach resonance as in the jargon of ultracold gases [31]. The Fano resonance gives high-$T_c$ domes around Lifshitz transitions in the energy range of $E_{Fn}$ of the order of the energy of the pairing cut-off and the $n$-th condensate is in the BCS-BEC crossover [32,33].

The configuration interaction between pairing channels is determined by the symmetry and interference between the wave functions of electron pairs at the coexisting multiple Fermi surfaces therefore the nanoscale material architecture plays a central role. In refs. [25,26] particular material architectures made by heterostructures on the atomic scale which could give high-$T_c$ superconductors have been disclosed. Panel (A) in fig. 1 shows one of these heterostructures at the atomic limit: a superlattice of stripes. In this case the material is made of nanoscale modules, metallic stripes of atomic thickness, as for example metallic graphene or phosphorene nanoribbons assembled in a superlattice of stripes separated by potential barriers from neighbor stripes in the same plane or in the neighbor plane. The size of the nanoscale units or modules and the superlattice period $\lambda_p$ is required to be in the nanoscale. In fact, in order to attain the highest $T_c$, it is necessary to tune the Fano resonance with the wavelength of the electrons at the Fermi level in the $n$-th band $\lambda_{Fn}$ in the range of $\lambda_p$. The crystalline structure of

![Fig. 1: (Colour online) (A) Drawing of the heterostructure at the atomic limit made of nanoscale stripes which promotes shape resonances according to ref. [26]. The stripes run along the $x$-direction of the $xy$-planes which are separated along the $z$-direction. (B) The p-Terphenyl crystal structure $P21/a$ (CCDC reference No. 847173) appears as a practical realization of the superlattice of stripes shown in panel (A) made of p-Terphenyl striped units of atomic thickness. In the $P21/a$ structure the $b$, $c$ and $a$ axis correspond to the $x$, $y$ and $z$ axes in the schematic drawing in panel (A). The p-Terphenyl stripes run along the $b$-direction and are well separated by the neighbor stripe along the $c$-axis and the $a$-axis directions.](image-url)
Undoped p-Terphenyl [34] with a monoclinic space group $P2_1/a$ is shown in panel (B) of fig. 1 where gray dots are carbon atoms and red dots are hydrogen atoms, which can be described as a packing of parallel p-Terphenyl nanoribbons or stripes of about 1.4 nm width running in the $b$-axis direction indicated by the black arrows. The figure shows the similarity of the arrangements of the p-Terphenyl nanoscale stripes with the schematic drawing of the superlattice of stripes shown in panel (A) of fig. 1 from ref. [26]. The projections in the $ac$, $bc$ and $ba$ crystal planes are shown in fig. 2. Two parallel stripes are clearly seen in the $bc$ projection. The $ba$ projection in fig. 2 shows a variable torsion angle (up to 14 degrees) of the middle ring relative to the two lateral ones. While the H-H bond is 0.32 nm between the lateral rings of the neighbor molecules very short H-H intermolecular bonds (dashed lines connecting neighbor molecules in the stripe in the $b$-direction) are established for the central benzene ring, as short as 0.22 nm, like the shortest values observed in the high-pressure phases of benzene [20,21]. The stripes are not connected with the neighbor stripes also in the $a$-axis direction indicating the quasi–one-dimensional electronic structure of the stripes.

The electronic structure of p-Terphenyl [24,35,36] confirms the presence of one-dimensional electronic states in the conduction band. A portion of the electronic structure of the conduction band [35] is shown in the upper part of fig. 3. The band structure, upper panel of fig. 3, displays in a clear way a strong anisotropic character in the wave-vector space. Indeed, in the irreducible representation of the band structure reported in the upper part of fig. 3 [24,35,36] shows two directions in the Brillouin zone for which the band dispersions are very narrow. A narrow bandwidth of the order of hundred meV indicates that large potential barriers have to be penetrated by the electrons to tunnel from one p-Terphenyl stripe to its neighbor stripe. Interestingly and relevantly for this work, all the bands of the band-bundle, due to the different overlapping orbitals of the p-Terphenyl, have this property and are very narrow along these two independent directions, indicating that the potential barrier formed by the crystal structure and by the characteristics of the electronic bands is felt by all the conduction and valence electrons.

Fig. 2: (Colour online) Three different projections of the p-Terphenyl crystal structure, monoclinic space group $P2_1/a$, with axis $a = 0.81$ nm, $b = 0.56$ nm, $c = 1.36$ nm and $\beta = 92^\circ$. The $bc$ projection shows two parallel p-Terphenyl stripes, made of linear p-Terphenyl molecules, running in the $b$-axis direction, the packing of these stripes form a superlattice of stripes with a period of 1.36 nm in the $c$-direction. The upper $ba$ projection shows the lateral view of the p-Terphenyl stripes. The lower $ac$ projection shows the packing of stripes, running in the $b$-axis direction, perpendicular to the page well separated by neighbor stripe forming a superlattice of stripes with period of 0.81 nm in the $a$-axis direction.

Fig. 3: (Colour online) The upper panel shows the Brillouin zone (BZ) representation of the conduction band of the p-Terphenyl from ref. [35]. The 2 eV wide conduction band is made by a bundle of many bands showing a large dispersion in the $Y$-direction, the direction of the p-Terphenyl stripes, and flat dispersions in the $ZX$-directions, orthogonal to the stripes direction. The red circle indicates a narrow energy range of about 600 meV around the band edge of the $n$-th electronic band which shows the narrow energy dispersion in the $XZ$-direction and wide dispersion in the $Y$-direction which coexist with other $(n-1)$-th dispersing bands. The lower panel shows that the dispersion of the electronic bands obtained by the solution of the Schrödinger equation for a superlattice of stripes with period 1.4 nm, separated by a potential barrier, determined by the hopping energy between stripes, in the transversal direction is such that the transversal energy dispersion in the periodic potential is 145 meV, the same as the assumed energy cut-off for the pairing $\omega_0 = 145$ meV. The narrow energy range of the dome of high $T_c$ is only of the order of $4\omega_0 = 580$ meV, where the Fano resonance near the Lifshitz transition is in action.
to predict the superconducting properties of the K-doped p-Terphenyl with numerical calculations through a simplified model of its nanoscale structure getting the key electronic structure near a band edge. The bands and wave functions are created by using a proper superlattice of stripes, which allow the solution of the Bogoliubov gap equations [37,38] without standard BCS approximations, giving high-$T_c$ superconducting state with multigaps and multicondensates at different BCS/BEC pairing regimes. The pairing is thought to be driven by an attractive interaction within each Fermi surface, but the non-diagonal interaction between condensates can be either repulsive or attractive. The multicomponent character of the pairing and the geometry of the system will determine shape resonances in the superconducting gaps and $T_c$, with peculiar features predicted for the isotope effect and the gap to $T_c$ ratios, which can be tested in future experiments, together with the expected anisotropic transport of electrons in doped (or out of equilibrium) single crystals. The presence of high-temperature superconducting domes where the chemical potential crosses the Lifshitz transitions is now well confirmed by experiments in iron-based superconductors. Here we present the possible scenario of high-temperature superconductivity in p-Terphenyl where the chemical potential is driven by potassium doping at a Lifshitz transition. Our model predicts that at the Lifshitz transition the Fermi surface is made of multiple components: circular Fermi surface pockets and Fermi arcs as shown in fig. 4. The superconducting properties have been calculated using the Bianconi-Perali-Valletta (BPV) theory which describes a solution of the Bogoliubov-de-Gennes (BdG) equations for inhomogeneous superconducting phase. The BPV theory has been used to predict the high-$T_c$ in striped cuprates [39–42], proposing the coexistence of Fermi arcs and Fermi pockets, which was confirmed in 2009 [43], and the anomalous isotope coefficient [44,45]. The BPV theory has been applied to diborides [46–48], and iron-based superconductors [49–51] where it has been confirmed by recent experiments [52–56]. In these experiments it has been reported compelling evidence that the high-$T_c$ domes occur in the proximity of the Lifshitz transitions for the appearing of a new Fermi surface pocket. Recently similar scenarios have been proposed for pressurized sulfur hydrides [57] and in superconducting nanofilms [58]. Let us consider a system made of multiple bands with index $n$. The energy separation between the chemical potential and the bottom of the $n$-th band defines the Fermi energy of the $n$-th band. This formulation was proposed for systems with a band crossing the chemical potential having a steep free-electron–like dispersion in the $x$-direction and a flat band-like dispersion in the $y$-direction. The wave functions of electrons at the Fermi level are calculated using a lattice with quasi-one-dimensional lattice potential modulation where the chemical potential is tuned near a Lifshitz transition, like in magnesium diborides, A15, cuprates, iron-based superconductors.

Fig. 4: (Colour online) Upper panel: drawing from the patent in ref. [26] where the Fermi level is tuned above the second peak of the conduction band density of states (DOS) of a superlattice of stripes to get the Fano resonance in superconducting gaps. Lower panel: the $n$-th DOS peak (solid line) of the conduction band of p-Terphenyl as a function of the Lifshitz parameter $x = (\mu - E_0)/\omega_0$, where $\mu$ is the chemical potential and $E_0$ is the bottom of the $n$-th band. Panels (A)–(D) show the evolution of the Fermi arcs and Fermi pockets for: (A) $x < 0$; (B) $0 < x < 1$, where a new circular Fermi pocket appears; (C) $x = 1$ at the 2D-1D topological Lifshitz transition, i.e., at the Van Hove singularity; and (D) $x > 1$.

In the $b$-axis direction in the real space, orthogonal to the upper surface of the Brillouin zone the band dispersion is much broader, of the order of 700 meV, pointing toward a quasi-free conduction of the electrons with a moderate effective mass along the $b$-direction. The energy scale of the pairing, 145 meV, is taken from the relevant phonons detected at 1171 cm$^{-1}$, due to a mode of the C–C bond, and/or the mode at 1222 cm$^{-1}$ of the C–H mode, detected by Raman spectroscopy in metallic K$_3$ p-Terphenyl [1]. We have simulated the band dispersion and the DOS with a periodic potential barrier with 1.4 nm periodicity which reproduces the narrow band dispersion in the transversal direction of the stripes shown in the lower panel of fig. 3. We have obtained an electronic structure which reproduce the key features observed when the chemical potential is tuned at a band edge in a superlattice of stripes as shown in the upper panel of fig. 4 showing the drawing of the patent for material design of heterostructures at atomic scale [26]. Once doped by K, the chemical potential will be raised in the conduction band and depending on the doping (and/or misfit strain, pressure, orientational disorder, magnetic field . . .) at the $n$-th band edge it gives rise to a complex network of Fermi surfaces, with electron and hole-like small pockets of Fermi surfaces and Fermi arcs. The key point of this work is
The superconducting critical temperature $T_c$ in the BPV theory is obtained by a numerical solution of the gaps equation [37,38] considering the simplest case of a two-dimensional system [41] of stripes, but the extension to a three-dimensional system [48] is straightforward. The $T_c$ is determined by solving the following self-consistent system of equations:

$$\Delta_{n,k_y} = \frac{1}{2N} \sum_{n',k_y'} V^{n,n'}_{k,k'} \frac{\tanh \left( \frac{E_{n',k_y'} + \epsilon_{k_y'} - \mu}{2T_c} \right)}{E_{n',k_y'} + \epsilon_{k_y'} - \mu} \Delta_{n',k_y'},$$

where $E_{n,k_y} + \epsilon_{k_y}$ is the energy dispersion and $\mu$ the chemical potential. We consider a superconductor with multiple gaps $\Delta_{n,k_y}$ in multiple bands $n$ with flat band-like dispersion in the $y$-direction and steep free-electron-like dispersion in the $x$-direction for a simple model of a two-dimensional metal with a one-dimensional superlattice modulation in the $y$-direction. The self-consistent equation for the gaps at $T = 0$ where each gap depends on the other gaps is given by

$$\Delta_{n,k_y} = \frac{1}{2N} \sum_{n',k_y'} V^{n,n'}_{k,k'} \Delta_{n',k_y'} \frac{1}{\sqrt{(E_{n',k_y'} + \epsilon_{k_y'} - \mu)^2 + \Delta^2_{n',k_y'}}}.$$ (2)

where $N$ is the total number of wave-vectors in the discrete summation and $V^{n,n'}_{k,k'}$ is the effective pairing interaction taken in the separable and energy cutoff approximation

$$V^{n,n'}_{k,k'} = \tilde{V}^{n,n'}_{k,k'} \theta(\omega_0 - |E_{n,k_y} + \epsilon_{k_y} - \mu|) \theta(\omega_0 - |E_{n',k_y'} + \epsilon_{k_y'} - \mu|).$$ (3)

Here we take account of the interference effects between the single-particle wave functions of the pairing electrons in the different bands, where $n$ and $n'$ are the band indexes, $k_y(k_y')$ is the superlattice wave-vector and $k_x(k_x')$ is the component of the wave-vector in the free-electron-like direction of the initial (final) state in the pairing process:

$$\tilde{V}^{n,n'}_{k,k'} = -\frac{\lambda_{n,n'}}{N_0} S \times \int_S \psi_{n',-k_y'}(y)\psi_{n,-k_y}(y)\psi_{n,k_y}(y)\psi_{n',k_y'}(y)dx dy,$$ (4)

$N_0$ is the DOS at the Fermi energy $E_F$ without the lattice modulation, $\lambda_{n,n'}$ is the dimensionless coupling parameter, $S = L_xL_y$ is the surface of the plane and $\psi_{n,k_y}(y)$ are the eigenfunctions in the 1D superlattice. We have used weak coupling intraband coupling constants 0.14 for the $(n-1)$-th bands, 0.2 for the appearing $n$-th band, a small 0.1 interband attractive or repulsive exchange interband pairing constant and the distribution of calculated intraband pairing terms $(n, n) (n-1, n-1)$ together with the $(n, n-1)$ interband terms is shown in fig. 5.

The system of equations for the gaps needs to be solved iteratively. The anisotropic gaps depend on the band index and on the superlattice wave-vector $k_y$. According to Leggett [59] the ground-state BCS wave function corresponds to an ensemble of overlapping Cooper pairs at weak coupling (BCS regime) and evolves to molecular (non-overlapping) local pairs with bosonic character in the BEC regime. This approach remains valid also if a particular band is in the BCS-BEC crossover and beyond Migdal approximation because all other bands are in the BCS regime and in the Migdal approximation. In this crossover regime the chemical potential $\mu$ results strongly renormalized with respect to the Fermi energy $E_{F,n}$ of the non-interacting system. In the case of a Lifshitz transition, as described in this paper, nearly all electrons in the new appearing Fermi surface condense forming a condensate having a BCS-BEC crossover character.

Therefore at any chosen value of the charge density $\rho$ for a number of the occupied bands, $N_0$, the chemical potential in the superconducting phase has to be renormalized by the gap opening solving the following equation:

$$\rho = \frac{1}{L_xL_y} \sum_{n,k_y} \sum_{n',k_y'} \frac{\lambda_{n,n'} S}{N_0} \int_S \psi_{n',-k_y'}(y)\psi_{n,-k_y}(y)\psi_{n,k_y}(y)\psi_{n',k_y'}(y)dx dy,$$ (5)

Three distinct regimes of multi-gap superconductivity are obtained as a function of the chemical potential tuned around the 2D-1D Lifshitz transition, as reported in fig. 6. At the $n$-th band bottom, when the new Fermi surface pocket starts to appear, there is a coexistence of a BCS-like condensate of the pairs of the $(n-1)$-th band together with a BEC-like condensate of the pairs of the $n$-th band, which, because of the very low density, condense completely in a bosonic liquid. In this regime the critical temperature is extremely low and small variations...
Fig. 6: (Colour online) Results of the BPV theory for the superconducting state properties as a function of the energy distance from the 2D-1D Lifshitz transition. Panel (A): superconducting gaps at zero temperature which open in the band $n$ and $n-1$, and gaps to $T_c$ ratios. Panel (B): superconducting critical temperature and corresponding isotope coefficient. The maximum gaps and $T_c$ are located at the 2D-1D dimensional crossover, with a broad resonance induced by the large value of the phonon energy $\omega_0 = 145$ meV.

of the parameters can lead to large variations in the gaps and in the $T_c$, determining a large peaked value of the isotope coefficient. The peak in the isotope coefficient reported in panel (B) is a finger print of our BPV theory and it signals the strong interplay between the Lifshitz transition at the band bottom and the onset of shape resonant superconductivity. Increasing the chemical potential trough the second Lifshitz transition, the resonant regime of maximum $T_c$ and gaps is obtained. This resonant regime is characterized by an interesting coexistence of BCS-like pair condensate of the $(n-1)$-th band and BCS-BEC crossover-like pair condensate of the $n$-th band. In the resonance regime the two gaps differ by a sizable $2.5$ factor, the isotope effect gets its smallest values and $T_c$ can reach the high value of $123$ K with coupling strengths in the different channels not exceeding $0.3$, values still typical of metals, as Nb. The large energy scale of the phonon (145 meV) determines not only a large prefactor for the critical temperature, but it also induces a large width of the resonant regimes, making it relatively simple to find the right doping levels giving the highest critical temperatures. Finally, for larger chemical potentials, a third regime of conventional two-band superconductivity is reached, with the coexistence of two-particles condensates having both BCS-like character, confirmed also by values of the isotope coefficient approaching $0.5$ and small values of the gaps typical of weakly coupled superconductors. The predicted zero-temperature superconducting gaps to $T_c$ ratios, panel (A), and the isotope coefficient as a function of the critical temperature, panel (B) are reported in fig. 7 so that the present theoretical work can be confirmed by direct experiments. This theory does not include superconducting fluctuations. However it should be noticed that in a multigap/multiband system another fundamental phenomenon helps in stabilizing high-temperature superconductivity: the screening of the superconducting fluctuations. In fact the multiband BCS-BEC crossover in a two-band superconductor (one condensate in the BCS regime, the other in the BCS-BEC regime) can determine the optimal condition to allow the screening of the detrimental superconducting fluctuations due to the large stiffness of the BCS-like condensate in the deep band. Finally, an arrested or frustrated phase separation is expected to occur at a topological Lifshitz transition $[60,61]$ as it was observed in cuprates $[62,63]$ and diborides $[64]$.

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