We study the effect of the spin-orbit coupling on the band structure and the Fermi surface of the three-orbital model within the two-iron Brillouin zone. Due to the presence of two irons in the crystallographically correct unit cell, the spin-orbit coupling can be divided into the intra- and intercell parts with respect to the one-iron unit cell. We show that the intercell part produces the reconstruction of the Fermi surface in the form of the pronounced splitting between the previously degenerate electron \((\pi, \pi)\)-pockets along the \((0, \pi) - (\pi, \pi)\) direction. Intracell part shifts the bands around \((0, 0)\) point and removes degeneracy there. There are also some other band shifts but they should not affect the low-energy physics because they occur at energy scales of about 1 eV below the Fermi level.

Keywords: Fe-based superconductors, spin-orbit coupling, band structure, Fermi surface.

where and a spin $k+4$.

1. Three-orbital model in 1-Fe BZ

Fermi surface in the 2-Fe BZ within the three-orbital model from Ref. [9].

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However, some experiments sensitive to the Fe positions, like neutron scattering on Fe
and DFT band structure are reported in the folded BZ since crystallographically it is the correct
approach was used before to study the spin response in model from Ref. [9] within the 1-Fe
BZ [12].

There is a complication coming from the As, which forms square lattice planes between the
lattice sites of, but also above and below, the square lattice of Fe. This alternating pattern of As
makes the correct real space unit cell twice the 1-Fe unit cell. The corresponding 2-Fe BZ is twice
as small as the 1-Fe one and called “folded BZ”. For the simplest case of single-layer Fe pnictides
the folding wave vector is two-dimensional and equal to $Q = (\pi, \pi)$. Most experimental results
and DFT band structure are reported in the folded BZ since crystallographically it is the correct
one. However, some experiments sensitive to the Fe positions, like neutron scattering on Fe
moments, have more meaning in the 1-Fe BZ (“unfolded” zone).

Here we study the role of the SO coupling in the formation of the band structure and the
Fermi surface in the 2-Fe BZ within the three-orbital model from Ref. [9].

1. Three-orbital model in 1-Fe BZ

We write the Hamiltonian of the three-orbital model [9] in the following form:

$$H_0 = \sum_{\mathbf{k},\sigma,l,m} \varepsilon_{lm}^{\mathbf{k}} c_{l\sigma}^\dagger c_{m\sigma},$$

where $l$ and $m$ are orbital indices, $c_{\mathbf{k}m\sigma}$ is the annihilation operator of a particle with momenta
$k$ and a spin $\sigma$. We choose the following numbering of orbitals, $d_{xy} \leftrightarrow 1$, $d_{yz} \leftrightarrow 2$, $d_{zx} \leftrightarrow 3$. The model consists of the three $t_{2g}$ orbitals and all of them are hybridized. Matrix of one-electron
energies and hoppings, $\hat{\varepsilon}_\mathbf{k}$, is given by

$$\hat{\varepsilon}_\mathbf{k} = \begin{pmatrix}
\varepsilon_{1\mathbf{k}} & 0 & 0 \\
0 & \varepsilon_{2\mathbf{k}} & \varepsilon_{4\mathbf{k}} \\
0 & \varepsilon_{4\mathbf{k}} & \varepsilon_{3\mathbf{k}}
\end{pmatrix},$$

where $\varepsilon_{1\mathbf{k}} = \varepsilon_{xy} - \mu + 2t_{xy}(\cos k_x + \cos k_y) + 4t'_{xy} \cos k_x \cos k_y$, $\varepsilon_{2\mathbf{k}} = \varepsilon_{yz} - \mu + 2t_x \cos k_x + 2t_y \cos k_y + + 4t' \cos k_x \cos k_y + 2t''(\cos 2k_x + \cos 2k_y)$, $\varepsilon_{3\mathbf{k}} = \varepsilon_{xz} - \mu + 2t_y \cos k_x + 2t_x \cos k_y + 4t' \cos k_x \cos k_y + + 2t''(\cos 2k_x + \cos 2k_y)$, $\varepsilon_{4\mathbf{k}} = 4t_{xzy} \sin k_x / 2 \sin k_y / 2$. The following set of parameters (in eV)
alows to reproduce the topology of the Fermi surface in iron pnictides: chemical potential $\mu = 0$,
$\varepsilon_{xy} = -0.70$, $\varepsilon_{yz} = -0.34$, $\varepsilon_{xz} = -0.34$, $t_{xy} = 0.18$, $t'_{xy} = 0.06$, $t_x = 0.26$, $t_y = -0.22$, $t' = 0.2$,$t'' = -0.07$, $t_{xzy} = 0.38$. 


2. Spin-orbit coupling in 1-Fe BZ

Following Ref. [13], we write the spin-orbit coupling terms, \( H_{SO} = \lambda \sum_{f} L_{f} \cdot S_{f} \), in the second-quantized form assuming that three \( t_{2g} \) states behave like an \( \ell = 1 \) angular momentum representation,

\[
H_{SO} = i \lambda \sum_{l,m,n} \epsilon_{l,m,n} \sum_{k,\sigma,\sigma'} c_{k2\sigma}^\dagger c_{k3\sigma'} \delta_{\sigma\sigma'}^{n} \delta_{\sigma\sigma'}^{n'},
\]

where \( \epsilon_{l,m,n} \) is the completely antisymmetric tensor, indices \( \{l, m, n\} \) take values \( \{x, y, z\} \) or equivalently \( \{d_{xz}, d_{xy}, d_{yz}\} \leftrightarrow \{2, 3, 1\} \), and \( \delta_{\sigma\sigma'}^{n} \) are the Pauli spin matrices. Explicit form of the Hamiltonian is the following:

\[
H_{SO} = i \lambda \sum_{k,\sigma} \left[ c_{k2\sigma}^\dagger c_{k3\sigma} \text{sgn}(\sigma) + ic_{k2\sigma}^\dagger c_{k1\sigma} \text{sgn}(\sigma) + c_{k3\sigma}^\dagger c_{k1\sigma} - h.c. \right].
\]

Let us introduce vector operators in the orbital space,

\[
\hat{\Psi}_{k\sigma}^\dagger = \left( c_{k1\sigma}^\dagger, c_{k2\sigma}^\dagger, c_{k3\sigma}^\dagger \right).
\]

Then,

\[
H_{0} = \sum_{k,\sigma,\sigma'} \hat{\Psi}_{k\sigma}^\dagger \hat{\sigma}_{\sigma'}^{n} \Psi_{k\sigma'},
\]

\[
H_{SO} = \sum_{k,\sigma,\sigma'} \hat{\sigma}_{\sigma'}^{n} \delta_{\sigma\sigma'}^{n'} \hat{\Psi}_{k\sigma}^\dagger \Psi_{k\sigma'}. \tag{5}
\]

Here

\[
\hat{\Psi}_{SO}^{\sigma\sigma'} = i \lambda \left( \begin{array}{cc} 0 & -i \delta_{\sigma',\sigma} \text{sgn}(\sigma) \\ i \delta_{\sigma',\sigma} \text{sgn}(\sigma) & 0 \\ -\delta_{\sigma',\sigma} \text{sgn}(\sigma) & \delta_{\sigma',\sigma} \text{sgn}(\sigma) \end{array} \right) = \hat{\Psi}_{SO}^{\sigma} \delta_{\sigma',\sigma} \left( \hat{\xi}^{\sigma} - i \hat{\eta}^{\sigma} \text{sgn}(\sigma) \right), \tag{6}
\]

\[
\hat{\xi}^{\sigma} = \left( \begin{array}{ccc} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{array} \right) = iJ_{x}, \quad \hat{\eta}^{\sigma} = \left( \begin{array}{ccc} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{array} \right) = -iJ_{y}, \quad \hat{\xi}_{SO}^{\sigma} = \left( \begin{array}{ccc} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{array} \right) = iJ_{z}. \tag{7}
\]

Here, \( J_{i} \) are the generators of the rotation group \( O(3) \). It is well known [14] that \( O(3) \) transformation of the \((x, y, z)\) vector is equivalent to the \( SU(2) \) transformation of the \((\xi_{1}, \xi_{2})\) spinor if \( x = \frac{1}{2}(\xi_{2}^{2} - \xi_{1}^{2}), \quad y = \frac{1}{2i}(\xi_{2}^{2} + \xi_{1}^{2}), \quad z = \xi_{1}\xi_{2} \).

The total Hamiltonian \( H = H_{0} + H_{SO} \) can be written explicitly as

\[
H = \sum_{k,\sigma} \left[ \hat{\Psi}_{k\sigma}^\dagger \left( \hat{\xi}_{k} + i \frac{\lambda}{2} \hat{\eta}_{k} \text{sgn}(\sigma) \right) \hat{\Psi}_{k\sigma} + i \frac{\lambda}{2} \hat{\Psi}_{k\sigma}^\dagger \left( \hat{\xi}_{k} - i \frac{\lambda}{2} \hat{\eta}_{k} \text{sgn}(\sigma) \right) \hat{\Psi}_{k\sigma} \right] =
\]

\[
= \sum_{k} \left[ \hat{\Psi}_{k1}^\dagger \left( \hat{\xi}_{k} + i \frac{\lambda}{2} \hat{\eta}_{k} \right) \hat{\Psi}_{k1} + \hat{\Psi}_{k1}^\dagger \left( \hat{\xi}_{k} - i \frac{\lambda}{2} \hat{\eta}_{k} \right) \hat{\Psi}_{k1} + \hat{\Psi}_{k2}^\dagger \hat{\xi}_{k} \hat{\Psi}_{k2} + \hat{\Psi}_{k2}^\dagger \hat{\eta}_{k} \hat{\Psi}_{k2} - \frac{\lambda}{2} \hat{\Psi}_{k3} \hat{\xi}_{k} \hat{\Psi}_{k3} + \frac{\lambda}{2} \hat{\Psi}_{k3} \hat{\eta}_{k} \hat{\Psi}_{k3} \right] =
\]

\[
= \sum_{k} \left( \hat{\Psi}_{k1}^\dagger \hat{\Psi}_{k1} + \hat{\Psi}_{k2}^\dagger \hat{\Psi}_{k2} \right) \cdot \hat{H} \cdot \left( \hat{\Psi}_{k1} \hat{\Psi}_{k2} \right), \tag{8}
\]

where

\[
\hat{H} = \left( \begin{array}{ccc} \hat{\xi}_{k} + \frac{\lambda}{2} \hat{\eta}_{k} & i \frac{\lambda}{2} \hat{\xi}_{k} + \frac{\lambda}{2} \hat{\eta}_{k} \\ i \frac{\lambda}{2} \hat{\xi}_{k} - \frac{\lambda}{2} \hat{\eta}_{k} & \hat{\xi}_{k} - i \frac{\lambda}{2} \hat{\eta}_{k} \end{array} \right). \tag{9}
\]
If one considers only the \( z \)-component of the SO coupling, then the expression for \( H \) simplifies significantly,

\[
H_z = H_0 + H_{SOz} = \sum_{k, \sigma} \hat{\psi}_{k\sigma}^\dagger \left( \xi_k + i \frac{\lambda}{2} \xi^z \text{sgn} (\sigma) \right) \hat{\psi}_{k\sigma} = \sum_k \left( \hat{\psi}_{k\uparrow}^\dagger \hat{\psi}_{k\downarrow} \right) \hat{H}_z \left( \hat{\psi}_{k\uparrow} \hat{\psi}_{k\downarrow} \right),
\]

(11)

where

\[
\hat{H}_z = \begin{pmatrix}
\xi_k + i \frac{\lambda}{2} \xi^z & 0 \\
0 & \xi_k - i \frac{\lambda}{2} \xi^z
\end{pmatrix}.
\]

(12)

Therefore, \( z \)-component of the SO interaction modifies one-electron energies only, but does it differently for spin-up and spin-down elements of the spin-resolved Hamiltonian matrix \( \hat{H} \). On the other hand, \( x \) - and \( y \)-components mix spin-up and spin-down matrix elements and thus effectively increase the dimensionality of the problem by a factor of two.

3. Spin-orbit coupling in 2-FeBZ

While working in the unfolded BZ as before, we are missing important effect of the SO hybridization between orbitals on neighboring irons. After such a hybridization the unfolding is not possible any more. Hereafter we utilize the following conjecture: the structure of the SO coupling between two orbitals on neighboring irons is the same as the structure between two orbitals with the same symmetry on the one iron. Thus, if SO coupling between \( d_{xz} \) and \( d_{yz} \) orbitals has the form \( i \frac{\lambda}{2} \xi^z \), the same form holds for \( d_{xz} \) on Fe-1 (some one-iron unit cell) and \( d_{yz} \) on Fe-2 (neighboring one-iron unit cell). For convenience, we assign different coupling constant, \( \lambda' \), to intercell SO interaction; one can always put it to be equal to \( \lambda \). Note that when we use a wording ‘intercell SO coupling’, it does not mean a long-range SO coupling. The SO interaction is always local but since orbitals of two neighboring irons hybridize directly and through As, the wave functions of electrons on these orbitals can overlap that opens up a possibility for the effectively intercell SO coupling.

Brillouin zone folding, i.e. transition from 1-Fe BZ to 2-Fe BZ, is done in two steps. First, momenta are transformed as \((k_x + k_y) / 2 \rightarrow k'_x, (k_x - k_y) / 2 \rightarrow k'_y\). Second, the Hamiltonian matrix is doubled by adding the shifted \( \xi_{k'+Q_F} \), where \( Q_F = (\pi, \pi) \) is the folding wave vector. Thus, the Hamiltonian (1) takes the form

\[
H_0 = \sum_{k', \sigma, l, m} \xi_{k', \sigma, l, m} + \sum_{k', \sigma, l, m} \xi_{k'+Q_F, \sigma, l, m}.
\]

(13)

Later we skip prime assuming that all momenta are within the 2-Fe BZ.

The Hamiltonian can be written in the matrix form analogous to Eq. (9),

\[
H = \sum_k \left( \hat{\psi}_{k\uparrow}^\dagger \hat{\psi}_{k\downarrow} \right) \hat{H} \left( \hat{\psi}_{k\uparrow} \hat{\psi}_{k\downarrow} \right),
\]

(14)

where \( \hat{\psi}_{k\sigma} (\hat{\psi}_{k\sigma}) \) corresponds to the first (second) set of iron orbitals.
In case of intracell SO coupling, \( \hat{H} \) has the form which immediately follows from Eq. (10):

\[
\hat{H} = \begin{pmatrix}
\hat{\varepsilon}_k + i\frac{\lambda}{2}\hat{\xi}^z & \frac{\lambda}{2}\hat{\xi}^x + \frac{\lambda}{2}\hat{\eta}^y \\
\frac{\lambda}{2}\hat{\xi}^x - \frac{\lambda}{2}\hat{\eta}^y & -i\hat{\varepsilon}_k + \frac{\lambda}{2}\hat{\eta}^z \\
0 & 0 \\
\end{pmatrix}.
\] (15)

For finite \( \lambda \), the result of diagonalization of Eq. (15) is the same as of Eq. (10). New effects come in once we add the intercell SO coupling:

\[
\hat{H}_{SO\text{inter}} = \begin{pmatrix}
0 & 0 & \frac{\lambda'}{2}\hat{\eta}^z & \frac{\lambda'}{2}\hat{\xi}^x + \frac{\lambda'}{2}\hat{\eta}^y \\
0 & 0 & \frac{\lambda'}{2}\hat{\xi}^x - \frac{\lambda'}{2}\hat{\eta}^y & -i\frac{\lambda'}{2}\hat{\eta}^z \\
\frac{\lambda'}{2}\hat{\eta}^z & \frac{\lambda'}{2}\hat{\xi}^x + \frac{\lambda'}{2}\hat{\eta}^y & 0 & 0 \\
-i\frac{\lambda'}{2}\hat{\eta}^z & -i\frac{\lambda'}{2}\hat{\xi}^x - \frac{\lambda'}{2}\hat{\eta}^y & 0 & 0 \\
\end{pmatrix}.
\] (16)

The total Hamiltonian is given by the sum of matrices (15) and (16),

\[
\hat{H} = \begin{pmatrix}
\hat{\varepsilon}_k + i\frac{\lambda}{2}\hat{\xi}^z & \frac{\lambda}{2}\hat{\xi}^x + \frac{\lambda}{2}\hat{\eta}^y \\
\frac{\lambda}{2}\hat{\xi}^x - \frac{\lambda}{2}\hat{\eta}^y & -i\hat{\varepsilon}_k + \frac{\lambda}{2}\hat{\eta}^z \\
0 & 0 \\
\end{pmatrix}. + \begin{pmatrix}
\frac{\lambda'}{2}\hat{\xi}^x + \frac{\lambda'}{2}\hat{\eta}^y \\
\frac{\lambda'}{2}\hat{\xi}^x - \frac{\lambda'}{2}\hat{\eta}^y & \frac{\lambda'}{2}\hat{\eta}^z \\
0 & 0 \\
\end{pmatrix}.
\] (17)

Again, if one considers only \( z \)-component of the SO coupling, the expression for \( H \) simplifies:

\[
\hat{H} \rightarrow \hat{H}_z = \begin{pmatrix}
\hat{\varepsilon}_k + i\frac{\lambda}{2}\hat{\xi}^z & \frac{\lambda'}{2}\hat{\xi}^z \\
0 & -i\frac{\lambda'}{2}\hat{\xi}^z \\
\frac{\lambda'}{2}\hat{\xi}^z & \frac{\lambda'}{2}\hat{\eta}^z \\
0 & 0 \\
\end{pmatrix}.
\] (18)

4. Results of the band structure and Fermi surface calculations

For \( \lambda = 0 \), the band structure and the Fermi surface are shown in Fig. 1. It is essentially the same as in Ref. [9] but within the folded BZ.

First, we switch on only the intercell SO interaction by setting \( \lambda = 0 \) and \( \lambda' = 100 \) meV. Corresponding band structure and the Fermi surface are shown in Fig. 2. There is a pronounced splitting between the previously degenerate electron \( M \)-pockets along the \( X-M \) direction. Now, the band structure can not be unfolded. Also, there is a splitting between bands at \( M \) point and along the \( M-\Gamma \) direction around \(-1 \) eV.
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**Band Structure Modification Due to the Spin-orbit . . .**

Fig. 1. Band structure and the Fermi surface in the three-orbital model without the SO coupling ($\lambda = \lambda^\prime = 0$) in the 2-Fe BZ

Now we also switch on the intracell SO interaction by setting $\lambda = \lambda^\prime = 100$ meV. The result is shown in Fig. 3. Apparently, the intracell SO coupling provides shift of the bands around $\Gamma$ point. Apart from that, there is no pronounced difference between Fig. 2 and Fig. 3.

Fig. 2. The same as in Fig. 1 but for the finite intercell SO coupling $\lambda^\prime = 100$ meV and the vanishing intracell SO coupling $\lambda = 0$

**Conclusions**

If working in the 2-Fe BZ, the SO coupling can be divided into the intra- and intercell parts, though both being local. We conclude that intercell coupling produces the reconstruction of the Fermi surface around the $M$ point. The new band structure can not be unfolded anymore. Intracell SO coupling removes degeneracy of the bands around $\Gamma$ point. There is also a splitting between bands at $M$ point and along the $M - \Gamma$ direction around $-1$ eV. However, these energies are far below the chemical potential and should not affect the low-energy physics.
Fig. 3. The same as in Fig. 1 but for the finite intra- and intercell SO coupling, $\lambda = \lambda' = 100$ meV

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References


Изменение зонной структуры из-за спин-орбитального взаимодействия в трехорбитальной модели пниктидов железа

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Исследовано влияние спин-орбитального взаимодействия на зонную структуру и поверхность Ферми трехорбитальной модели в зоне Бриллюэна двух атомов железа на ячейку. Из-за присутствия двух атомов железа в кристаллографической элементарной ячейке спин-орбитальное взаимодействие можно разделить на внутри- и межъячеечную части по отношению к элементарной ячейке решетки железа. Показано, что межъячеечная часть приводит к реконструкции поверхности Ферми в виде выраженного расщепления между ранее вырожденными электронными карманами в точке $(\pi, \pi)$ вдоль направлений $(0, \pi)$ и $(\pi, 0)$. Внутрьжечейная часть приводит к сдвигу зон вблизи точки $(0, 0)$ и снимает там вырождение. Также имеют место другие сдвиги зон, но они не должны влиять на низкоэнергетическую физику, поскольку возникают на энергиях порядка 1 eV ниже уровня Ферми.

Ключевые слова: сверхпроводники на основе железа, спин-орбитальное взаимодействие, зонная структура, поверхность Ферми.