Lifshitz transitions in multi-band Hubbard models for topological superconductivity in complex quantum matter

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How the macroscopic quantum coherence can resist to the decoherence attacks of high temperature is a major challenge for the science of the 21st century. Superstripes 2017 conference held in Ischia on June 2017 has been focused on the new physics of high $T_c$ superconductors made of complex quantum matter. Today the standard model of high $T_c$ superconductivity which grabs the physics of complex quantum matter is the multi-band Hubbard model where the dome of $T_c$ occurs by driving the chemical potential in the proximity of a topological Lifshitz transition. The multi-gap superconductivity in the $T_c$ dome is driven by exchange interaction between a first condensate in the BEC-BCS crossover which coexists with second BCS condensates. The proximity to Lifshitz transitions in correlated electronic systems gives the ubiquitous arrested phase separation observed in all high temperature superconductors. Non Euclidean filamentary hyperbolic geometry is needed for the space description of superstripes textures produced by the coexistence of short range CDW puddles, hole poor SDW puddles and self organized dopants rich puddles. A road map to room temperature superconductors in particular organic compounds made of superlattices of quantum wires driven by Fano resonances with one of the condensates in the BEC-BCS crossover has been proposed.

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I. INTRODUCTION.

High temperature superconductivity has been found in a sequence of exotic complex materials: ceramics, intermetallies, diborides, iron pnictides and chalcogenides, with the record for the highest critical temperature $T_c$ in pressurized sulfur hydride near structural phase transitions. These superconductors show a dome of high critical temperature in a particular range of interstitials or defects concentration and in a particular range of pressure or misfit strain. Each system shows a different complex landscape characterized by a different type of multi-scale arrested phase separation with local-lattice-distortion, orbital, charge and spin modulations forming textures of puddles of stripes from atomic-scale to nanoscale, mesoscale and micron-scale. These exotic systems are clearly far away from a typical conventional BCS superconductor made of homogeneous metal with a single large Fermi surface.

Experimental evidence for stripes due to anharmonic incommensurate lattice and orbital modulation has been found since 1990 by novel experimental methods using synchrotron radiation. The early results have been reported and discussed at several international conferences focusing on lattice complexity and phase separation [1–5].

The date of birth of the stripes physics in high temperature superconductors can be fixed on Dec 7, 1993 which is the priority date of the patent for material design of heterostructures at atomic limit formed by superlattices of quantum stripes [6]. In this stripes scenario a Fermi liquid coexists with an incommensurate 1D charge density wave (CDW) forming a multigap superconductor near a Lifshitz transition where the critical temperature amplification is driven by Fano resonances involving different condensates. This stripes scenario for the high $T_c$ mechanism was presented at several international conferences in 1994-1996 [3, 9]. The series of conferences on stripes in high temperature superconductors started three years later on Dec 1996 following the confirmation for the presence of stripes by other standard experimental methods like neutron diffraction and NMR [10]. The first Stripes 1996 conference was followed by the second very large conference Stripes 1998 [11] where the very simple Emery model of spin stripes with wave-vector $q_{sdw}$, locked with a charge stripes with wave-vector $q_{cdw}$ became very popular within the scientific community. The series of stripes conference have kept open the discussion on many different proposals for the stripes scenarios like the coexistence of short range charge stripes puddles unlocked from spin stripes puddles [12]. A major problem in the field was the diversity of the stripes scenarios in different families of hole doped cuprates which was solved in 2000 by the disclosure of the key role of the lattice strain field with a critical strain value for the appearing of short range stripes ordering [13]. Moreover at the stripes conference the term superstripes [14] has been coined to indicate the complex landscape generated by an arrested phase-separation near a critical strain point, forming a texture of nano puddles of short range striped charge density wave order [15–19].

At that time, in the year 2000, the proposed heterogeneous landscape of superstripes was in contrast with the most popular paradigm i.e., the single-band Hubbard model. Later many Scanning Tunneling Microscopy.
(STM) experiments have confirmed this scenario providing compelling evidence for electronic nanoscale phase separation. Today the presence of nanoscale puddles of electronic pseudogap matter competing with superconducting condensate puddles with different symmetries is well established. In the new emerging paradigm high temperature superconductors are described as particular forms of complexity where particular forms of complexity are not detrimental (like normal disorder in the majority of disordered superconductors) but they favor higher critical temperatures.

The name of the series of stripes conferences changed its name into superstripes conferences in 2008 driven by clear evidence for phase separation in iron based superconductors. This decision marked the shift of the scientific interest toward quantum phenomena in complex materials. Paul Chu discussed the role of lattice architecture, internal strain and strong electron-phonon coupling and high density of states (DOS) at the van Hove singularity.

On the contrary experiments have shown the failure of these predictions since the parent compounds are antiferromagnetic insulators with an energy gap of about 2 eV. The insulating phase was explained by two different schools. The first school assumed the opening of a Peierls gap over the full Fermi surface with wave-vector $2k_F$ associated with the formation of a 2D Peierls charge density wave. The 2D Peierls CDW can be described as the ordering of polarons in the real space. The CDW competes with the ordering of polaron pairs (bipolarons) in the k-space forming a superconducting phase in the strong coupling limit where below $T_c$ a Bose Einstein Condensation (BEC) occurs. The second school proposed that the insulating phase was due to the opening of a Peierls singularity.

The chemical potential is tuned at the electronic topological Lifshitz transition from the hole-like to the electron-like Fermi surface. Here the system shows a peak in the Density of States (DOS) and strong electron-phonon scattering at the nesting wave-vector $2k_F$ connecting opposite sides of the square Fermi surface. Therefore high temperature superconductivity was expected according with BCS theory because of strong electron-phonon coupling and high density of states (DOS) at the van Hove singularity.

II. FROM THE WOODSTOCK OF PHYSICS TO SUPERSTRIPES 2017

The international conference Superstripes 2017 has been held on June 4-10, 2017 at the Ischia island of the Neapolitan archipelago in Italy. Scientists leaders in the field have been invited to discuss the latest advances in this field. Some discussions at Superstripes 2017 have given an answer to topics open since the APS March meeting held in New York, on 18 March 1987, the so called Woodstock of Physics, where 30 years ago Alex Muller presented the discovery of high temperature superconductivity in ceramic La-Ba-Cu-O materials. Paul C.W Chu reported superconductivity above liquid nitrogen temperature in $YBa_2Cu_3O_{6+y}$ (Y123). At Ischia 2017 conference Alex Muller, presented a review on the key role of complexity in cuprates recently reported in the book on high-$T_c$ copper oxide superconductors presenting the scenario of high temperature superconductivity in complex materials. Paul Chu discussed the role of interfaces in the enhancement of $T_c$ above 77 K including the role of lattice architecture, internal strain and pressure. He pointed out the fact that a single-band Hubbard model is not sufficient for describing high $T_c$, why multi-band Hubbard models are needed. Vladimir Kresin who proposed at the 1987 APS March meeting the theoretical scenario of strong electron-phonon coupling in a complex lattice discussed in Ischia the strong coupling limit in the pairing involving high energy phonons in view of explaining 203 K superconductivity in pressurized $H_3S$ which is today object of active research.

Band structure calculations of the parent compounds $La_2CuO_4$ and $YBa_2Cu_3O_6$ presented at the Woodstock of Physics predicted that the Fermi level is at half filling in a wide band due to the covalent bond between $Cu(3d)$ [ml=2] and $O(2p_{x,y})$ orbital in the metallic $CuO_2$ layers. Considering a perfect tetragonal bcc lattice including only first-neighbor hopping $t$, the 2D Fermi surface at half filling is predicted to have a square shape. The chemical potential is tuned at the electronic topological Lifshitz transition from the hole-like to the electron-like Fermi surface. Here the system shows a peak in the Density of States (DOS) and strong electron-phonon scattering at the nesting wave-vector $2k_F$ connecting opposite sides of the square Fermi surface. Therefore high temperature superconductivity was expected according with BCS theory because of strong electron-phonon coupling and high density of states (DOS) at the van Hove singularity.

III. FROM SINGLE-BAND TO MULTI-BAND HUBBARD MODEL AND LIFSHITZ TRANSITIONS

It was well known that in the frame of a single-band Hubbard model the Mott insulator occurs if $U_{dd}$ is larger than the conduction band-width $W$. At the 1987 APS March meeting it was assumed by the scientific community that chemical doping form itinerant $Cu^{3+}$ impurity states, with $3d^8$ configuration, moving in a background made of $Cu^{2+}$ ions with the $3d^9$ configuration.

Three weeks later on Apr 8th 1987 in the Symposium on High $T_c$ Superconductivity at the 7th General Conference of the Condensed Matter Division of the European Physical Society held in Pisa, Italy, it was reported that the doped holes in doped metallic $Y123$ do not form the expected $Cu^{3+}$ with $3d^8$ configuration but they form the unexpected $Cu^{2+}$ $O^{1-}$ states called $3d^9L$, where L indicates the hole in the ligand oxygen $2p$ orbital.
This result was obtained by Cu $L_{2,3}$-edge x-ray absorption near edge structure (XANES) spectroscopy of the high $T_c$ superconductor Y123 measured using ACO storage ring in Orsay, France in March 1987 [44, 45] and by the Cu $K$-edge XANES measured at the Adone storage ring in Frascati, Italy [46].

These results have been possible thanks to the development of XANES spectroscopy as a probe of both of multiple scattering resonances or shape resonances [47–51] and of many body electronic configurations in valence fluctuation materials, heavy fermions and charge transfer correlated transition metal oxides like NiO, CeO$_2$ and PrO$_2$ [51, 52].

The Cu $L_{2,3}$ X-ray photoelectron spectroscopy (XPS) spectra of Y123 were measured to get $U_{dd}$ in the Italian ENEA Laboratory [53] and the results were found to be in agreement with the XPS experiments made by Fujimori in Tokyo [54] at the same time.

These works have been confirmed in different cuprate families like in $La_{1+0.15}Sr_{0.85}CuO_4$ (La124) [55]. The results have been presented at the four major international conferences in 1987: 1) the Pisa EPS April meeting [56]; 2) at the Special Adriatico Research Conference on High Temperature Superconductors held on 6-8 Jul 1987 in Trieste, Italy [60]; 3) at the tenth Taniguchi international symposium held on October 19-23, 1987 in Kashiokima, Japan [61]; and 4) at the 14th International Conference on X-ray and inner-shell processes, held in Paris on September 14-18, 1987 [62]. The relevance of these results was recognized on 8 Dec 1987 at the Nobel prize ceremony where Alex Muller reported that:

> [early photoelectron core-level spectra (XPS and UPS) by Fujimori et al. [55] and Bianconi et al. [57] in $La_{1-0.15}Sr_{0.85}Cu_2O_4$ and $YBa_2Cu_3O_7$ did not reveal a final state owing to a Cu$^{3+}$ 3d$^0$ state]

In fact the XPS experiments [49, 57] have clearly shown that the parent compounds are Mott insulators with the Coulomb repulsion between two holes in the Cu 3d orbitals $U_{dd} = 6 \, \text{eV}$ [48, 57], larger than the conduction bandwidth which was calculated by band structure calculations for non interacting fermions. The Cu $L_3$ XANES experiments have shown that the carriers, created by doping, are states with 3d$^0$L many body configuration in the correlation gap.

The correlation gap in both La124 and Y123 compounds is not $U_{dd}$ as expected for a single-band Hubbard model but the charge transfer gap for the excitation from the $[\text{Cu}(3d^0), O(2p^6)]$ to the $[\text{Cu}(3d^{10}), O(2p^5)]$ many body configuration, called also the $3d^0$ to $3d^{10}L$ gap, which was predicted for the correlated charge transfer transition metal oxides [58].

A month after the EPS 1987 Pisa conference, Emery understood that the results of the Cu $L_3$-edge experiment [44] had falsified the single-band Hubbard model and proposed in June 1987 the three-band Hubbard model [63] involving p and d orbitals for hole doped cuprates.

The experimental evidence of the 3d$^0$L by A. Bianconi [60] and the V. Emery theory paradigm of the p-d three-band Hubbard model were presented together at the Adriatico Trieste meeting in July 1987. After the Adriatico 1987 meeting the fact that doped holes are in the oxygen orbital in cuprates was widely accepted by the community as recognized by Alex Muller in the opening talk at the 3rd international conference on Materials and Mechanisms of Superconductivity in 1991 at Kanazawa Japan [65]:

> [The carriers in these type of conducting cuprates are holes on the oxygens. To me the first indication came from X-ray absorption spectroscopy by Prof. Bianconi at University of Rome]

Evidence for the 3d$^0$L states induced by doping in the correlation gap was presented in 1988 at the first $M^2S$ conference in Interlaken [66, 68], and at the international Symposium on the Electronic Structure of High $T_c$ Superconductors, Rome, 5-7 October 1988 [69], where it was confirmed by many authors [70, 74]. These results have been confirmed by experiments and theories published in 1989 [75, 76]; and in 1990 [77, 78]; in 1991 [79, 81]; in 1992 [82, 83]; in 1993 [84, 85]; in 1995-1997 [86, 87] and in these last 10 years [88, 90].

It was established that the correct model for high temperature superconductors is the multi-band Hubbard model, where the domes of high $T_c$ occur in the proximity of electronic topological transitions called Lifshitz transitions.

Boguliobov equations for a multigap superconductor near a band edge have been solved by numerical calculations for the cases of sulfur hydrides, cuprates, diborides, and iron based superconductors [37, 91–99]. Recently it was shown that this mechanism for high $T_c$ can be in action in particular filamentary organic compounds [100] where the condensate in the new appearing Fermi surface is in the BEC-BCS crossover regime.

Also the ubiquitous nanoscale phase separation occurring in high temperature superconductors has been shown to be driven by the proximity to a Lifshitz transition in multi-band Hubbard models [101, 102].

IV. RECENT ADVANCES

At superstripes 2017 conference it was proposed that the origin of the multiple Fermi surfaces could be determined by oxygen interstitials self-organization as it has been shown in the case of HgBa$_2$CuO$_{4-y}$ (Hg1201) where the oxygen interstitials (O-i) are not homogeneously distributed but form one-dimensional atomic wires which can dramatically enhance the critical temperature. [103]. The complex interplay of charge, spin [104, 105] and orbital degrees of freedom including spin-orbit interaction in topological matter [110, 111] are now object of investigation as key ingredients. The rich physics of unconventional superconductivity in cuprates and their asymmetry between electron doped and hole doped families continue to attract theory and experimental research [112–117]. Ivanov has shown the noncentrosymmetric struc-
ture of a Bi2212 crystal at optimum doping in a high magnetic field by using x-ray magnetic circular dichroism, XMCD. This new result suggests a possible role of spin-orbit coupling. Investigation of basic physics in low dimensional quasi 1D superconductors \[118, 119\] and in the 2D electron gas \[120, 121\] have been object of high interest to unveil key features of dimensionality in unconventional superconductors. Iron based superconductors continue to provide a clear case for the study of the interplay of nanoscale phase separation and multi-gap superconductivity \[122-124\]. New topics in physics and materials science are provided by systems out-of-equilibrium \[125\], novel silver based materials \[126\] and granular materials \[127\]. Finally key advances in the quantum electronics using superconducting devices \[128, 129\] and on metal-to-insulator transition in \(\text{VO}_2\) \[130\] have been reported at Superstripes 2017.

V. CONCLUSIONS

There is today after many years of discussion a growing agreement in the scientific community on some key common physical features of high temperature superconductors. All high \(T_c\) superconductors are highly inhomogeneous and different multi-band Hubbard models are needed to describe unconventional high temperature superconductors. Topology, Lifshitz transitions, and spin-orbit coupling are opening new fields of research in condensed matter of strongly correlated materials. Further works will be addressed to exchange interaction giving Fano resonances between condensates in the strong coupling regime in hot spots of the Fermi surface coexisting with condensates in other portions of the Fermi surfaces in the weak coupling regime, which can be manipulated in metalorganic materials to get room temperature superconductors \[100\].

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