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I.2

FESHBACH SHAPE RESONANCES IN MULTIBAND HIGH T_C SUPERCONDUCTORS

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Abstract: We describe particular nanoarchitectures (superlattices of superconducting wires and layers) where a mechanism to evade temperature decoherence effects in a quantum condensate is switched on by tuning the charge density. The superlattice structure determines the subbands and the corresponding Bloch wavefunctions of charge carriers at the Fermi level *with different parity* and *different spatial locations.* The disparity and negligible overlap between electron wave-functions in different subbands suppress the single electron interband impurity scattering rate and allow the multiband superconductivity in the clean limit. The quantum trick that bestows to the system the property to resist to the decoherence attacks of high temperature is the Feshbach shape resonance in the interband off-diagonal exchange-like pairing term i.e., in the quantum configuration interaction between pairing channels in different subbands. It occurs by tuning the chemical potential at a particular point near a Van Hove singularity (vHs) in the electronic energy spectrum, or a Lifshitz electronic topological transition (ETT), associated with the change of the dimensionality of the Fermi surface topology of one of the subbands.

Key words: Feshbach resonance; Shape resonance; Diborides; Heterostructure at atomic limit.

1. INTRODUCTION

Understanding the mechanism that allows a quantum condensate to resist to the decoherence attacks of temperature is relevant in many fields going from high T_c superconductivity [1] to quantum computing and quantum biophysics [2]. It is possible that the evolution has refined the living matter to acquire a quantum phase coherence for its biochemical reactions. In fact the living matter displays a dynamical and spatial order with collective properties and non-local interactions as a superfluid. So the research is focusing on the nanoarchitectures deploying quantum tricks for the decoherence-evading qualities at room temperature

The macroscopic quantum phase coherence in superfluids [3-5] appears only below a critical temperature T_c much lower than the earth temperature because the phase coherence is suppressed by decoherence effects at high temperature. While the research for high T_c superconductors has been focused for many years to systems at the borderline between superconducting and ferromagnetic or antiferromagnetic phases it is now shifting toward the identification of a particular nanoscale heterogeneity suppressing decoherence effects at high temperature. The key for solving the problem could be in subtle structural and electronic details.

Looking for details in the theory of superconductivity one has to go beyond the standard BCS approximations [3] for a generic homogeneous system (i) the high Fermi energy: the Fermi energy is assumed at an infinite distance from the top or the bottom of the conduction band, (ii) the isotropic approximation: the pairing mechanism is not electronic state dependent. The BCS wave-function of the superconducting ground state has been constructed by configuration interaction of all electron pairs (+k with spin up, and -k with spin down) on the Fermi surface in an energy window that is the energy cut off of the interaction,

$$|\Psi_{BCS}\rangle = \prod_k (u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow})|0\rangle \qquad (1)$$

where $|0\rangle$ is the vacuum state, and $c^+_{k\uparrow}$ is the creation operator for an electron with momentum k and spin up. The Schrieffer idea [3] of this state with off-diagonal long range order came from the configuration interaction theory by Tomonaga involving a pion condensate around the nucleus [6].

In anisotropic superconductivity one has to consider configuration interaction between pairs, in an energy window ΔE around the Fermi level, in different locations of the k-space with a different pairing strength, that gives a k-space dependent superfluid order parameter i.e., a k-dependent superconducting gap.
A particular case of anisotropic superconductivity is multiband superconductivity, where the order parameter and the excitation gap are mainly different in different bands.

The advances in this field are related with the development of the theory of configuration interaction between different excitation channels in nuclear physics including quantum superposition of states corresponding to *different spatial locations* for interpretation of resonances in nuclear scattering cross-section [7] related with the Fano configuration interaction theory for autoionization processes in atomic physics [8].

The theory of two band superconductivity, including the configuration interaction of pairs of oppositive spin and momentum in the *a*-band and *b*-band, was developed on basis of the Bogolyubov transformations [9-13] where the many body wave function [14] is given by

$$\left|\Psi_{Kondo}\right\rangle = \prod_{k}(u_k + v_k a^{+}_{k\uparrow} a^{+}_{-k\downarrow}) \prod_{k'}(x_{k'} + y_{k'} b^{+}_{k'\uparrow} b^{+}_{-k'\downarrow})\left|0\right\rangle \qquad (2)$$

The element corresponding to the transfer of a pair from the *a*-band to the *b*-band or vice versa appears with the negative sign in the expression of the energy. This gain of energy is the origin of the increase of the transition temperature driven by interband pairing.

The two band superconductivity has been proposed for metallic elements and alloys [10-42], for doped cuprate perovskites [43-114], for magnesium diboride [115-184] and for few other materials as Nb doped $SrTiO_3$ [185], Sr_2RuO_4 [186-188] YNi_2B_2C, $LuNi_2B_2C$ [189] and $NbSe_2$ [190]. We provide a nearly complete reference list on this subject since it is not available elsewhere.

The multiband superconductivity shows up only in the "clean limit", where the single electron mean free path for the interband impurity scattering satisfies the condition $l > hv_F/\Delta_{av}$ where v_F is the Fermi velocity and Δ_{av} is the average superconducting gap [24,28,30,35].

The criterium that the mean free path should be larger than the superconducting coherence length must be met. This is a very strict

condition that implies also that the impurity interband scattering rate γ_{ab} should be very small $\gamma_{ab} << (1/2)(K_B/\hbar)T_c$. Therefore most of the metals are in the "dirty limit" where the interband impurity scattering mixes the electron wave functions of electrons on different spots on bare Fermi surfaces and it reduces the system to an effective single Fermi surface.

The "interchannel pairing" or "interband pairing" that transfers a pair from the "a"-band to the "b"-band and viceversa in the multiband superconductivity theory is expressed by

$$\sum_{k,k'} J(k,k')(a^+_{k\uparrow} a^+_{-k\downarrow} b_{-k'\downarrow} b_{k'\uparrow}) \qquad (3)$$

where a^+ and b^+ are creation operators of electrons in the "a" and "b" band respectively and $J(k,k')$ is an exchange-like integral. This interband pairing interaction may be repulsive as it was first noticed by Kondo [14]. Therefore it is a non-BCS pairing process since in the BCS theory an attractive interaction is required for the formation of Cooper pairs.

Another charateristic feature of multiband superconductivity is that the order parameter shows the sign reversal in the case of a repulsive interband pairing interaction [26].

The non-BCS nature of the interband pairing process is indicated also by the fact that, when it is dominant, the isotope effect vanishes even if the intra-band attractive interaction in each band is due to the electron-phonon coupling.

Moreover the effective repulsive Coulomb pseudopotential in the Migdal-Eliashberg theory is expected to decrease (so the effective coupling strength increases) where the interband pairing is dominant.

In this work we will discuss the particular case of multiband superconductivity where a Van Hove-Lifshitz feature [191] in the electronic energy spectrum associated with a change of Fermi surface topology shown in Fig. 1 occurs within an energy window around the Fermi energy. The width of this windows is the cut-off energy for the pairing that is determined by the energy of the exchanged excitation of phononic or electronic or magnetic origin.

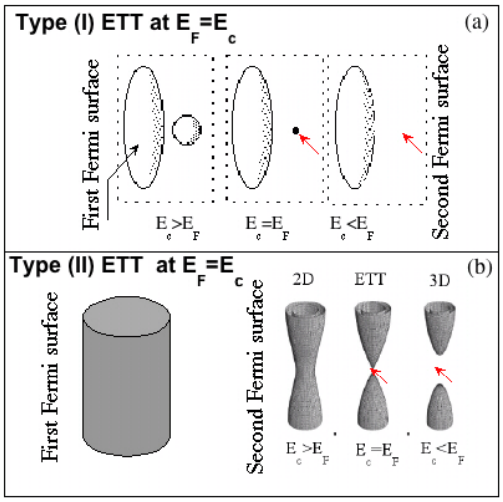

Figure: I:2:1. The different types of 2.5 Lifshitz electronic topological transition (ETT): The upper panel shows the type (I) ETT where the chemical potential E_F is tuned to a Van Hove singularity (vHs) at the bottom (or at the top) of a second band with the appearance (or disappearance) of a new detached Fermi surface region. The lower panel shows the type (II) ETT with the disruption (or formation) of a "neck" in a second Fermi surface where the chemical potential E_F is tuned at a vHs associated with the gradual transformation of the second Fermi surface from a two-dimensional (2D) cylinder to a closed surface with three dimensional (3D) topology characteristics of a superlattice of metallic layers.

2. FESHBACH SHAPE RESONANCES

The "shape resonances" have been described by Feshbach in elastic scattering cross-section for the processes of neutron capture and nuclear fission [7] in the cloudy crystal ball model of nuclear reactions. These scattering theory is dealing with configuration interaction in multi-channel processes involving states with *different spatial locations.* Therefore these resonances can be called also Feshbach shape resonances. These resonances are a clear well established manifestation of the non locality of quantum mechanics and appear in many fields of physics and chemistry [8,192] such as the molecular association and dissociation processes.

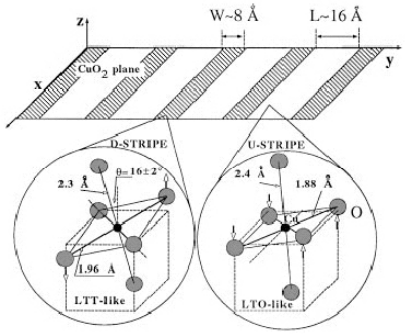

*Figure **I**:2:2.* The pictorial view of the superlattice of stripes of mesoscopic lattice fluctuations in La124, and Bi2212 systems determined by EXAFS [87] and resonant anomalous x-ray diffraction [88].

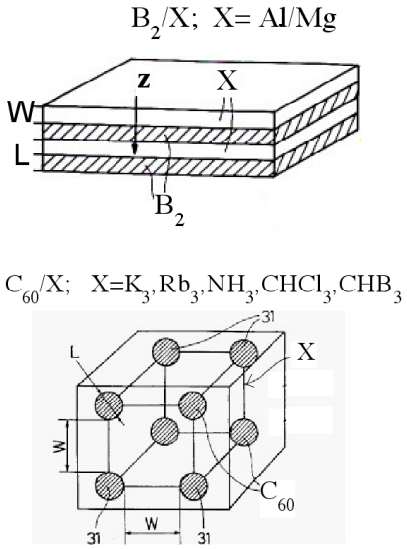

*Figure **I**:2:3.* The metal heterostructures at the atomic limit: a superlattice of superconducting layers and a superlattice of superconducting spheres

Feshbach resonances for molecular association and dissociation have been proposed for the manipulation of the interatomic interaction in ultracold atomic gases. In fact the interparticle interaction shows resonances tuning the chemical potential of the atomic gas around the energy of a discrete level of a biatomic molecule controlled by an external magnetic field [193]. This quantum phenomenon has been used by Ketterle to achieve the Bose-Einstein condensation (BEC) in the dilute bosonic gases of alkali atoms [194]. Feshbach resonances have recently been used to get a BCS-like condensate in fermionic ultra-cold gases with large values of T_c/T_F [195].

The process for increasing T_c by a Feshbach "shape resonance" was first proposed by Blatt and Thompson [15,16,19] in 1963 for a superconducting thin film. The shape resonance described by Blatt occurs in a superconducting thin film of thickness L where the chemical potential crosses the bottom E_n of the n-th subband of the film, a quantum well, characterized by $k_z = n\pi/L$ with n>1. Therefore it occurs where the chemical potential E_F is tuned near the critical energy $E_F=E_n$ for a 2.5 Lifshitz electronic topological transition (ETT) [191] of type (I) as shown in Fig. 1. At this ETT a small Fermi surface of a second subband disappears while the large 2D Fermi surface of a first subband shows minor variations. In the "clean limit" the single electrons cannot be scattered from the nth to the (n-1)th subband and viceversa, but configuration interaction between pairs in different bands is possible in an energy window around $E_F=E_n$. Therefore the Feshbach shape resonance occurs by tuning the Lifshitz parameter $z=E_F-E_n$ around z=0. In the Blatt proposal z is tuned by changing the film thickness. The prediction of Blatt and Thompson of the oscillatory behavior of T_c as a function of film thickness L has been recently confirmed experimentally for a superconducting film [196] although phase fluctuations due to the electron confinement in the two dimension is expected to reduce the critical temperature.

In 1993, following the experimental evidence of nanoscale striped lattice fluctuations in cuprates shown in Fig. 2, we have proposed to increase T_c via a Feshbach shape resonance in a different class of systems: superlattices of superconducting units as shown in Fig. 3 [75,76,80,81,87-89,93-97,102,109,110].

The idea is that the particular heterogeneous architectures formed by a superlattice of metallic superconducting units intercalated by a different material can bestow decoherence evading qualities to the system. The superconducting units can be dots, spheres, wires, tubes, layers, films and

some practical realizations of these architectures are shown in Fig. 3: (i) superlattices of fullerene (quantum spheres), or graphene layers (quantum wells) using carbon atoms intercalated by different atoms can be a practical realization of heterostructures at atomic limit; (ii) superlattices of lead layers intercalated by germanium or silicon layers; (iii) superlattices of bcc metallic layers intercalated by fcc rocksalt layers of a different metal rotated by 45 degrees; (iiii) superlattices of superconductiving honeycomb monolayers intercalated by hcp metallic monolayers.

The quantum tricks to realize high T_c superconductors are based on the generic feature of the electronic structure of the superlattices: the presence of different subbands where the charge density associated with each subband is non homogenously distributed in the real space and single electron interband hopping is forbidden by symmetry.

First, the disparity and negligible overlap between electron wavefunctions of different subbands suppress the impurity scattering rate that allows multiband superconductivity in the clean limit. Second, tuning the chemical potential in superlattices of metallic layers shown in Fig. 3 it is possible to approach the type (II) ETT characterized by the opening or closing of a neck in the one of the Fermi surfaces. This simple case is shown in Fig. 1 where the chemical potential is tuned in the region where one Fermi surface changes from a the three-dimensional (3D), for $E_F>E_c$ to a two-dimensional (2D) topology, for $E_F<E_c$.

3. SHAPE RESONANCE IN SUPERLATTICES OF QUANTUM WIRES

The calculation of a Feshbach shape resonance has been carried out for a 2D superlattice of carbon nanotubes of period λ_p on a 2D x,y plane shown in Fig. 4. The electronic structure is similar to the case of a superlattice of stripes [93-96,102] and this type of heterostructures at atomic limit can be classified as “superlattices of quantum wires". While the charge carriers move as free charges in the x direction, the wire direction, they have to overcome a periodic potential barrier V(x,y), with period λ_p, amplitude V_b

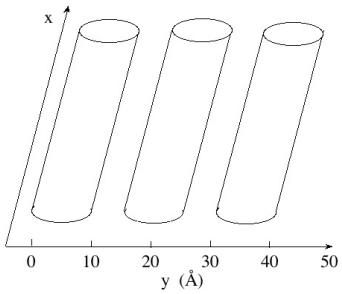

Figure I:2:4. The pictorial view of a 2D superlattice of carbon nanotubes with a period λ_p =1.55 nm in the y direction.

and width W along the y direction, constant in the x direction, expressed for x=constant as:

$$V(y) = -V_b\theta\left(\frac{L}{2} - \tilde{y}\right) \quad where \quad \tilde{y} = y - q\ \lambda_p - \frac{\lambda_p}{2} \tag{4}$$

and q is the integer part of y/λ_p.

The solution of the Schrödinger equation for this system, $-\frac{\hbar^2}{2m}\nabla^2\psi(x,y) + V(x,y)\,\psi(x,y) = \mathrm{E}\,\psi(x,y)$ is given as

$$\psi_{n,k_x,k_y}(x,y) = e^{ik_x x} \cdot e^{ik_y q\lambda_p}\,\psi_{n,k_y}(y) \tag{5}$$

where in the stripe

$$\psi_{n,k_y}(y) = \alpha e^{ik_w\tilde{y}} + \beta e^{-ik_w\tilde{y}} \quad for\,|\tilde{y}| < L/2$$

$$k_w = \sqrt{2m_w\left(E_n\left(k_y\right) + V_b\right)/\hbar^2}$$

and in the barrier

$$\psi_{n,k_y}(y) = \gamma e^{ik_b\tilde{y}} + \delta e^{-ik_b\tilde{y}} \quad for\,|\tilde{y}| \geq L/2$$

$$k_b = \sqrt{2m_b E_n(k_y)/\hbar^2}$$

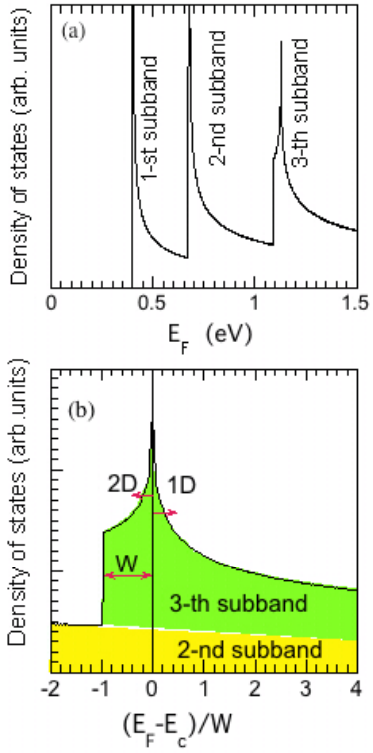

Figure I:2:5. Panel (a) The total density of states (DOS) of a superlattice of nanotubes. The partial DOS of each subband n=1,2,3 gives a peak near the bottom of each subband. Panel (b) shows the details of the DOS near the bottom of the third subband as function of the reduced Liftshitz parameter $"z" = (E_F - E_c)/W$ where W=36.6 meV is the dispersion of the third subband in the y direction of the superlattice, transversal to the nanotube direction. The type (I) ETT occurs at the subband edge ("z"=-1) where the partial DOS of the third subband gives the step-like increase of the DOS. The type (III) ETT occurs at "z"=0 where the DOS shows the main peak.

The coefficients α, β, γ and δ are obtained by imposing the Bloch conditions with periodicity λ_p, the continuity conditions of the wave function and its derivative at L/2, and finally by normalization in the surface unit. The solution of the eigenvalue equation for E gives the electronic energy dispersion for the n-th subband with energy

$$\varepsilon_n\left(k_x, k_y\right) = \varepsilon\left(k_x\right) + E_n\left(k_y\right) \text{ where } \quad \varepsilon\left(k_x\right) = \left(\hbar^2/2m\right)\, k_x^2$$

is the free electron energy dispersion in the x direction and $E_n\left(k_y\right)$ is the dispersion in the y direction.

There are N_b solutions for $E_n\left(k_y\right)$, with $1 \leq n \leq N_b$, for each k_Y in the Brillouin zone of the superlattice giving a dispersion in the y direction of the N_b subbands with $k_X=0$.

The partial density of states (DOS) of the n-th subband gives a step-like increase of the total DOS when the chemical potential reaches the bottom of the subband n=1,2,3 where a type (I) ETT occurs as shown in Fig. 5. The DOS peaks in Fig. 5 are due to partial DOS of each subband tuning the chemical potential by electron doping at the vHs associated with the type (III) ETT in each subband. The panel (b) of Fig. 5 shows the details of the DOS near the type (III) ETT at E_c in the third subband as a function of the reduced Liftshitz parameter $"z" = (E_F - E_c)/W$ where W is the dispersion of the third subband in the y direction of the superlattice, transversal to the nanotube direction.

The pictorial view of the Fermi surfaces of the third and second subbands is shown in Fig. 6. The variation of the Fermi surface topology going through the type (III) ETT is shown. The Fermi surface of the third subband changes from the 1D topology to 2D going from $E_F > E_c$ to $E_F < E_c$ respectively.

The superlattice with its characteristic wavevector $q=2\pi/\lambda_p$ induces a relevant k dependent interband pairing interaction $V_{n,n'}\left(k, k'\right)$. This is the non BCS interband effective pairing interaction (of any repulsive or attractive nature [14,26]) with a generic cutoff energy $\hbar\omega_o$.

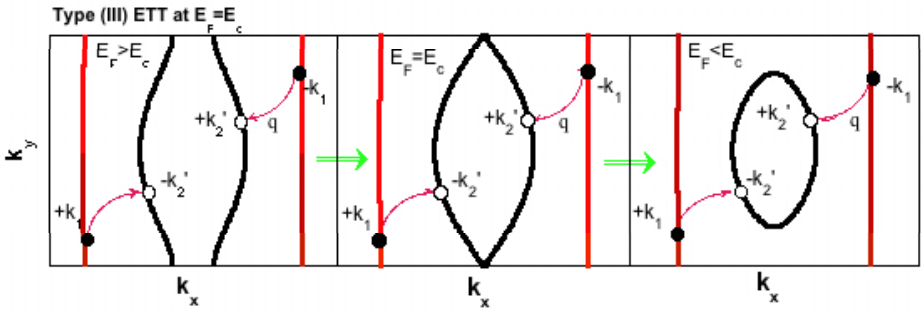

Figure I:2:6. The Fermi surface of the second (red) and third subband (black) of a 2D superlattice of quantum wires near the type (III) ETT where the third subband changes from the one-dimensional (left panel) to two-dimensional (right panel) topology. Going from the left panel to the right panel the chemical potential E_F crosses a vHs singularity at E_c associated with the change of the Fermi topology going from $E_F>E_c$ to $E_F<E_c$, while the Fermi surface of the second subband retains its one-dimensional (1D) character. A relevant inter-band pairing process with the transfer of a pair from the first to the second subband and viceversa is shown.

The interband interaction is controlled by the details of the *quantum superposition of states corresponding to different spatial locations i.e,* between the wave functions of the pairing electrons in the different subbands of the superlattice

$$V_{n,n'}\left(k,k'\right)=V^{o}_{n,k_y;n',k_y}\theta(\hbar\omega_0-\left|\varepsilon_n(k)-\mu\right|)\,\theta(\hbar\omega_0-\left|\varepsilon_{n'}(k')-\mu\right|) \qquad (6)$$

where $k=\left(k_x,k_y\right)$ and

$$V^{o}_{n,k_y;n',k'_y}=-J\int_S dx\,dy\,\psi_{n,-k}(x,y)\psi_{n',-k'}(x,y)\psi_{n,k}(x,y)\psi_{n',k'}(x,y)$$

$$=-J\int_S dx\,dy\left|\psi_{n,k}(x,y)\right|^2\left|\psi_{n',k'}(x,y)\right|^2$$

n and n' are the subband indexes. k_X (k_X') is the component of the wavevector in the wire direction (or longitudinal direction) and k_Y, (k_Y') is the superlattice wavevector (in the transverse direction) of the initial (final) state in the pairing process, and μ is the chemical potential.

In the separable kernel approximation, the gap parameter has the same energy cut off $\hbar\omega_o$ as the interaction. Therefore it takes the values Δ_n (k_y) around the Fermi surface in a range $\hbar\omega_o$ depending from the subband index and the superlattice wavevector k_y.

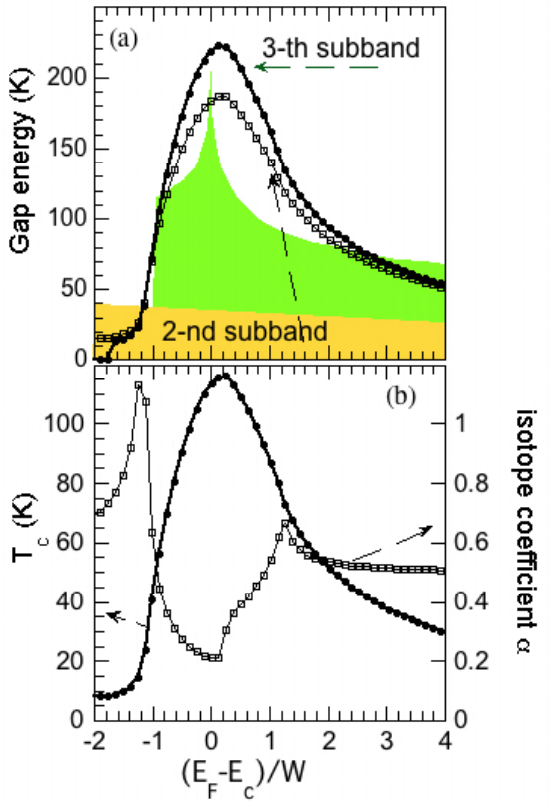

Figure I:2:7. Panel (a): The superconducting gaps in the second, Δ_2, and third, Δ_3, subband in a superlattice of quantum wires as a function of the reduced Lifshitz parameter "z". Panel (b) The critical temperature T_c and the isotope coefficient α at the shape resonance as a function of "z".

The self consistent equation, for the ground state energy gap Δ_n (k_y) is:

$$\Delta_n(\mu, k_y) = -\frac{1}{2N}\sum_{n' k_y' k_x'} \frac{V_{n,n'}\left(k,k'\right)\cdot \Delta_{n'}(k_y')}{\sqrt{(E_{n'}(k_y') + \varepsilon_{k_x'} - \mu)^2 + \Delta_{n'}^2(k_y')}} \tag{7}$$

where N is the total number of wavevectors. Solving iteratively this equation gives the anisotropic gaps dependent on the subband index and weakly dependent on the superlattice wavevector k_y. The structure in the interaction gives different values for the gaps Δ_n giving a system with an anisotropic gaps in the different segments of the Fermi surface.

The superconducting gaps in the second, Δ_2, and third, Δ_3, subband in a superlattice of quantum wires as a function of the reduced Lifshitz parameter "z" are shown in Fig. 7a, where E_F is tuned at E_c for "z"=0, the energy cut off for the pairing interaction is fixed at 500K. The increase of the gap Δ_2 is driven only by the Feshbach resonance in the interband pairing since the partial DOS of the second subband has not peaks.

The critical temperature T_c of the superconducting transition can be calculated by iterative method

$$\Delta_n(k) = -\frac{1}{N}\sum_{n' k'} V_{nn'}(k,k')\frac{\mathrm{tgh}(\frac{\xi_{n'}(k')}{2T_c})}{2\xi_{n'}(k')}\Delta_{n'}(k') \tag{8}$$

where $\xi_n(k)=\varepsilon_n(k)-\mu$.

The interband pairing term enhances T_c [93-97,102] by tuning the chemical potential in an energy window around the Van Hove singularities, "z"=0, associated with a change of the topology of the Fermi surface from 1D to 2D (or 2D to 3D) of one of the subbands of the superlattice in the clean limit.

The critical temperature T_c and the isotope coefficient α at the shape resonance are shown in Fig. 7. The result shows the characteristic feature of the T_c amplification by a shape resonance at the maximum critical temperature $T_{c,max}$ the isotope coefficient is close to zero or negative, and

shows large positive values up to 1.2 much larger that the standard BCS value α=0.5 at the border of the resonance.

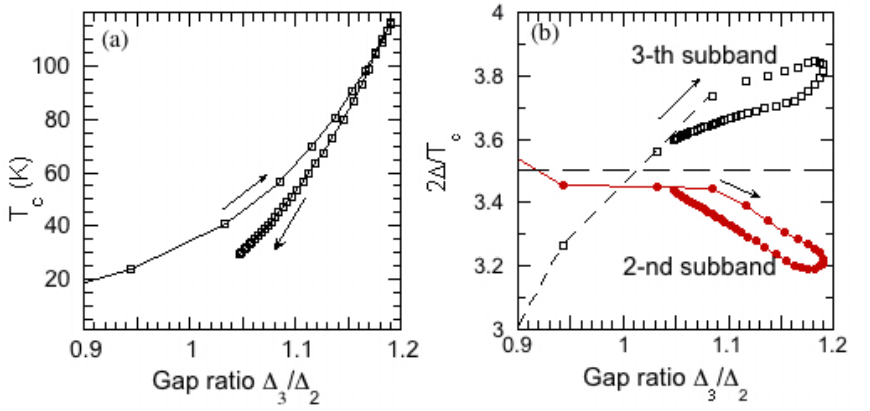

Figure I:2:8. Panel (a) The variation of T_c as a function of the gap ratio $R=\Delta_3/\Delta_2$ at the shape resonance. The maximum T_c is reached for the maximum gap ratio. Panel (b) the ratio $2\Delta_2/T_c$ and $2\Delta_3/T_c$ as a function of the gap ratio Δ_3/Δ_2. The largest deviation from the single band BCS value $2\Delta/T_c=0.35$ is reached at the highest gap ratio indicating the key effect of multiband superconductivity.

In Fig. 8 we report the variation of T_c as a function of the gap ratio Δ_3/Δ_2 showing that the critical temperature increases by increasing the gap ratio. This provides direct evidence that is a measure of the relevance of the shape resonance in interband pairing. Also the ratio $2\Delta_2/T_c$ and $2\Delta_3/T_c$ show large deviations from the BCS value $2\Delta/T_c=0.35$ for a single band indicating the key effect of multiband superconductivity. These calculations show that the interband pairing enhances T_c [93, 95] by tuning the chemical potential at the shape resonance.

4. SHAPE RESONANCES IN SUPERLATTICES OF QUANTUM WELLS

MgB_2 provides the simplest high T_c superconductor therefore it could play a key role for understanding high T_c superconductivity as atomic hydrogen for quantum mechanics. There is now growing evidence that MgB_2 is a practical realization of the proposed T_c amplification process driven by Feshbach shape resonances in interband pairing [116,120,132,139,144,162, 176,177,180] representing the case of a superlattice of quantum wells

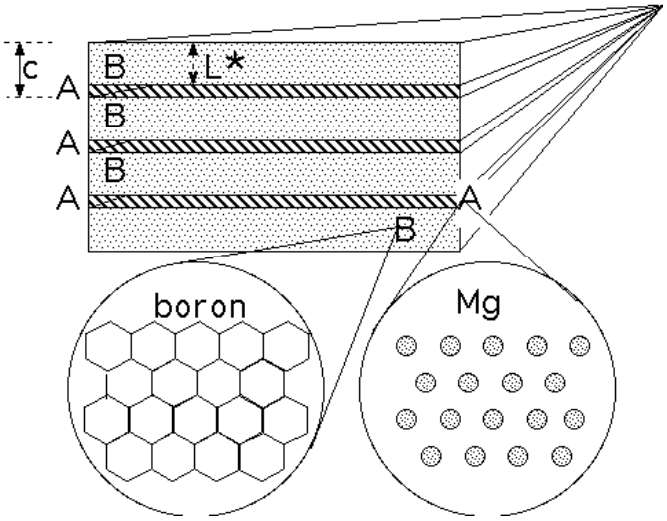

Figure I:2:9. The superlattice of metallic layers (B) made of graphite-like honeycomb boron planes separated by hexagonal Mg layers (A) forming a superlattice ...ABABAB… where the c-axis is the period of the superlattice.

The light-metal diborides AB_2 (A=Mg, Al) are not common natural compounds. They have been discovered as residuals in the chemical

processing [197,198] for the reduction of boron oxide with electropositive metals to obtain elemental boron. Following the synthesis and characterization of aluminum diboride (AlB_2) in 1935 [199] magnesium diboride (MgB_2) was synthesized in 1953 [200-201] when the chemical interest in borides was driven by nuclear power industry for control rods and neutron shields.

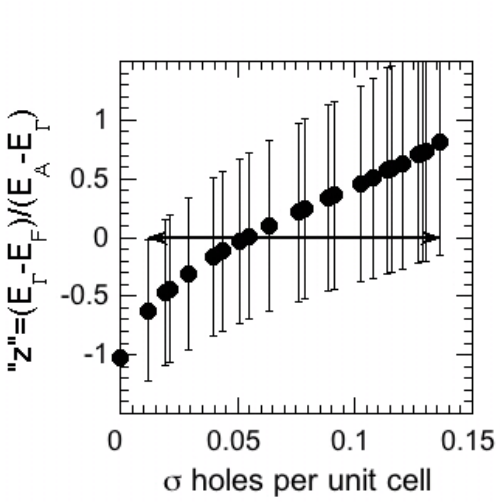

Figure I:2:10. The reduced Lifshitz parameter $"z" = (E_\Gamma - E_F)/(E_A - E_\Gamma)$, where ($E_A$- E_Γ) is the full energy band dispersion in the c-axis direction, as a function of the number of holes in the σ subband in Al doped MgB_2. The quantum uncertainty in the z value is indicated by the error bars that are given by $D\sqrt{\langle\sigma_{z,y}^2\rangle}/(E_A - E_\Gamma)$ where D is the deformation potential and $\langle\sigma_{x,y}^2\rangle$ is the mean square boron displacement at T=0K associated with the E_{2g} mode measured by neutron diffraction [139]. The T_c amplification by Feshbach shape resonance occurs in the σ hole density range shown by the double arrow indicating where the 2D-3D ETT sweeps through the Fermi level because of zero point lattice motion, i.e., where the error bars intersect the z=0 line.

For many years MgB_2 was not considered as a possible superconductor by the scientific community on the basis of conventional theories or material science rules for search of high T_c superconductors. The AlB_2 crystalline

structure is a heterostructure at the atomic limit made of superconducting layers (boron monolayers) intercalated by different layers (Al or Mg hcp monolayers) shown in Fig. 9.

The σ band is usually fully occupied in non superconducting diborides where there are no holes in the σband, so these diborides, as AlB_2 have a Fermi surface of the type shown for the case $E_F>E_A$ in Fig. 10. In MgB_2 the σ band is partially unoccupied due to the electron transfer from the boron layers to the magnesium layers. In fact the chemical potential E_F in MgB_2 is at about 750 meV below the energy E_A of the top of the σ band. Moreover the chemical potential E_F in MgB_2 is also at about 350 meV below the energy of the Γ point in the band structure ($E_\Gamma>E_F$). Therefore the σ Fermi surface of MgB_2 where $E_F<E_\Gamma<E_A$ has the corrugated tubular shape with a two-dimensional topology of the type shown in Fig. 10 for the case $E_F<E_\Gamma$. Going from below ($E_F<E_\Gamma<E_A$) to above the energy of the Γ point the σ Fermi surface becomes a closed Fermi surface with 3D topology like in $AlMgB_4$ that belongs to the Fermi surface type for the case $E_\Gamma<E_F<E_A$.Therefore by tuning the chemical potential E_F, by electron doping the σ subband, it is possible to reach the point where E_F is tuned at the 2D/3D Van Hove singularity. This is a type (II) 2.5 Lifshitz electronic topological transition (ETT) with the disruption of a "neck" in the σ Fermi surface with the critical point at $E_F=E_\Gamma$. The changes of physical properties near the ETT transition are studied here as a function of the reduced Lifshitz parameter "z"=$(E_\Gamma-E_F)/(E_A-E_\Gamma)$, where W=$(E_A-E_\Gamma)$ is the energy dispersion in the c-axis direction due to electron hopping between the boron layers (W=0.4 eV in MgB_2 but it changes with chemical substitutions). The influence of the proximity to a type (II) electronic topological transition on the anomalous electronic and lattice properties of MgB_2 is shown by the anomalous pressure dependence of the E_{2g} phonon mode and T_c (202, 203).
The response of the superconducting properties of diborides to Fermi level tuning has been studied by electron doping using atomic substitutions, in fact it is possible to reduce the number of holes in the σ band from about 0.15 holes per unit cell in MgB_2 up to reach zero σ holes at the top of the σ band for "z"=-1 where $E_F=E_A$.

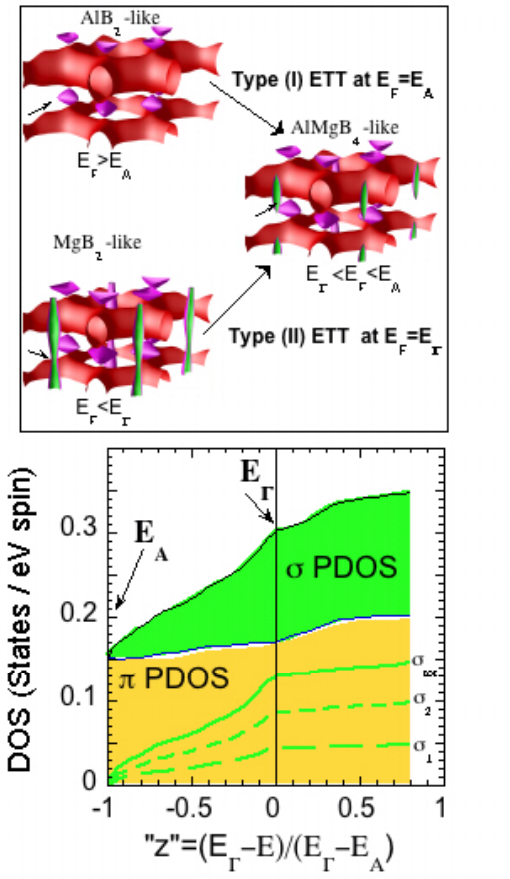

Figure I:2:11. The total density of states (DOS) in MgB_2 and the partial DOS (PDOS) of the σ and π band as a function of the reduced Lifshitz parameter 'z". The upper curve shows two different types of 2.5 Lifshitz electronic topological transition (ETT) in electron doped MgB_2 associated with changes of the Fermi surface topology. The type (I) ETT: with the appearance of the closed 3D σ Fermi surface by tuning the Fermi energy at the critical point $E_F=E_A$ where E_A is the energy of the A point in the band structure. The type (II) ETT with the disruption of a "neck" in the σ Fermi surface by tuning the chemical potential E_F at the critical point in the band structure $E_F=E_\Gamma$ where the σ Fermi surface changes from a 2D corrugated tube for $E_\Gamma>E_F$ to a closed 3D Fermi surface for $E_\Gamma<E_F$ while the large π Fermi surface keeps its 3D topology [163].

We report in Fig. 11 the variation of the reduced Lifshitz parameter "z" as a function of the number of holes in the σsubband for the case of Al doped $Mg_{1-x}Al_xB_2$. In order to understand the physics of superconductivity in diborides we have to consider that the Lifshitz parameter "z" has an intrinsic uncertainty due to quantum fluctuations. The error bars in Fig. 11 indicate the quantum uncertainty in the "z" value induced by zero point lattice fluctuations. In fact the in-plane boron phonon mode with E_{2g} symmetry near the zone-center, split the partially occupied σ bands. The energy splitting of the two degenerate σ bands is given by $\Delta E=D\sqrt{\langle\sigma^2_{x,y}\rangle}$ where D is the deformation potential and $\sqrt{\langle\sigma^2_{x,y}\rangle}$ is the mean square in plane displacement at T=0K of the boron atoms due to zero point motion measured by neutron scattering [132,139]. The energy splitting is ΔE=±0.4 eV in MgB_2 and it decreases a little going to $AlMgB_4$ where there are about 0.02 σholes per unit cell. Therefore the quantum lattice fluctuations induce the electronic quantum fluctuations of the Γpoint relative to the Fermi level, i.e., of the Lifshitz parameter z.

This induces quantum charge fluctuations between the two σ bands and between the σ and π bands involving electronic states within the energy window of ±0.4 eV around the Fermi level. These charge fluctuations control the energy window of the states involved in the pairing processes therefore we can estimate from Fig. 11 the expected width of the Feshbach shape resonance. The high T_c amplification by Feshbach shape resonance should occur in the range –0.8< "z" <+0.8 where the 2D/3D Van Hove singularity sweeps through the Fermi level that is represented in Fig. 11 where the value z=0 follows within the error bars of z.

The Lifshitz parameter z as a function of x in the case of the Al and Sc substitutions for Mg in the $Mg_{1-x}Al_xB_2$, and $Mg_{1-x}Sc_xB_2$ systems and for the C for B substitution in the $MgB_{2-x}C_x$ system has been calculated by R. De Coss et al. by band structure calculations described elsewhere [204] therefore it has been possible to convert the variation of the critical temperature as a function of the number density of substituted ions x to the variation of T_c versus the universal reduced Lifshitz parameter "z" for all doped magnesium diborides.

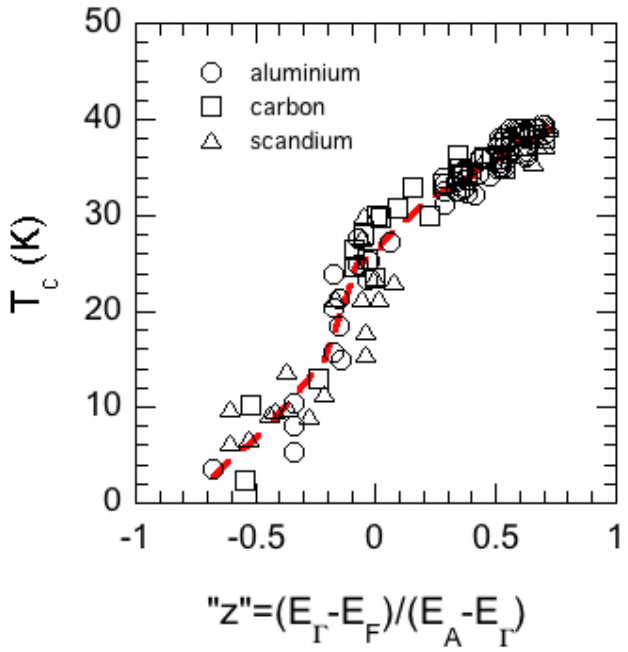

Figure I:2:12. The critical temperature in aluminum, scandium and carbon doped magnesium diborides as a function of the Lifshitz parameter "z"= $(E_\Gamma-E_F)/(E_A-E_\Gamma)$

The critical temperature T_c obtained by aluminium [143], carbon [183,184] and scandium [177] substitutions are reported in Fig. 12. The universal scaling of the critical temperature T_c, versus "z" show the negligible effects of impurity scattering in different substitutions because of the suppression of interband impurity scattering in the superlattice.

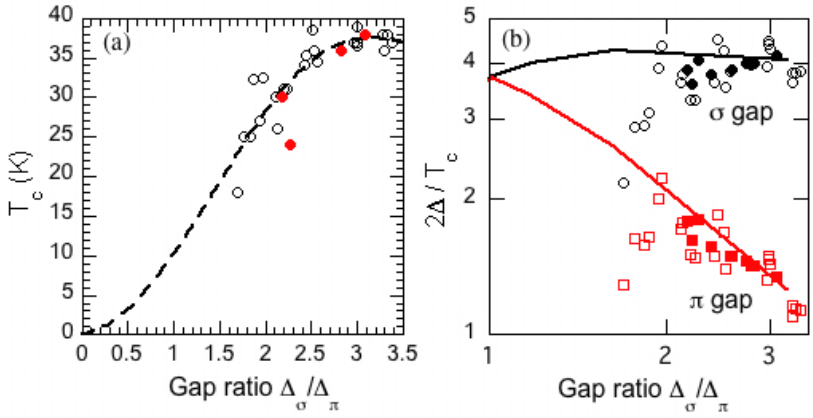

Figure I:2:13. Panel a): The experimental T_c in C for B (filled symbols) [183] and in Al for Mg (empty symbols) substituted MgB_2 as a function of the gap ratio Δ_σ/Δ_π . Panel b): The ratio $2\Delta/T_c$ for the σ gap (circles) and for the π gap (squares) as a function of the gap ratio Δ_σ/Δ_π . The solid lines are the theoretical prediction (published before the experiments have been done [162]) where the effect of atomic substitutions in this superlattice of boron layers do not introduce interband impurity scattering effects but only tune the chemical potential toward the 2D/3D vHs in the Feshbach shape resonance range.

We report in Fig. 13 the superconducting critical temperature T_c obtained by aluminium [143], carbon [183,184] and scandium [177] substitutions as a function of the superconducting gap ratio Δ_σ/Δ_π. The experimental results clearly show that the critical temperature increases by increasing the gap ratio as it was shown by theoretical calculations for a superlattice of wires in Fig. 8. In Fig. 13 we report the experimental ratio $2\Delta_\sigma/T_c$ and $2\Delta_\pi/T_c$ for the π and in the σ band as a function of the gap ratio. The highest T_c occurs for the largest deviation from the BCS value 3.5

These results show that the two gaps behaviour is present over all the range of the reduced Lifshitz parameter -0.8<"z"<+0.8. These results support the predictions that the doped materials remain in the clean limit for interband pairing although the large number density of impurity centres. This result falsifies the predictions of the multigap suppression because of impurity scattering due to substitutions.

In order to identify the Feshbach shape resonance we have plotted in Fig. 14 the ratio T_c/T_F(exp) for the aluminum doped case where T_F is the Fermi temperature $T_F=\varepsilon_F/K_B$ and $\varepsilon_F=E_A-E_F$ is the Fermi energy of the holes in the σ band, and T_c is the measured critical temperature. The T_c/T_F ratio is a measure of the pairing strength $(k_F\xi_0)^{-1}$ where k_F is the Fermi wavevector and ξ_0 is the superconducting coherence length. In fact in the single band BCS theory this ratio is given by $T_c/T_F = 0.36/k_F\xi_0$.

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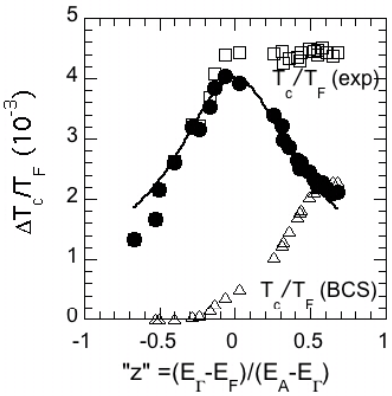

Figure I:2:14. The ratio T_c/T_F(exp) (open squares) for the aluminium doped case where T_F is the Fermi temperature $T_F=E_F/K_B$ for the holes in the σ band and T_c is the measured critical temperature for Al doped samples as a function of the reduced Lifshitz parameter "z". The expected ratio T_c/T_F(BCS) (open triangles) for the critical temperature in a BCS single σ band, The ratio $\Delta T_c / T_F = (T_c(\exp) - T_c(BCS))/T_F$ (solid dots) that measures the increase due to the interband pairing, for the Feshbach shape resonance, fitted with a asymmetric Lorentzian with Fano line-shape centred at z=0, a half width $\Gamma/2$=0.47 and asymmetry parameter q=5.

In Fig. 14 we have plotted also the expected ratio T_c/T_F(BCS) for the critical temperature in the single σ band of MgB_2 calculated by the standard BCS approximations using the McMillan formula, the density of states and electron phonon coupling obtained by band structure theory that gives for MgB_2 $T_c(BCS)$=20K [148].

The increase of the critical temperature determined by the Feshbach shape resonance [118,120,205] of the interband pairing is given by $\Delta T_c/T_F = (T_c(\exp) - T_c(BCS))/T_F$ that is plotted in Fig. 14 as a function of Lifshitz parameter "z". It has been fitted with an asymmetric Lorentzian with Fano line-shape [8] centred at z=0, with the half width $\Gamma/2$=300meV and an asymmetry parameter q=4. This experimental curve provides the clear experimental evidence for the T_c enhancement driven by interband pairing shows a resonance centred at z=0, as expected for Feshbach shape resonanceIn conclusion we have discussed the Feshbach shape resonances around a type (I), type (II) and type (III) ETT in heterostructures and in the particular case of MgB_2 where the two band scenario is well established [205-207], we have shown that the Feshbach shape resonance in interband pairing occurs in a superlattice of superconducting layers near a type (II) ETT in this particular multiband superconductor in the clean limit. The Feshbach shape resonance increases the critical temperature from low T_c diborides up to T_c =40K in MgB_2 and it provides the most clear case of T_c amplification beyond the limit of 20K. These results confirm that the Feshbach shape resonance in interband pairing could be a possible mechanism for high T_c i.e., the quantum trick for suppressing decoherence effects at high temperature.

We finally summarize the physical conditions to get a Feshbach shape resonance suppressing decoherence effects of temperature and driven by quantum superposition of pairs in states corresponding to different spatial locations and different parity. *First*, the material architecture is made of a superlattice of superconducting units (B) at atomic limit intercalated by a different material (Al, Mg) like in AlB_2 diborides; *second*, the chemical potential is tuned in an energy window around a 2.5 Lifshitz topological electronic transition associated with the change of the topology of theFermi surface of one of the subbands; *third*, the energy window of the resonance is controlled by quantum fluctuations driven by the zero point lattice vibrations that sweep the Van Hove singularity through the Fermi level.

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