Article

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BIANCONI, Antonio, JARLBORG, Thomas N. Lifshitz transitions and zero point lattice fluctuations in sulfur hydride showing near room temperature superconductivity. *Novel Superconducting Materials*, 2015, vol. 1, no. 1, p. 37-49

DOI : 10.1515/nsm-2015-0006

Research Article **Open Access**

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DOI 10.1515/nsm-2015-0006
Received September 7, 2015; accepted October 3, 2015

Abstract: Emerets's experiments on pressurized sulfur hydride have shown that H_3S metal has the highest known superconducting critical temperature T_c = 203 K. The Emerets data show pressure induced changes of the isotope coefficient between 0.25 and 0.5, in disagreement with Eliashberg theory which predicts a nearly constant isotope coefficient. We assign the pressure dependent isotope coefficient to Lifshitz transitions induced by pressure and zero point lattice fluctuations. It is known that pressure could induce changes of the topology of the Fermi surface, called Lifshitz transitions, but were neglected in previous papers on the H_3S superconductivity issue. Here we propose that H_3S is a multi-gap superconductor with a first condensate in the BCS regime (located in the large Fermi surface with high Fermi energy) which coexists with second condensates in the BCS-BEC crossover regime (located on the Fermi surface spots with small Fermi energy) near the Γ and M points. We discuss the Bianconi-Perali-Valletta (BPV) superconductivity theory to understand superconductivity in H_3S since the BPV theory includes the corrections of the chemical potential due to pairing and the configuration interaction between different condensates, neglected by the Eliashberg theory. These two terms in the BPV theory give the shape resonance in superconducting gaps, similar to Feshbach resonance in ultracold fermionic gases, which is known to amplify the critical temperature. Therefore this work provides some key tools useful in the search for new room temperature superconductors.

PACS: 74.20.Pq,74.72.-h,74.25.Jb

1 Introduction

Following early claims of 190 K superconductivity in sulfur hydride at very high pressure [1], new results of superconductivity with T_c=203 K[2], i.e. at about 10 ^{o}C above the coldest temperature in Antartica, have been presented on June 17, 2015 at Superstripes 2015 conference in Ischia, Italy [3] triggering a very high scientific interest [4]. The recent work of Emerets's group [2] shows the Meissner effect and the pressure dependent critical temperature of H_3S and D_3S. These results have triggered today the materials research for room temperature superconductors in different hydrides at extreme high pressures [5–9].

The experimental discovery of high temperature superconductivity in H_2S at very high pressure was predicted by [10] to occur in the high pressure metallic H_3S phase, with $Im\bar{3}m$ lattice symmetry. Disproportion from 2(H_2S) + H_2 to 2(H_3S) occurs at very high pressure. The theoretical prediction of Duan et al. [10] has been obtained by using the successful algorithm USPEX (Universal Structure Predictor Evolutionary Xtallography) for the prediction of crystalline structures at high pressure in material science [11].

Many of preceding theoretical studies on this issue conclude that the superconducting phase in pressurized H_3S is described by the Eliashberg theory [10, 12–19] while Hirsh proposes the hole superconductivity model [20].

The Eremets's group research was motivated by the search for high temperature superconductivity predicted to emerge in metallic hydrogen and hydrides [21–29].

The BCS theory [30] has given a microscopic description of the superconducting condensate wave-function made of interacting Cooper pairs in a weak coupling regime, where the pairing is mediated by the conventional attractive phonon-exchange mechanism. However the standard BCS theory formulas [30] have been obtained

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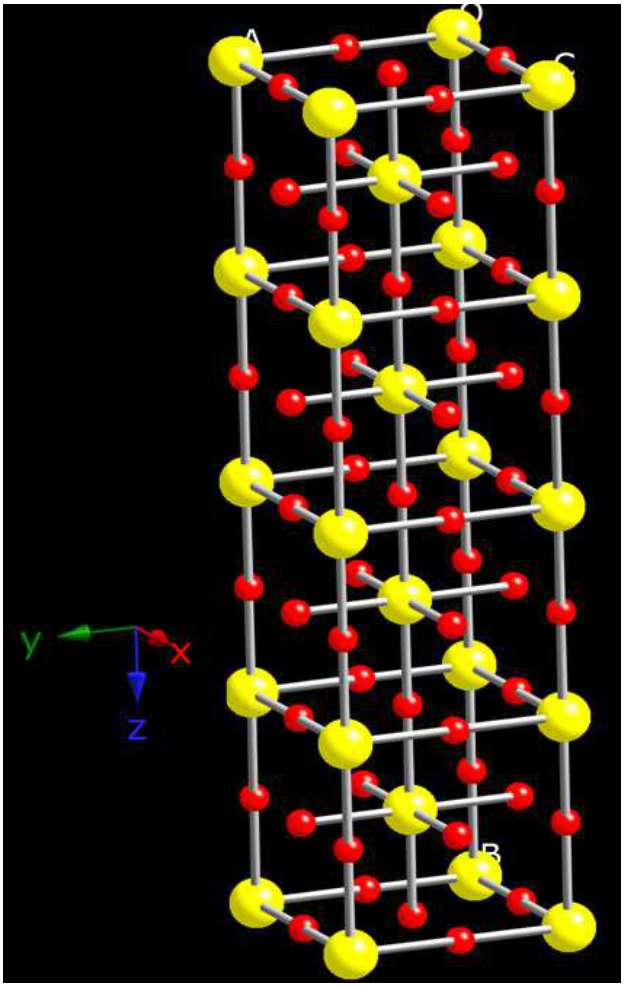

Figure 1: (Color online) The crystalline structure of H_3S with $Im\bar{3}m$ lattice symmetry, with two formula units per unit cell, with sulfur (yellow large spheres) and hydrogen atoms (red small spheres). The linear S-H-S hydrogen bonds along the a,b and c axis in the $Im\bar{3}m$ lattice of H_3S, form a first 3D network of three linear chains of covalent bonds crossing at the sulfur atom at the (0,0,0) lattice point which coexists with a second 3D network of other three linear chains of covalent bonds (solid black lines) crossing at the sulfur atom at the (0.5,0.5,0.5) lattice point.

using many approximations on the metallic phase: i) a simple homogeneous lattice; ii) a single electronic band where the multiple bands of a metal are reduced to a single effective band (called dirty limit); iii) a single value of the density of states at the Fermi level N_0; iv) a constant electron-phonon coupling constant λ (isotropic pairing). The basic assumption of the standard BCS theory is a very small energy of the phonon ω_0 and a very high electron density i.e., a high Fermi energy, $\omega_0/E_F << 1$, which is called the Migdal approximation [31]. This is a particular case of the common adiabatic Born-Oppenheimer approximation, where the electronic and ionic degrees of freedom are assumed to be rigorously separated. The McMillan [32, 33] and the Eliashberg [34] formulas for the superconducting critical temperature have been obtained in the frame of the BCS standard theory introducing corrections for the electron-electron repulsive interaction and for the strong electron-phonon coupling.

In the sixties it was well accepted that the superconducting critical temperature cannot be larger than 23 K in the frame of standard BCS theory. In fact in the single band approximation T_c increases with both phonon energy and coupling strength but for extreme strong electron-phonon coupling the electron liquid at low temperature prefers to order in the real space, forming electronic crystals (charge density waves, and Wigner crystals) which compete with the superconducting phase. Moreover if superconductivity survives increasing electron-phonon coupling, the critical temperature decreases since the phonon energy is pushed toward zero. In this regime the lattice structure collapses and the system is in the verge of a catastrophe. Therefore the materials research for room temperature superconductivity was not driven simply by looking for a high phonon energy and a high coupling strength in the Cooper pairing. The theoretical predictions of high T_c in solid metallic hydrogen and hydrides at high pressure [22, 24, 28] were based on the search of materials characterized by high frequency phonons mediating the pairing and by a negative dielectric constant controlling the electron-electron interaction and the Coulomb energy [21–29].

The textbook treatments of superconductivity describe the properties of the superconductors using models within the standard BCS approximations. However the fundamental properties of superconductivity may be explained without introducing any unnecessary approximation using the general theory of superconductivity called by Weinberg *superconductivity for particular theorists* [35]. The general theory of superconductivity is based on the self consistent theory developed by Bogoliubov [36], providing the spectrum of excited quasiparticles, and on the fact that the electromagnetic gauge invariance is spontaneously broken in a superconductor as shown by Nambu[37]. The general theory of superconductivity includes the contributions of Gorkov[38], Josephson [39], Kondo[40], Blatt[41], Leggett [42] and others as described in two recent books[43, 44]. This general theory of superconductivity allows the description of superconductors with complex anisotropic or granular structure in the momentum space and in the real space as described by Coleman[45]. The weak coupling limit of this theory gives the standard BCS superconductivity or the Ginzburg Landau regime, while the strong coupling limit gives the Bose-Einstein condensation (BEC). The fundamental interaction

in the general theory, missing in the standard BCS scenario, is the *configuration interaction* between multiple condensates. Starting from the general theory of superconductivity developed by Blatt [41] and Leggett [42] a different roadmap for high temperature superconductivity was proposed in 1994 [46–50] including the exchange terms due to the configuration interaction between multiple condensates. It was based on experimental results showing that multiple electronic components coexist in cuprates at optimum doping in different Fermi arcs[46–50].
A first component is a Fermi liquid, within the Migdal approximation $\omega_0/E_F << 1$, making a condensate in the BCS limit below T_c and a second component is a strong interacting electronic liquid, where the Migdal approximation is violated $\omega_0/E_F \sim 1$, which is the polaron limit, forming paired charge density wave or Wigner crystal made of polaron pairs below T_c.
The high temperature superconductivity was assigned to the role of the shape resonance, belonging to the class of Fano resonances and synonym of Feshbach resonance[51], which is due to the exchange term between a free electrons pairs in the first condensate and a bipolaron in the second condensate.

In 1996-1998 a theory for high temperature superconductivity or high T_c superconductivity in cuprates was developed by Bianconi, Perali and Valletta (BPV) [52–56] based on the Blatt [41] and Leggett [42] theories, in the frame of the general theory of superconductivity for multi-components electronic systems avoiding the standard BCS approximations. The first standard BCS approximation which is not used in the BPV theory is the *dirty limit* approximation which reduces all multiband superconductors into a single effective band used by all proposed theories for high temperature superconductors assumed for both conventional or unconventional pairing mechanisms. The electronic structure of cuprates is described in the BPV theory in the *clean limit* by multiple bands forming Fermi arcs.

The variation of the critical temperature with doping is predicted considering Lifshitz transitions [54] for a new appearing Fermi arc driven by doping and misfit strain. While some Fermi arcs host BCS-like condensates, the new Fermi arc appearing at the Lifshitz transition hosts a condensate in the BEC or in the BCS-BEC crossover regime, violating the Migdal approximation. The wave-functions of electrons at the Fermi level are obtained by solving the Schroedinger equation in an artificial lattice superstructure which gives a band dispersion in a narrow range of about 1 eV around the chemical potential like in the real material. The k dependent exchange contact interaction, due to configuration interaction between pairs in different Fermi arcs, is calculated numerically by the overlap of the pair wave-functions without approximations. The key point to treat these complex systems is to solve the multiple gaps equation together with the density equation, which allows a correct quantum description of Fermi surfaces including Fermi portions beyond the Migdal approximation.

A similar mechanism called Feshbach resonance,[57] was proposed independently in ultracold gases, based on the configuration interaction between a pair of atoms in the first diluted gas of fermionic atoms (analogous to the Fermi liquid) and the atomic pair forming a diatomic molecule (analogous to the polaron pairs). There is no intraband Cooper pairing in the diluted fermionic gas and the Feshbach resonance is the only way to generate an attractive pairing mechanism of the contact type for atomic fermions which is tunable by using an external magnetic field. The exchange contact interaction increases the critical temperature giving high temperature superconductivity, with $K_B T_c/E_F \sim 0.2$, which was experimentally identified [57, 58] and fully explained by the theory [59–61].

Details of the normal metallic phase, neglected in the BCS theory, become key ingredients in the BPV theory: a) the complex Fermiology, beyond the single band model; b) the formation of charge density waves and polaronic Wigner crystals involving the electronic component in n-th Fermi surfaces beyond the Migdal approximation $\omega_0/En_F \sim 1$; c) the strong electronic correlations in the electron fluid with very low Fermi energy, beyond the usually assumed Fermi gas approximation; e) the anomalous or negative dielectric constant controlling the electron-electron interaction; f) the complex inhomogeneous spatial geometry in systems with nanoscale phase separation [62] induced by electron-lattice interaction and lattice misfit strain [63] which can give also insulator to superconductor phase transitions [64].

The numerical calculation of the critical temperature includes the condensation energy which has been proposed in superconductors and superfluids by other authors [65, 66].

2 Superconductivity in binary intermetallics: A15 and diborides

The overall features of superconductivity in H_3S are similar to superconductivity in A15 and diboride compounds. Figure 2 shows the evolution of the maximum critical temperature in diatomic intermetallics discovered in these last years. A15 compounds (like Nb_3Ge) have the same $Im\bar{3}m$

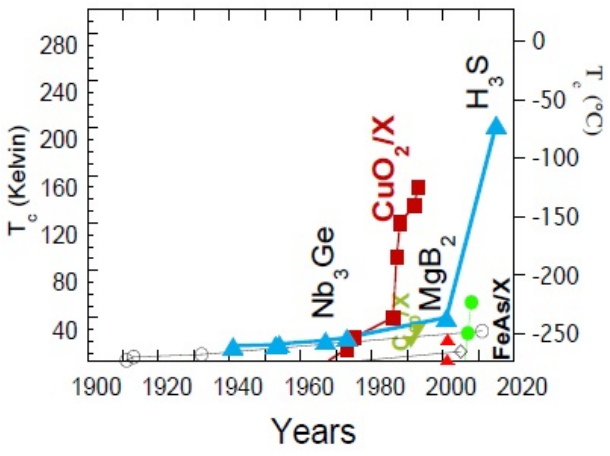

Figure 2: (Color online) The superconducting critical temperature of superconducting elements, open black circles, binary intermetallics, filled blue triangles, and ternary and quaternary oxide layered perovskites made of CuO_2-atomic layers with different X spacer layers (filled red squares) coefficient as a function of the year of the discovery.

lattice structure [67] as H_3S above 100 GPa (shown in Fig.1) and are made of atomic wires of transition metals as noticed by Friedel [68, 69] embedded into a 3D metal [70–72]. Superconductivity in A15 compounds appears in a highly inhomogeneous phase at the edge of a lattice catastrophe due incipient structural phase transitions [73–75] giving complex pattern of defects and local lattice fluctuations [76–78].

Few days after the discovery of superconductivity in MgB_2 in 2001 it was noticed [79] that it was a practical realization of the predictions of the BPV theory for a superlattice of quantum wells. This superconducting phase could not be understood in the frame of the standard BCS approximations.The standard BCS formulas failed to predict accurately the anomalous specific heat of MgB_2 and the direct evidence of two superconducting gaps [80]. The BCS *dirty limit* approximation was very clearly falsified by many experiments. Also the multi-band BCS superconductivity theory in the weak coupling [81] failed to explain the data. It was clear that in one of the Fermi surfaces, the tubular small σ Fermi surface, the pairing was in the strong coupling limit, while pairing in the large π Fermi surface is in the very week coupling limit [82, 83]. The coupling is so weak there that the Fermi gas made by only π electrons at the Fermi level, as in the isostructural AlB_2 system, does not superconduct. It starts to superconduct only when the chemical substitution of Mg for Al ions pushes the top of the σ band above the chemical potential giving a Lifshitz transition for the appearing of the small hole-like σ Fermi surface pocket[80]. Therefore here the particles in the small σ band play the role in MgB_2 of polaron pairs, in cuprates or diatomic molecules in the ultracold gases. Moreover it was shown that because of zero point atomic fluctuations[84–87], the Fermi energy in the σ bands is time and space dependent with energy fluctuations of about 600 meV of same order of magnitude as the Fermi energy in the small σ Fermi surface. Therefore also the Migdal approximation $\omega_0/E_F < 1$, is violated in the σ band while it is valid in the large π band.

In spite of the conventional phonon mediated pairing, the 40 K superconducting phase in magnesium diboride as provided the experimental evidence that the high critical temperature was associated with the breakdown of two key BCS approximations: the *dirty limit* and the *Migdal approximation*.

Moreover in the standard BCS approximations the shift of the chemical potential going from the normal to the superconducting phase below T_c, is considered to be negligible while in BPV theory this is taken into account solving the self consistent gaps equation and the density equation together step by step.

Considering the data collected in diborides doped with substitutions of Sc or Al for Mg and of C for B it was possible to track the variation of the critical temperature across the Lifshitz transition for the appearing of the new σ Fermi surface. Using the BPV theory is was possible to get a quantitative description of the variation of the critical temperature across the Lifshitz transition also where $\omega_0/E_F \sim 1$ and to quantify the role of the shape resonance which drives the system to the highest critical temperature known in a binary intermetallics, before the recent discovery of Eremets's group [88]. The maximum critical temperature occurs where the small appearing σ Fermi surface is in the BCS-BEC crossover $\Delta_n/E_{Fn} \sim 1$ (where n indicates the σ band) [60, 61] while the other condensate in the large π Fermi surface is in the BCS regime. These results [88] have shown that the BPV theory, avoiding standard BCS approximations, was successful to describe high temperature superconductivity in a multiple condensates superconductor where only one of the Fermi surface spots are in the BCS-BEC crossover.

3 Lifshitz transitions and the iron based superconductors

The topological changes of the Fermi surface of the normal phase caused by the lattice strain (as a response to pressure), misfit strain, chemical substitution, variation of the

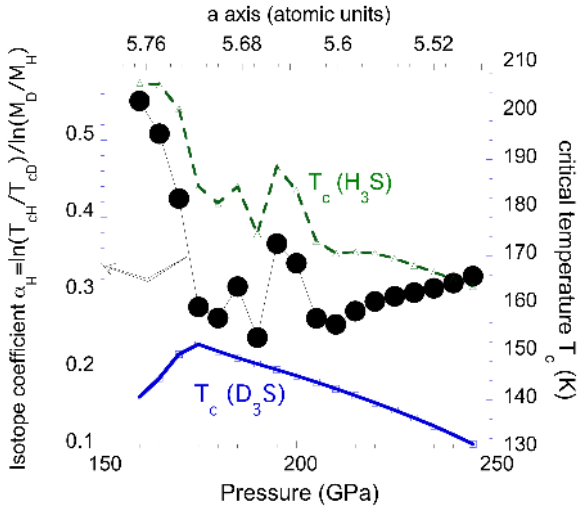

Figure 3: (Color online) The pressure dependent isotope coefficient as a function of pressure (filled circles) calculated by interpolation of the experimental data of the critical temperature of H_3S (dashed green line) and D_3S) solid blue line reported by Drozdov et al. [2]

electronic density) are called Lifshitz transitions [89]. In many cases Lifshitz transitions appear on points or lines of high symmetry in the Brillouin zone and are associated with changes of the symmetry or dimensionality of the wave functions of the electrons at the Fermi level in critical Fermi surfaces. The Lifshitz transitions are revealed experimentally by anomalies in lattice parameters, in the density of states near the Fermi energy, in elastic properties, in anomalous thermodynamic and transport properties of metallic materials [90]. Lifshitz [89]. noted that at zero temperature, T = 0, Lifshitz transitions are true phase transitions of order 2.5 (as in Ehrenfest's classification) therefore are called "2.5 Lifshitz transition". A sharp Lifshitz transition at T=0, at high temperature shows a crossover character. In presence of strong interactions the 2.5 phase transition becomes first order with a phase separation between two phases where the chemical potential in each phase is shifted above and below the Lifshitz transition respectively[87, 91, 92] driving the system well tuned at a Lifshitz transition on the verge of a lattice catastrophe as shown in the case of A15 and diborides. While in the early times the interest was focused on Lifshitz transitions in single band metals, now the interest is addressed to Lifshitz transitions in multi-band metals with different Fermi surfaces showing multi-gap superconductivity. The shape resonance mechanism considers the relevant contribution, near the Lifshitz transition, of the exchange interaction between pairs in the hot spots and in all other points of the Fermi surfaces in the k space. We have learn that the "Devil is in the details", in fact for the optimization of a high critical temperature it is necessary to reach particular Lifshitz transitions where a small number of electrons in a new appearing Fermi surface (the hot spot) are in the extreme strong coupling regime in the antiadiabatic $\omega_0/E_{Fn} \sim 1$ regime in the normal phase without the lattice catastrophe since the majority of the electron gas is in large Fermi surfaces well in the Midgal approximation $\omega_0/E_{Fn} < 1$.

The BPV theory was proposed and confirmed to be successful to describe the high temperature superconductivity in iron based superconductors [97–106]. We discuss below the failure of the standard Migdal approximation and of the breakdown of Eliashberg theory in H_3S. The large electron-phonon coupling and the high frequencies of H-phonons contribute to rise T_c [10, 15, 19] but we claim the need of the BPV theory to describe the gaps in the new small Fermi surfaces appearing at the Lifshitz transitions controlled by pressure and their configuration interaction with the gap in the large Fermi surface.

4 Isotope effect in H_3S.

The isotope effect in H_3S [1] has provided a direct evidence of the involvement of the lattice degree of freedom in the pairing process. Therefore the isotope effect in sulfur hydride at high pressure H_3S has been interpreted as ruling out theories of unconventional superconductivity (based only on spin liquid models or magnetic interactions) and supporting conventional theories of superconductivity based on the role of lattice fluctuations. However the standard BCS theory predicts a pressure independent isotope coefficient 0.5 while in non standard BCS theories, like in the BPV theory [55, 95, 96] the isotope coefficient deviates from 0.5 as in magnesium diboride where it is 0.26 [107]. From the new results reported by Drozdov et al. [2] we have extracted the isotope coefficient as a function of pressure shown in Figure 3. We can see in Figure 3 large variations of the isotope coefficient reaching a minimum of 0.2 and first maximum reaching 0.5 at 170 GPa and a second peak at 240 GPa. The anomalous pressure dependent isotope coefficient has been found in cuprates superconductors as a function of doping [55, 95, 96] with anomalies where the chemical potential crosses Lifshitz transitions driven by pressure. Therefore the data in Figure 3 indicate the possible presence of Lifshitz transitions in the pressure range showing near room temperature superconductivity.

5 Band structure calculation of H_3S as a function of pressure

We have performed preliminary band structure calculations[108] of H_3S with $Im\bar{3}m$ lattice symmetry made using the linear muffin-tin orbital (LMTO) method [109, 110] and the local spin-density approximation (LSDA) [111]. We show in Fig. 4 the dispersion of the bands crossing the chemical potential in the $\Gamma - M$ direction.

Self-consistent paramagnetic calculations are made for a simple cubic unit cell containing 8 sites totally, used for A15 compounds with the same crystalline structure. The technical information on the method have been published earlier [112–115]. The present calculations are in good agreement with previous band structure calculations [15–19]. We confirm the presence of a narrow peak of the occupied total Density of States (DOS) very close to the chemical potential. We show that the high energy threshold of the narrow DOS peak crosses the chemical potential at a=5.7 a.u. i.e., at a pressure of about 180 GPa. The narrow peak in the total DOS in a narrow energy range around the chemical potential is shown in Fig. 5. While previous papers have stated that this peak is pinned at the zero energy, we show in Fig. 5 that the energy position of this peak relative to the chemical potential shifts with pressure. The narrow peak of the DOS is pushed toward high energy by pressure and it crosses the chemical potential at the highest P for the lattice constant smaller than a=5.7 a.u..

The narrow peak of the DOS peak is related with the flat dispersion of bands in the $\Gamma - M$ direction in the energy range of 2 eV below the chemical potential. shown in Fig. 4. The band structure shows a first steep band with very large energy dispersion with its band edges at about 20 eV away from the chemical potential. This first band gives the large Fermi surface shown in [13]. There are three other small Fermi surface pockets centered around the Γ point shown in Fig. 4 for different lattice parameter a.

The tops of the hole-like bands near the Γ point are below E_F at low pressure P but they move above the chemical potential for a pressure higher than 130 GPa as shown in Fig.4. The edges of these bands cross the chemical potential as function of P giving topological Lifshitz transitions with the appearing of new Fermi surfaces. Moreover there is a Lifshitz transition due to the crossing of one band at about 2/3 of the $\Gamma - M$ distance indicated by δ in Fig. 4 which appears only for lattice parameters smaller than $a \sim 5.7$. a.u., i.e. in the pressure range of highest P when T_c is highest. The top of this band goes from -0.2 eV below the chemical potential to +0.1 eV when a decreases from 6.2 to 5.6 a.u.. Finally we associate the crossing of the chemical potential by this band at the δ point in Fig. 4 with the Fermi level crossing of the narrow DOS peak in Fig. 5. When the pressure decreases a Fermi surface tubular neck disappears near the N point seen in the common bcc BZ.

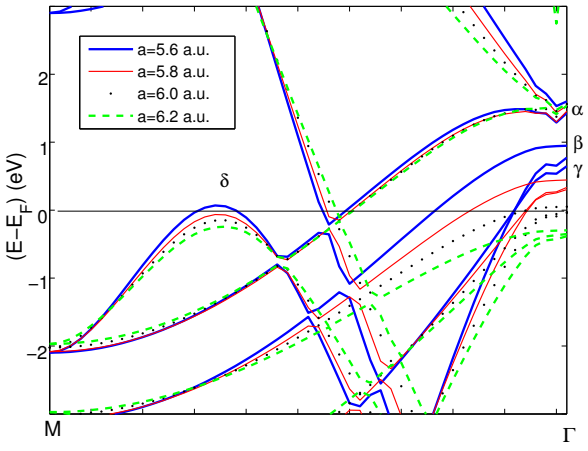

Figure 4: (Color online) The dispersion of the bands in the electronic structure of H_3S calculated using the simple cubic Brillouin zone (sc BZ) used for A15 compounds with $Im\bar{3}m$ structure, between M and Γ points. The band dispersion in this direction gives the narrow DOS peak near the Fermi energy. We show the variation of the band dispersion at different pressures by changing the lattice parameter between a=6.2 a.u and a=5.6. We show that there are three bands (β, $\gamma 1$, $\gamma 2$) forming 3 small Fermi surfaces at the Γ point and a band crosses the zero energy at the point δ at about 2/3 of the Γ-M distance which is saddle point associated with a Fermi surface topology change i.e., a neck disrupting Lifshitz transition by decreasing pressure

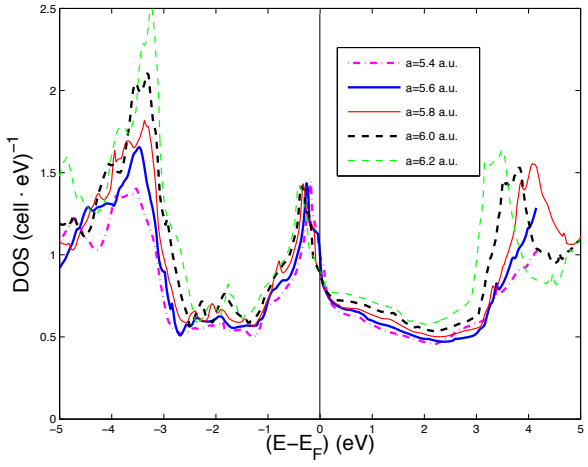

Figure 5: (Color online) The total DOS for H_3S at different lattice constants a. A sharp peak of the DOS near the chemical potential crosses the chemical potential at high pressure. The high energy side of the narrow flat DOS peak corresponds with the energy of the top of the band at δ point shown in Fig.4.

Let us now consider the fact that because of the zero-point motion (ZPM) the different Fermi energies in the small pockets show large energy fluctuations like in magnesium diboride. The ZPM is large because of the small mass of H atoms and it has large effects on the fluctuations of electronic structure. Such effects have been shown to be important in several different materials, even if their atomic masses are larger [119–121]. Lattice fluctuations can perturb spin waves and phonons in high-T_c cuprates and it cannot be neglected if superconductivity relies on few phonons coupled with particular bands [122]. The Debye temperature for H phonons is high ($\sim 1800K$ or 155 meV) in H_3S and the amplitude of lattice fluctuations from ZPM is large already at low T. With a force constant $K = M\omega^2$ of 7 eV/Å^2 we obtain an average amplitude u of the order 0.15 Å. As seen in Fig. 5, the first high lying valence band has a width is about 27 eV. This makes the band dispersion and Fermi velocities high in the first band forming the Fermi surface. The large effect of the zero point motion is on the small Fermi pockets near the Γ point. The low-T energy band fluctuations in materials with narrower band widths has been found to be about 20 meV for u in the range 0.03-0.04 Å [119, 120, 122]. From an extrapolation of these values to the conditions in H_3S we estimate that the band energy fluctuation can be of the order of 160 meV for H-bands. Therefore when the chemical potential is tuned by pressure near a Lifshitz transition, so that the En_F in one of the bands is of the order of 160 meV the topology of the small Fermi surfaces made of small pockets show strong dynamical fluctuations controlled by the zero point lattice fluctuations.

Figure 6 shows the energy position of the top of the 3 bands at the Γ point and the top of the band at about 2/3 of the $\Gamma - M$ distance as a function of pressure. The energy spread due to zero point lattice fluctuations is indicated by the red area for states at the Γ point by the yellow area for the states at $\Gamma - M$ point. The shift of the energy position of the top of the narrow peak in the DOS near the chemical potential tracks the top of the band at 2/3 of Γ-M direction, indicating the Lifshitz transition L_2 around 180 GPa for the 3D-2D change of Fermi surface topology with the formation of a Fermi neck. Finally these results show that in superconducting pressurized sulfur hydride metal the Fermi surface topology shows Lifshitz transitions, L_1 and L_2 in Fig. 6, by increasing the pressure. This scenario can be compared with the Lifshitz transitions for the appearing new Fermi surface arcs observed in cuprates as a function of doping and misfit strain [47, 52, 55].

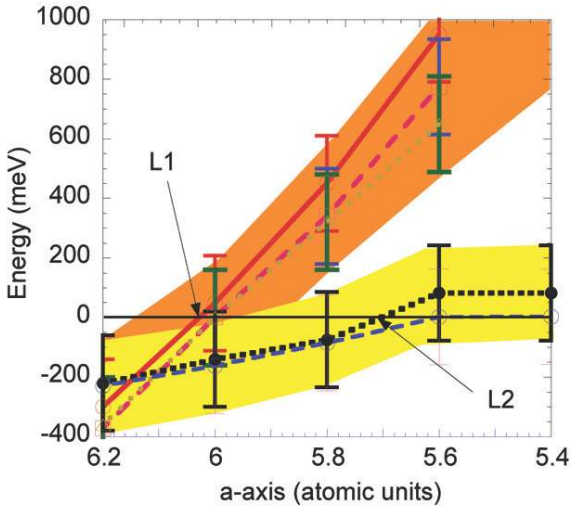

Figure 6: (Color online) Energy shift of the tops of the three hole-like bands at the Γ point (solid red line, dashed red line and dotted yellow line) crossing the chemical potential at around 100 GPa. The errors bars and the red region indicate the zero point energy fluctuations of the band edges. The filled black dots and the dotted black line show the energy shift of the top of the band crossing the chemical potential at about 2/3 of the $\Gamma - M$ distance of the Brillouin zone. The open circles and the blue dashed line shows the energy shift of the high energy side of the narrow peak of DOS near the chemical potential. L_1 indicates the first Lifshitz transition at around 100 GPa for the appearing of the new small Fermi surface pockets at the Γ point. L_2 indicates the second Lifshitz transition at around 180 GPa for the Fermi surface 3D to 2D topology change with the formation of tubular neck.

6 BPV theory for multi-gaps superconductors at the BCS-BEC crossover

The proposals of high temperature superconductivity based Eliashberg theory can be classified in different groups. Let us start with a first group considering a single effective band, in a dirty limit, giving a single condensate:

1A) the standard Eliashberg theory considering a high energy phonon or vibron (a quantum of intramolecular vibration) interacting with electrons having a large Fermi energy $\omega_0/E_F << 1$;

1B) the theories considering the case of a low density electron gas beyond the Migdal approximation $\omega_0/E_{Fn} > 1$ where the single condensate is formed by BEC condensation or by BCS-BEC crossover $\Delta_n/E_F \sim 1$;

1C) non standard BCS theories which consider pairing mediated by electronic excitations, called exciton theories.

The second group of non standard BCS theories considers the anisotropic BCS theory, in the clean limit. These non standard BCS theories consider metals with multiple bands with different symmetry crossing th chemical potential and multiple gaps are formed in different in different spots of the k-space.

2A) The multiband BCS model where all multiple Fermi surfaces are in the BCS limit;

2B) the Fermi-Bose model where the Fermi level of a first band is degenerate with a single level, occupied by paired electrons. Here a BCS condensate coexist with bosons which undergoes a Bose condensation;

2C) the extreme case of superconductivity driven mostly by exchange like interband pairing with very weak, or no intraband pairing in all Fermi surfaces;

2D) The BPV theory for multiple condensates with a second condensate in the BEC- BCS crossover, beyond Migdal approximation, in a small Fermi surface which coexists with a majority of charges in large Fermi surfaces forming BCS condensates.

A third group of theories consider the case of systems with relevant electronic and lattice inhomogeneity observed in cuprates [62], diborides [86] and iron based superconductors [97]. In these systems the nanoscale and mesoscale phase separation can be associated with the Lifshitz transitions in strongly correlated multiband systems [91, 92]. The general theory of superconductivity has been proposed for nanoscale disordered systems using the reduced density matrices [45] and considering the insulator to superconductor transitions [64].

We recall bellow the fundamentals features of the BPV (Bianconi, Perali, Valletta) theory for multi gap superconductors at the BCS-BEC crossover including shape resonances. This theory is proposed here for sulfur hydride at very high pressure following the evidence for Lifshitz transitions driven by high pressure shown in this work. This theory was proposed before for cuprates, [47, 52, 55, 56, 94–96], for diborides [80, 88] and iron based superconductors [97–99].

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 wavefunctions of electrons at the Fermi level are calculated using a lattice with one-dimensional lattice potential modulation where the chemical potential is tuned near a Lifshitz transition like in magnesium diborides, A15, cuprates, iron based superconductors and we propose here for sulfur hydride at high pressure.

The formula for the superconducting critical temperature T_c in the BPV theory is given by the linearized BCS equation considering the simplest case of a two dimensional system [55] but the extension to three dimensional system [88] is trivial.

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

where the energy dispersion is measured with respect to the chemical potential.

We consider a superconductor with multiple gaps Δ_{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

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

where N is the total number of wave-vectors in the discrete summation, μ is the chemical potential, $V^{n,n'}_{\mathbf{k},\mathbf{k}'}$ is the effective pairing interaction

$$V^{n,n'}_{\mathbf{k},\mathbf{k}'} = \widetilde{V}^{n,n'}_{\mathbf{k},\mathbf{k}'} \times \theta(\omega_0 - |E_{n,k_y}+\epsilon_{k_x}-\mu|)\theta(\omega_0 - |E_{n',k'_y}+\epsilon_{k'_x}-\mu|) \quad (3)$$

Here we take account of the interference effects between the 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.

$$\widetilde{V}^{n,n'}_{\mathbf{k},\mathbf{k}'} = -\frac{\lambda_{n,n'}}{N_0}S \times \int_S \psi_{n',-k'_y}(y)\psi_{n,-k_y}(y)\psi_{n,k_y}(y)\psi_{n',k'_y}(y)dxdy, \quad (4)$$

Here N_0 is the DOS at 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. The gap equation need to be solved iteratively. The anisotropic gaps dependent on

the band index and on the superlattice wave-vector k_y. According with Leggett [42] the ground-state BCS wave function corresponds to an ensemble of overlapping Cooper pairs at weak coupling (BCS regime) therefore evolves to molecular (non-overlapping) pairs with bosonic character and 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.

However in this anomalous regime, where Eliashberg theory breakdown, by increasing coupling or decreasing the density by approaching the band edge, the chemical potential μ results strongly renormalized with respect to the Fermi energy E_F of the non interacting system, and approaches minus half of the molecular binding energy of the corresponding two-body problem in the vacuum. In the case of a Lifshitz transition, described in this paper, all electrons in the new appearing Fermi surface condense forming a condensate in the BCS-BEC crossover. Therefore at any chosen value of the charge density for a number of the occupied bands N_b, the chemical potential in the superconducting phase should be renormalized by the gap opening at any chosen value of the charge density ρ using the following formula:

$$\rho = \frac{1}{L_x L_y}\sum_{n}^{N_b}\sum_{k_x,k_y}\left[1-\frac{E_{n,k_y}+\epsilon_{k_x}-\mu}{\sqrt{(E_{n,k_y}+\epsilon_{k_x}-\mu)^2+\Delta^2_{n,k_y}}}\right]$$
$$= \frac{\delta k_y}{\pi}\sum_{n=1}^{N_b}\sum_{k_y=0}^{\pi/l_p}\int_0^{\epsilon_{min}} d\epsilon\frac{2N(\epsilon)}{L_x}+\int_{\epsilon_{min}}^{\epsilon_{max}} d\epsilon\frac{N(\epsilon)}{L_x} \quad (5)$$
$$\times\left(1-\frac{E_{n,k_y}+\epsilon_{k_x}-\mu}{\sqrt{(E_{n,k_y}+\epsilon_{k_x}-\mu)^2+\Delta^2_{n,k_y}}}\right).$$

taking the increment in k_y as $\delta k_y = 2\pi/L_y$ for a size of the considered surface aL_x L_y and in the range

$$\epsilon_{min} = max\left[0, \mu-\omega_0-E_{n,k_y}\right],$$
$$\epsilon_{max} = max\left[0, \mu+\omega_0-E_{n,k_y}\right],$$
$$N(\epsilon) = \frac{L_x}{2\pi\sqrt{\frac{\epsilon}{2m}}},$$

This theory does not include superconducting fluctuations. However it should be noticed that in a multigap / multiband system another fundamental phenomenon helps in stabilizing room temperature superconductivity: the screening of the superconducting fluctuations. In fact the multi-band BCS?BEC crossover in a two-band superconductor can determine the optimal condition to allow the screening of the detrimental superconducting fluctuations. [125, 126]

7 Conclusion.

In this work we have presented the breakdown of the Eliashberg theory for H_3S, in fact the electronic structure of sulfur hydride H_3S with $Im\overline{3}m$ lattice structure as function of pressure shows Lifshitz transitions revealed by band crossings at E_F and by the shift of the narrow peak in the density of states below the chemical potential pushed above it by lattice fluctuations associated with the hydrogen zero point motion. We have discussed the presence of two topological Lifshitz transitions at two critical pressures P_1 = 110 Gpa, and P_2 = 180 GPa by pressure dependent electronic structure calculations of H_3S. At the first Lifshitz transition, around P_{c1} = 110 Gpa, three new Fermi surface spots appear at the γ point pushed up by pressure. These anisotropic bands are characterized by a flat dispersion in the $\Gamma - M$ direction and a steep dispersion in the $\Gamma - R$ direction. The second Lifshitz transition at P_{c2} = 180 GPa is due the appearing of a tubular Fermi surface neck.

The amplitude of the energy fluctuations of this band edge due to atomic zero point motion has been calculated and we have found that it pushes this DOS peak above the chemical potential. Therefore dynamical energy fluctuations of the band edge due to zero point motion of the hydrogen atoms is of high relevance. We find a colossal zero point energy fluctuation which induces a 160 meV energy fluctuation of the Lifshitz transitions. The present results show that the condensates in the 4 small hole pockets around the Γ point and the small Fermi surface in the $\Gamma - M$ direction are beyond the Migdal approximation $\omega_0/E_F \sim 1$, including lattice dynamical zero point fluctuations. In particular the condensate in the hole-like δ Fermi surface pocket, associated with the sharp quasi-1D peak in the DOS, pushed at the chemical potential by pressure, is clearly in the BCS-BEC crossover regime, coexisting with other condensates in the BCS regime in other large Fermi surfaces in the pressure range where the superconducting critical temperature is near room temperature.

The emerging scenario for pairing in sulfur hydride at high pressure in a dynamical landscape where key energy parameters have all the same magnitude i.e, of the order of 160 meV: 1. the energy separation between the average position of the nth band edge and the chemical potential, defined as the nth Fermi energy controlling the "appearing or disappearing Fermi surface spot" Lifshitz transition in the Fermi surface topology, 2. the energy separation of a peak in the Density of States and the band edge, usually controlling the "Neck opening" Lifshitz transition 3. the amplitude of the energy fluctuation of the critical Fermi surfaces associated with zero point lattice fluctuations 4. The

energy of the pairing interaction defining the energy of the cut-off for the formations of pairs away from the chemical potential

In this scenario the BCS approximations used in the standard BCS theory are no more valid and the critical temperature is controlled not only by the energy of the changed boson, w_0, and the effective electron-phonon coupling (given by the product of the density of states times the electron-phonon coupling constant) but also by the condensation energy. While in the standard Eliashberg theory, the correction to the chemical potential induced by electron-phonon coupling is ignored on the verge of the Lifshitz transition, this correction, which has much impact, is included in the BPV theory. In this situation the chemical shift from the normal to the condensed phase below T_c is no more negligible, and the coupling is renormalized by a factor, given by the quantum overlap of the condensed pairs in cuprates [52, 55, 56, 94] diborides [82, 86, 88] and iron based superconductors[97–103].

Finally this paper shows the breakdown of Eliashberg theory for pressurized sulfur hydride, supports the role of phonons [10, 15–19] but claims the presence of Lifshitz transitions tuned by pressure and the need of the BPV theory including shape resonances, to describe superconductivity in H_3S.

Further work is needed to investigate i) the divergent amplitude of lattice fluctuations near the R3m to $Im\bar{3}m$ 2nd order structural transition around 180 GPa, ii) the large mass difference between H an S which requires the consideration of different amplitudes of u for the two types of atoms, and it should allow for E and k dependences for the energy fluctuations of Lifshitz transitions. The electronic band calculations should be extended to large supercells needed for more precise estimates of energy fluctuations of the electronic structure associated with spacial structural fluctuations. We think that the discovery of superconductivity in sulfur hydride very near room temperature has narrowed the number of possible road maps toward new functional superconducting materials. Further fundamental research on the mechanism of room temperature superconductivity in these new phase of matter are needed to clarify this emerging physical scenario and they will allow the definition of a protocol for the material design of new functional room temperature superconductors.

Finally we would like to mention that a preprint, posted when this paper was in press, confirms our results on the presence of Lifshitz transitions in H_3S in the high pressure range where the high temperature superconductivity emerges[127].

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