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RPA Analysis of a Two-orbital Model for the BiS$_2$-based Superconductors

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The random-phase approximation (RPA) is here applied to a two-orbital model for the BiS$_2$-based superconductors that was recently proposed by Usui et al., arXiv:1207.3888. Varying the density of doped electrons per Bi site, n, in the range 0.46 ≤ n ≤ 1.0, the spin fluctuations promote competing $A_{1g}$ and $B_{2g}$ superconducting states with similar pairing strengths, in analogy with the $A_{1g}$-$B_{1g}$ near degeneracy found also within RPA in models for pnictides. At these band fillings, two hole-pockets centered at (0, 0) and $(\pi, \pi)$ display nearly parallel Fermi Surface segments close to wavevector $(\pi/2, \pi/2)$, whose distance increases with n. After introducing electronic interactions treated in the RPA, the inter-pocket nesting of these segments leads to pair scattering with a rather “local” character in k-space. The similarity between the $A_{1g}$ and $B_{2g}$ channels observed here should manifest in experiments on BiS$_2$-based superconductors if the pairing is caused by spin fluctuations.

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Introduction.—The recently discovered family of layered bismuth oxy-sulfide superconductors$^{1-22}$ has immediately attracted considerable attention from the Condensed Matter community due to its close similarities with the famous iron-pnictide superconductors.$^{23-27}$ As in the case of other layered unconventional superconductors, such as the cuprates and the aforementioned iron pnictides/chalcogenides, this new family displays a layered structure involving BiS$_2$ planes where the observed superconductivity is believed to reside. The first report of superconductivity originated in Bi$_4$O$_3$S$_3$, with $T_c = 4.5$ K.$^1$ Superconductivity has also been reported in ReO$_{1-x}$F$_x$BiS$_2$, where Re = La, Nd, Ce, and Pr, with corresponding $T_c = 10.6, 5.6, 3.0, 15$ and 5.5 K.$^{17}$ These compounds are metallic in the normal state and Density Functional Theory calculations indicate that the relevant bands crossing the Fermi surface (FS) originate mainly from the Bi 6p orbitals, as shown, e.g., for LaO$_{1-x}$F$_x$BiS$_2$. However, contrary to the majority of the Cu- and Fe-based unconventional superconductors, no magnetically ordered phase has been detected thus far in the BiS$_2$ compounds. This apparent absence of magnetism in the BiS$_2$ compounds may still locate them in the same category as LiFeAs, FeSe, and possibly Sr$_2$VO$_3$FeAs,$^{24}$ which are also non magnetic but their pairing properties are widely believed to still originate in short-range magnetic fluctuations. For these reasons, and despite the absence of observed long-range magnetism in BiS$_2$, it is important to study the potential role of spin fluctuations in these novel materials and the pairing channels that those fluctuations tend to favor, to help in the analysis of experimental data. It is important to note that there is experimental support for considering, at least Bi$_4$O$_3$S$_3$, as an unconventional superconductor (see Ref. 4 for details). Recent theoretical work has interpreted superconductivity as originating from electron-phonon coupling.$^{11,28}$ However, subsequent neutron scattering experiments$^{29}$ have not given support to this scenario.

In this manuscript, the two-orbital (2-orbital) model recently introduced by Usui et al.$^3$ is adopted.$^3$ The fact that the relevant orbitals in BiS$_2$ compounds are p-type, where Coulomb interactions should be smaller than in d orbitals, turns RPA into a suitable technique, whose results deserve a careful analysis if electron correlations are found to be important for superconductivity in these materials. Similar calculations for a related four-orbital model$^3$ are underway. Note that in Ref. 3 a brief discussion of RPA calculations has already been presented. The results discussed by Usui et al. consisted of a single set of couplings (equivalent to our J/U = 0.2 calculations below) at n = 0.5. Their early weak-coupling RPA analysis is here expanded via a systematic study of the influence of the band filling $n$ and the identification of the dominant channels for superconductivity under the assumption of a spin fluctuations mechanism. The main novel contribution of our present effort is the identification of closely competing $B_{2g}$ and $A_{1g}$ gap functions as the dominant pairing channels, particularly for band fillings around $n = 0.5$. At quarter filling ($n = 1.0$), another pair of almost degenerate gap functions (with symmetries $A_{2g}$ and $B_{1g}$) is found to closely compete with the previously mentioned dominant pair, especially at $J/U = 0.3$.$^{30}$

Hamiltonian. The 2-orbital model described by Usui et al.$^3$ contains hopping parameters up to fourth neighbors, and in k-space is given by

$$H_{TB}(k) = \sum_{\mathbf{k, \sigma, \mu, \nu}} T^{\mu\nu}(\mathbf{k}) d_{\mathbf{k, \mu, \sigma}}^\dagger d_{\mathbf{k, \nu, \sigma}} ,$$

where

$$T^{XX} = 2t_x^X (\cos k_x + \cos k_y) + 2t_{x+y}^X \cos (k_x \pm k_y)$$
$$+ 2t_{x-y}^X [\cos (2k_x \pm k_y) + \cos (k_x \pm 2k_y)] + \epsilon_X ,$$
$$T^{YY} = 2t_y^Y (\cos k_x + \cos k_y) + 2t_{x\pm y}^Y \cos (k_x \mp k_y)$$
$$+ 2t_{x\pm y}^Y [\cos (2k_x \pm k_y) + \cos (k_x \pm 2k_y)] + \epsilon_Y ,$$
$$T^{XY} = T^{YX} = 2t_x^{XY} (\cos k_x - \cos k_y)$$
$$+ 4t_x^{XY} (\cos 2k_x - \cos 2k_y)$$
$$+ 4t_{x+y}^{XY} (\cos 2k_x \cos k_y - \cos k_x \cos 2k_y) .$$

The operator $d_{\mathbf{k, \nu, \sigma}}^\dagger$ (or $d_{\mathbf{k, \nu, \sigma}}$) in Eq. (1) creates (annihilates) an
TABLE I: Tight-binding parameters (eV) for 2-orbital model.

<table>
<thead>
<tr>
<th>$\epsilon_{X,Y}$</th>
<th>$t_{X,Y}$</th>
<th>$t_{X+Y}$</th>
<th>$t_{X,Y}$</th>
<th>$t_{X+Y}$</th>
<th>$t_{X,Y}$</th>
<th>$t_{X+Y}$</th>
<th>$t_{X,Y}$</th>
<th>$t_{X+Y}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.811</td>
<td>-0.167</td>
<td>0.880</td>
<td>0.004</td>
<td>0.069</td>
<td>0.014</td>
<td>0.107</td>
<td>-0.028</td>
<td>0.020</td>
</tr>
</tbody>
</table>

FIG. 1: (Color online) (a) Hole-pockets for four different electronic fillings: $n = 0.46$ (solid red), $n = 0.50$ (dashed green), $n = 0.65$ (dotted blue), and $n = 1.00$ (dot-dashed magenta). Note that close to the $(\pi/2, \pi/2)$ wavevector, where the $n = 0.46$ pockets almost touch, the increase of $n$ decreases the area of the hole-pockets and, more importantly, the adjacent FS segments (inside the dashed box) become more and more parallel. (b) Lindhard function $\chi_0$ for the same fillings as in panel (a). Note that the position of the leftmost peaks in $\chi_0$ agree (within a few percent) with the vectors indicated in the inset (see text for details, especially Fig. 5). Obviously, there are additional nesting vectors that become evident in a 2-d plot of $\chi_0$ [Fig. 5(b)].

The Coulomb interaction in the Hamiltonian is given by

$$H_{\text{int}} = U \sum_{i,\alpha} n_{i,\alpha} n_{i,\alpha} + (U' - J/2) \sum_{i,\alpha < \beta} n_{i,\alpha} n_{i,\beta} - 2J \sum_{i,\alpha < \beta} S_{i,\alpha} \cdot S_{i,\beta} + J \sum_{i,\alpha < \beta} (d_{i,\alpha \alpha}^\dagger d_{i,\beta \beta}^\dagger + h.c.),$$

where the notation is standard and the many terms have been described elsewhere. The usual relation $U' = U - 2J$ is assumed, and $J/U$ is a parameter. Calculations were done for $0.1 \leq J/U \leq 0.4$, in steps of 0.1, for the four fillings $n = 0.46, 0.50, 0.65,$ and $1.0$. The multi-orbital RPA calculations performed here follow closely those described in Ref. 33, and previous works by the authors. All results were obtained at temperature $T = 10^{-4}$ and an imaginary part $\eta = 10^{-5}$ was used to regularize the Green’s functions.

Our RPA results for spin-singlet pairing link the dominant superconducting gap functions to spin fluctuations, which originate in FS nesting and are enhanced by electronic interactions. The particular relative topology of the two adjacent hole-pockets (see Fig. 1) promotes pairing whose strength is independent of the global symmetry of the pairing functions [see Fig. 4(b)]. Indeed, the $B_{2g}$ and $A_{1g}$ symmetries have essentially the same pairing strength, which is determined by pair scattering between these two adjacent FS segments (see Fig. 5) close to $\pi/2, \pi/2$ in the Brillouin Zone (BZ). In addition, our results show that both dominant gap functions change sign between these two segments (Figs. 2 to 4), and the pairing is through the intraorbital scattering channel [Fig. 3(b) and (c)]. The near degeneracy $A_{1g} - B_{2g}$ is the analog of the near degeneracy $A_{1g} - B_{1g}$ found also in RPA calculations for the pnictides, since the pocket structures in both cases can be related by a $45^\circ$ rotation. Results for spin-triplet pairing are presented in the supplemental material.

**Results and Discussion.** As mentioned above, the most important feature of the FS for fillings between 0.46 and 1.0 is that the hole-pockets centered at the $\Gamma$ and $M$ points present almost parallel segments close to the $(\pi/2, \pi/2)$ wavevector, becoming more and more parallel as the pockets shrink, with
increasing filling [see Fig. 1(a) and inset in Fig. 1(b)]. In Figs. 2 and 3 it will be shown that this has important consequences for the spin fluctuations and the superconducting pairing associated to this 2-orbital model. Indeed, as displayed in the main panel of Fig. 2(a) (solid red curve), there is a divergence in the RPA spin susceptibility for very small $k$ values: $k_{0.46} \sim (\pi/25, 0)$ for $n = 0.46$, and $k_{0.50} \sim (\pi/8, 0)$ for $n = 0.50$ [panel (b)]. A divergence in the spin susceptibility $\chi_{\text{RPA}}$ may point to magnetic order, or at least to strong spin fluctuations with wave vector $k_\text{s}$. Figure 3(a) shows the same calculations, but now for $n = 0.65$. Note that although $\chi_0$ displays a broad-peak structure around $(\pi, \pi)$ [see Fig. 1(b)], $\chi_{\text{RPA}}$ does not present a divergence in this region. In the insets to Figs. 2(a) and (b), and Fig. 3(a), it is shown that the dominant gap function at the FS has symmetry $A_{1g}$ for the three cases, showing that despite the changes in the size of the hole-pockets the results are qualitatively the same. Figures 3(b) and (c) contain the orbital contribution ($X$, red solid curve; $Y$, green dashed curve) of the BZ states at the FS for the $\Gamma$ and $M$ pockets, respectively. It is interesting to note that the modifications in the position of the peak in $\chi_{\text{RPA}}$ correlates well with the “separation” between the $\Gamma$ and $M$ hole-pockets in the region around $(\pi/2, \pi/2)$. For the purposes of describing our results, this separation will be defined as the horizontal distance between two parallel lines tangent to the hole-pockets at the points where each intercepts the $\Gamma - M$ ($\Sigma$) line. As described in more detail in Fig. 5(a) [and already mentioned in connection with Fig. 1(a)], as the filling increases these segments of FS approach more and more the parallel lines just defined, justifying the definition just given.

The RPA results for the gap functions also point to an interesting effect, namely, the small value of $k_\text{s}$ for fillings $0.46 \leq n \leq 1.0$ results in the pairing strength depending on very “local” properties of the gap function at the adjacent segments of the hole-pockets. This implies that the pairing strength of gap functions with different symmetries is very similar, as long as they have the same “local” properties. To demonstrate that, in Fig. 4(a) the dominant gap function (with $A_{1g}$ symmetry) is shown for $n = 1.0$ and $J/U = 0.3$. It is clear that it is very similar in structure to the subdominant ones shown in the previous figures. In the inset to Fig. 4(b) the subdominant gap function with symmetry $B_{2g}$ is displayed for the same parameters. Note that comparing it with the dominant gap function in panel (a), despite having different symmetries, the two gap functions are identical in the two adjacent hole-pocket segments that cross the $\Sigma$ line. For this reason, their pairing strengths as measured by $\lambda$ (the eigenvalues of the Eliashberg Equation), and shown in the main panel of Fig. 4(b), are the same to the third decimal place. Note that the two eigenvalues for symmetries $A_{1g}$ and $B_{2g}$ are not degenerate. This seems a strong indication that the “local” aspect of the pair scattering, as mentioned above, seems to be determinant to establish the pairing properties of this model, at least

FIG. 3: (Color online) (a) RPA spin susceptibility and dominant gap function for $n = 0.65$. Orbital composition for the $(0, 0)$ and $(\pi, \pi)$ FS pockets ($n = 0.65$), (b) and (c), respectively. The winding angle $\theta$ runs counter-clockwise, starting from the $k_x$ direction. Assuming the nesting described in the inset to Fig. 1(b) as producing the spin fluctuations that provide pairing, the pair coupling is then intra-orbital.

FIG. 4: (Color online) (a) Dominant gap function with symmetry $A_{1g}$ at $n = 1.0$. (b) Main panel: normalized pairing strengths $\lambda$ for the dominant $(A_{1g},$ solid red curve) and subdominant $(B_{2g},$ dashed green curve) gap functions. Although the two curves are very close, the eigenvalues are not degenerate. In the inset, the structure of the subdominant gap function ($B_{2g}$) is shown. When compared to that of the dominant one [$A_{1g}$ in panel (a)], it is clear that the structure around $(\pi/2, \pi/2)$ is very similar to each other, explaining why the pairing strengths (eigenvalues) are the same. The region inside the dashed box, in panel (a), is analyzed in detail in Fig. 5(a).

FIG. 5: (Color online) (a) Region around point $(\pi/2, \pi/2)$ of the BZ [dashed box in Fig. 4(a)], showing the dominant $(A_{1g})$ gap-function for $n = 1.0$ and $J/U = 0.3$. (b) Two dimensional contour plot of $\chi_0$ also for $n = 1.0$. The horizontal (blue) vector in panel (a) connects the maximum amplitude of the gap-function in both pockets. Note also the horizontal (blue) vector in panel (b) along the $k_x$ direction, indicating the position of the maximum value of $\chi_0$. These two vectors agree up to a difference smaller than the width of this maximum peak in $\chi_0$. Therefore, it can be shown (see text) that the line describing the position of the points in the $M$ pocket in relation to the points in the $\Gamma$ pocket, as indicated by the two additional vectors (black and red) in panel (a), satisfies $k_x \sim -k_x + k_y$, where $(k_x, 0)$ and $(0, k_y)$ are the positions of the maxima in $\chi_0$ (with $n = 1.0$). This equation also describes the line of local maxima of $\chi_0$, as seen in panel (b), originating from FS nesting.
in our RPA weak-coupling approach. It should be noted that the rest of the BZ.

Fig. 5(a) where the gap function has a very pronounced peak, should be highlighted: the four points in the hole-pockets in Fig. 3(b) and the gap structure in Fig. 4 it appears that the symmetry of the B1g and A1g pairing operators is determined by the orbitals, while the spatial form in both cases is characterized by symmetric nearest-neighbor pairing with rotational invariance. Thus, the pairing operators have the form \( \Delta^\dagger = f(k)(d^\dagger_{k,x^\uparrow}d^\dagger_{-k,x^\downarrow} \pm d^\dagger_{k,y^\uparrow}d^\dagger_{-k,y^\downarrow}) \) where the + (−) sign corresponds to A1g (B2g) symmetry with \( f(k) = \cos k_x + \cos k_y \), plus higher harmonics with A1g symmetry.

Figure 5(a) shows in more detail the almost parallel FS segments of the two hole-pockets for \( n = 1.0 \). In this figure, the horizontal (blue) vector that was defined above as the separation between the two FS segments is displayed. A vector with the same length is reproduced in panel (b), where a 2d plot of \( \chi_0 \) in the first quadrant of the BZ is also shown. It clearly indicates that the position \( k_0 \) of the main peak in \( \chi_0 \) is exactly given by the horizontal separation. Not only that, the (red) vector along the \( \Sigma \) line in panel (a) is also reproduced in panel (b) and it too coincides exactly with a local maximum of \( \chi_0 \). In fact (see in both panels the black vectors located at angle \( \alpha \)), the locus of the ridge of local maxima in \( \chi_0 \) in panel (b) exactly coincides with the BZ points defined by the vectors connecting the two FS segments for \( 0 \leq \alpha \leq \pi/2 \). Figure 6 shows the RPA spin susceptibility for \( n = 1.0 \). The similarity between these results and those in Fig. 5(b) is clear, indicating that the FS nesting for the interacting system is the one described by the vectors in Fig. 5. Finally, an important issue should be highlighted: the four points in the hole-pockets in Fig. 5(a) where the gap function has a very pronounced peak, are exactly the two pairs of points (one in each pocket) connected by \( (k_{1,0}, 0) \) and \( (0, k_{1,0}) \). This fact clearly links the pairing properties with the spin fluctuations. Note also that for \( n = 1.0 \) and \( J/U = 0.3 \), the second pair of eigenvalues \( (\lambda_3 = 0.9038 \text{ and } \lambda_4 = 0.9036) \) corresponds to symmetries \( A_{2g} \) and \( B_{1g} \), respectively (not shown). The same occurs for \( J/U = 0.1 \) and \( J/U = 0.2 \), also for \( n = 1.0 \) (but the eigenvalues are smaller). Yet, the same explanation as described in Fig. 5 applies. See the supplemental material\(^{35}\) for a connection between the emergence of a \( B_{1g} \) symmetry at \( n = 0.50 \) with the one-dimensionality of the bands.

Conclusions. Summarizing, a weak-coupling RPA analysis of a minimal 2-orbital model was used to investigate the pairing properties of the BiS\(_2\)-based superconductors. Fillings between 0.46 and 1.0 were analyzed. The Hund’s coupling was varied in the range \( 0.1 \leq J/U \leq 0.4 \). Qualitatively, the results are similar for all values of \( J/U \) and different fillings. In the RPA results described here, a clear relationship is found between quasi FS nesting, spin fluctuations, and superconductivity: the topology of the two hole-pockets is such that they present almost parallel segments close to the \((\pi/2, \pi/2)\) wavector in the BZ. It is found that the horizontal distance \( (k_n, 0) \) between the tangents to these segments at the points where they cross the \( \Sigma \) line is also where the non-interacting susceptibility \( \chi_0 \) has a pronounced peak at \( (k_n, 0) \), for \( 0.46 \leq n \leq 1.0 \). Once interactions are introduced, this peak will diverge at a certain critical coupling \( U \) for each filling, and all the values of \( J/U \) studied (with exception of one: \( n = 0.5, J/U = 0.1 \)). In addition, a line of local maxima, connecting the BZ points \( (k_n, 0) \) and \( (0, k_n) \), is clearly observed in a 2d plot of \( \chi_0 \). As expected, this line can also be associated to FS nesting. This nesting structure gives origin to pairing functions with similar eigenvalues, i.e., similar pairing strengths, and symmetries \( B_{2g} \) and \( A_{1g} \). This close competition originates in the FS quasi nesting properties, which determine the spin-fluctuation-mediated inter-pocket pair scattering. This pair scattering is overwhelmingly between two adjacent FS segments, therefore the properties of the pairing functions, including the pairing strength, are quite “local”, having almost no dependence on their global symmetry. One can then predict that pairing symmetry measurements may contain a mixture of both symmetries if the pairing mechanism is driven by spin fluctuations.

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30. Although the experimentally relevant electron density is $n \sim 0.5$, the study of higher $n$ values had the sole purpose of verifying the consistency of our results and interpretation for a larger set of qualitatively similar FS geometries to ascertain that the results did not depend fundamentally on some feature of the FS. Our results lead to the same interpretation for the full range of density values analyzed.
31. Note that in Ref. 3 (Fig. 4(c), $n = 0.5$), there are small pockets around the $(\pi, 0)$ points. To obtain these pockets, hopping matrix elements to considerably larger distances have to be added to the Hamiltonian described here. The authors of Ref. 3 ascertained that the presence or not of these pockets does not alter the main RPA results (private communication).
35. See supplemental material at http://...