Comment on "Nonmagnetic Impurity Resonances as a Signature of Sign-Reversal Pairing in FeAs-Based Superconductors"

In a recent Letter [1], the energy band structure of Fe-As-based superconductors is fitted with a tight-binding model with two Fe ions per unit cell and two degenerate d_{xz} and d_{yz} orbitals per Fe ion. The author claims that the proposed model, which differs markedly from a model previously used by other authors for the same two orbitals in the same compounds [2,3], possesses the symmetry required to describe the Fe-As planes in iron-pnictide superconductors. In this Comment we argue that this is not the case.

As discussed in Ref. [1], the unit cell of the Fe-As planes contains two iron ions, and the Hamiltonian Eq. (1) employed there reflects this. However, each two-iron unit cell also has an internal symmetry that the Hamiltonian needs to obey. To see this, consider the square lattice made up by all iron ions, i.e., with one iron per unit cell, and the Fe-Fe distance as a new basis vector. The Fe-As planes are invariant under (a) translation by one unit along the Fe-Fe direction, followed by (b) a reflexion on the Fe-Fe plane. At first sight, the Hamiltonian of Ref. [1] appears to take this into account, because a translation by one Fe-Fe distance and an additional exchange of hoppings t_2 (mediated by an As *above* the plane) and t_3 (via an As *below* the plane) indeed leaves it invariant. But since the Fe-As-Fe distances and angles are the same for As ions above and below the plane, these two hopping paths are very symmetric, which induces additional restrictions [4] and the two paths actually give the same hopping [5].

This missing symmetry of the Hamiltonian also reveals itself in the momentum-dependent band structure. The d_{xz} and d_{yz} orbitals should be degenerate at the Γ point [4,6], as it can also be seen in band structures obtained from the local density approximation [7–11] or by a Slater-Koster approach [6,12]. Another consequence of the internal symmetry of the two-iron unit cell is that all bands have to be twofold degenerate at the boundaries of the Brillouin zone (BZ) corresponding to the two-Fe unit cell [4], which is clearly violated in the Hamiltonian presented in Ref. [1], see the data for the $(\pi, 0)$-(π, π) path in Fig. (2) [13]. In fact, any tight-binding Hamiltonian for the Fe-As planes can be written in block form, where each block is expressed in terms of the orbitals of one single Fe per unit cell [4,6]. Instead of studying both blocks for the BZ of the original two-iron unit cell, one can then consider just one block, but in the extended BZ corresponding to a unit cell with just one Fe ion, because the two blocks correspond to momenta $\mathbf{k}$ and $\mathbf{k} + (\pi, \pi)$ in the extended BZ. In this description, the system has D_{4h} symmetry which means that all the eigenstates at the center of the BZ should transform according to irreducible representations of D_{4h}. In particular, the orbitals d_{xz} and d_{yz} transform according to the two-dimensional representation E_g leading to the

degeneracy at the center of the BZ, which is missing in the Hamiltonian of Ref. [1].

Finally, t_3 is 5 times larger than t_2 in Ref. [1]. This difference is extreme even for the orthorhombic phase of the pnictides, where a slight oxygen distortion of 1% (6%) in bulk (on surfaces) [14] might in principle justify a small difference.

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