Solid State Communications 244 (2016) 57–63

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Communication

Applying experimental constraints to a one-dimensional model for BiS_2 superconductivity

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ARTICLE INFO

Article history:
Received 15 April 2016
Received in revised form
29 June 2016
Accepted 1 July 2016
Available online 2 July 2016

Keywords:
Superconductivity
Pressure effects
One-dimensional models
Multi-gap superconductivity
BiS_2 compounds

ABSTRACT

Recent ARPES measurements [Sugimoto et al., Phys. Rev. B 92 (2015) 041113] have confirmed the one-dimensional character of the electronic structure of $CeO_{0.5}F_{0.5}BiS_2$, a representative of BiS_2-based superconductors. In addition, several members of this family present sizable increase in the superconducting transition temperature T_c under application of hydrostatic pressure. Motivated by these two results, we propose an effective one-dimensional three-orbital model, whose kinetic energy part, obtained through ab initio calculations, is supplemented by pair-scattering terms, which are treated at the mean-field level. We solve the gap equations self-consistently and then systematically probe which combination of pair-scattering terms gives results consistent with experiment, namely, a superconducting dome with a maximum T_c at the right chemical potential and a sizable increase in T_c when the magnitude of the hoppings is increased. For these constraints to be satisfied multi-gap superconductivity is required, in agreement with experiments, and one of the hoppings has a dominant influence over the increase of T_c with pressure.

1. Introduction

The recently discovered $LnOBiS_2$ family of superconductors, containing BiS_2 planes [1], presents interesting characteristics that have attracted much attention: a layered structure, similar to cuprates and pnictides [2]; a possible double superconducting gap as in MgB_2 [3]; its minimal model contains two bands [4], and Fermi surface nesting effects seem to be important [5] (as in the iron pnictides); because it contains a heavy element (Bismuth), spin-orbit effects are enhanced and some proposals linking BiS_2 to spin-triplet pairing and a weak topological superconducting state have been made [6–8]; based on first-principles electronic structure calculations, it has been pointed out the 'subtle' one-dimensional (1d) character of its band structure [4], which has been recently confirmed experimentally through polarization-dependent Angular Resolved Photoemission Spectroscopy (ARPES) measurements [9]; finally, a few members of the BiS_2 family have semiconducting parent compounds that become metallic/superconducting with electron doping or application of moderate hydrostatic pressure, which also can lead to sizable increase in T_c [10].

In this work, to advance the understanding of superconductivity (SC) in BiS_2, where there is no consensus yet if it is of conventional or unconventional type [11], we concentrate in these last two aspects: one-dimensionality of the electronic structure and the pronounced effects pressure has over the superconducting phase. To model that, the authors take the following approach: (i) adopt a 1d three-orbital model for BiS_2, adding the Cooper-pairing by hand, (ii) solve the gap equations at the mean-field level, (iii) study the dependence of the superconducting gap with the variation of the hopping terms, whose magnitude one expects to increase under applied pressure, (iv) decide on the acceptance or not of specific pair-scattering terms based on semi-quantitative agreement with experiments. Regarding this last point, we look specifically in what range of electron-filling a superconducting dome is obtained (see Fig. 2(a)) and how SC varies with hopping parameters [see Fig. 3(a) and (b)]. To make the connection with BiS_2 more explicit, and thus obtain semi-quantitative agreement with experiments, all the parameter values of the single-particle Hamiltonian were obtained through first-principles Density Functional Theory (DFT) calculations for a two-dimensional (2d) five-band model (see Table 1).

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http://dx.doi.org/10.1016/j.ssc.2016.07.001
0038-1098/

Table 1
Partial list of tight-binding parameters (in eV) for the 2d five-orbital model. The same parameters are used for the 1d three-orbital model depicted in Fig. 1(a). The chemical potential corresponds to 1/8-filling of the p_b orbital in the 1d model.

$\epsilon_{s,n}$	$\epsilon_{p_a,n}$	$\epsilon_{p_b,n}$	t_{sp}	t_{pp}	μ
−11.2840	−1.2691	0.1635	−0.9952	−0.8155	0.5007

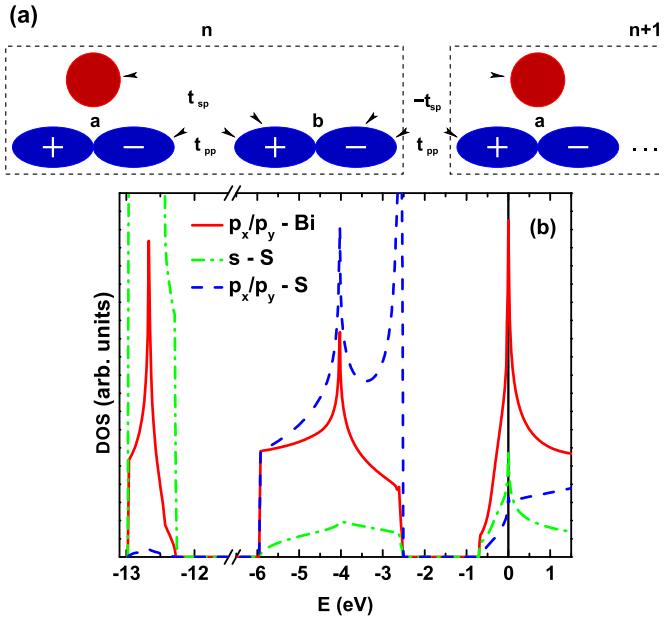

Fig. 1. (Color online) (a) 1d model for BiS_2. t_{pp} and t_{sp} are the hopping terms in our model. The dashed box indicates the unit cell with atoms a (Sulfur, with orbitals s and p) and b (Bismuth, with just one p orbital). (b) Density of states obtained through DFT for the *two-dimensional* five-orbital model of the $SrFBiS_2$ compound. Note the importance of the Sulfur s-orbitals [dot-dashed (green) line] at the Fermi energy (E_F=0), justifying its inclusion in the model described in panel (a). In addition, the van Hove singularities at the bottom of the conduction band and at the top of the valence band indicate the quasi-1d character of the electronic structure.

We can summarize our results as follows: taking into account a three-orbital model, where Sulfur contributes with orbitals s and p, and Bismuth with a p orbital [see Fig. 1(a)], we considered all possible pair-scattering terms (intra- and interband, restricted to pairs formed by same-band electrons), individually and in conjunction, and solved the resulting gap equation at the mean-field level. We obtain that (i) no single-band pair-scattering process, acting isolatedly, can describe the experiments (as specifically defined above), unless an unrealistic coupling is assumed ($g > 0.1$ eV); this seems to indicate that multi-gap SC is a natural consequence of our model, (ii) two different types of multi-gap SC (see detailed description below) are in semi-quantitative agreement with experiments, (iii) the gap dependence with hopping [see Fig. 3(a)] indicates a qualitative difference between the two hoppings considered in our model. These important results establish an appropriate effective 1d model to simulate the properties of BiS_2. We expect that our work will motivate other groups to investigate other similar purely 1d effective models.

Before describing the model and the results obtained, it is important to clarify the main objectives of the work presented here, in order to justify some of the approximations made and clearly state what was left out of our analysis. As already mentioned, the main objective is to explore the intriguing electronic-structure one-dimensionality aspect of BiS_2 and assess its relevance to SC. In doing that, our model assumes singlet-pairing and an s-wave-type order parameter as experimental facts [12]. In addition, SC is not derived from an assumed type of pairing, but introduced by hand, no assumption being made about its origin being conventional or unconventional, as this has not been experimentally settled yet [11]. The choice of a mean-field formalism is made with the clear understanding that, especially in 1d, it will not be able to capture the competition between superconducting and charge density wave phases. Furthermore, it is clear that, despite the indications of one-dimensionality mentioned above, the real system is *pseudo*-1d, in the sense that we are implicitly assuming a coupling between the chains that reduces the fluctuations and allows us to use a mean-field approximation. Therefore, the superconducting phase transition is a fully 3d phenomenon, where all chains become superconducting at T_c. Notice that this is an underlying assumption of almost all (pseudo) low-dimensional models for high-T_c cuprates and pnictides (2d), as well as Chevrel phases and organic superconductors (1d). Assuming the pair-scattering couplings as band independent constants conveniently decrease the number of self-consistent parameters from four to two. The full parameter space could be considered, but at the cost of a much larger computational effort, which will be avoided, as we believe this would only change the details of the results, not modifying our main conclusions. Finally, given the characteristics of our model, the simulation of an applied hydrostatic pressure is done in the most direct and objective way possible, i.e., by varying accordingly the tight-binding hoppings.

2. Model

We consider a linear chain with a unit cell consisting of two sites denoted a and b, see Fig. 1(a). The a sites (Sulfur) have orbitals s and p, while b sites (Bismuth) have just one p orbital. In second quantization notation, the annihilation operator for an s orbital in unit cell n is denoted as c_n, and those for Sulfur and Bismuth p orbitals are denoted $p_{a,n}$ and $p_{b,n}$, respectively. The non-interacting part of the Hamiltonian can then be written as

$$\mathcal{H} = \sum_n \{(\epsilon_{s,n} - \mu)n_{s,n} + \sum_{i=a,b} (\epsilon_{p_i,n} - \mu)n_{p_i,n}$$

$$+ t_{pp}[p^\dagger_{a,n}p_{b,n} + p^\dagger_{b,n}p_{a,n+1} + \text{h. c. }]$$

$$+ t_{sp}[c^\dagger_n p_{b,n} - p^\dagger_{b,n}c_{n+1} + \text{h. c. }]\}, \quad (1)$$

where $\epsilon_{s,n}$ and $\epsilon_{p_i,n}$ describe the energy levels of orbitals s and p (for site $i = a, b$) at unit cell n, respectively; $n_{s,n} = c^\dagger_n c_n$ and $n_{p_i,n} = p^\dagger_{i,n}p_{i,n}$ are the number operators, and μ is the chemical potential. In addition, we took into account the anti-symmetric nature of the hybridization between the s and p orbitals [note the negative sign in the last line of Eq. (1)]. The hopping parameters are indicated in Fig. 1(a) and the values used in this work (along with orbital energies and chemical potential) are listed in Table 1 in eV units. These parameter values were obtained through a DFT calculation performed on a representative BiS_2 system $SrFBiS_2$ using the full-potential linearized augmented plane-wave code WIEN2k [13] and the generalized gradient approximation [14] was employed. Hopping parameters were extracted using Wannier functions' technique as implemented in the code Wannier90 [15]. The hoppings kept for the 1d model here studied were all the nearest neighbor hoppings in excess of 0.5 eV.

An early 2d minimal model for BiS_2 contains two orbitals: Bismuth p_x and p_y orbitals [4]. Therefore, before deriving the self-consistent gap equations, the inclusion of the Sulfur p and s orbitals should be justified, mainly the latter one, which lies deep below the Fermi energy (see DFT parameter values in Table 1). Fig. 1(b) shows the density of states (DOS) obtained for a 2d model