Effect of tetrahedral distortion on the electronic properties of iron pnictides

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Abstract. We study the dependence of the electronic structure of iron pnictides on the angle formed by the arsenic–iron bonds. Within a Slater–Koster tight binding model which captures the correct symmetry properties of the bands, we show that the density of states and the band structure are sensitive to the distortion of the tetrahedral environment of the iron atoms. This sensitivity is extremely strong in a two-orbital (dₓ²−ᵧ², dₓz) model due to the formation of a flat band around the Fermi level. Inclusion of the dₓᵧ orbital destroys the flat band while keeping considerable angle dependence in the band structure.

Contents

1. Introduction 1
2. Two-orbital model 3
3. Three-orbital model 6
Acknowledgments 8
References 8

1. Introduction

The recent discovery of high-temperature superconductivity in iron arsenides [1] has triggered intense research in the condensed matter community. The characteristic building blocks of these materials are FeAs layers with each Fe atom surrounded by four arsenic atoms in a distorted tetrahedral geometry. Fe atoms form a square lattice, while As atoms located at the
center of each square are displaced above and below from the Fe plane in a checkerboard form (see figure 1). Undoped compounds are compensated semimetals that undergo a structural and a magnetic transition [2, 3]. Upon chemical doping, the structural distortion and magnetic order disappear and superconductivity emerges. Superconductivity has been reported so far in four families: the rare-earth oxyselenides [1] ReFeAsO (also called the 1111 systems) with Re a lanthanide atom, TFe$_2$As$_2$ with T an alkaline-earth metal and two FeAs planes per unit cell [4], also called the 122 family, LiFeAs [5] and AFFeAs (where A = Ca, Sr) [6]. Iron arsenides can be considered part of a larger family, the iron pnictides, with As substituted by an isovalent pnictogen element, such as P [7]. Superconductivity has also been observed in related compounds with Ni [8] (Se [9]) instead of Fe (As).

Hopping between Fe atoms via As is expected to give the dominant contribution to the kinetic energy [10] and to the exchange interaction [11]. Therefore, some dependence of the electronic properties on the angles formed by the Fe–As bonds, i.e. on the distortion of the As tetrahedron, is expected. This dependence is of crucial importance for both weak coupling models [12]–[14], based on nesting properties, and strong coupling models [11], based on superexchange interaction, aimed at explaining the properties of these systems. For each family of iron pnictides, the As tetrahedron presents different distortions. It is almost regular [3] in the 122 family with the four As–Fe–As angles close to the ideal value, 109.47°, while it is elongated in LiFeAs [5], with As atoms further away from the Fe plane than in the regular tetrahedron (the $\text{As}^{\text{top}}$–Fe–As$^{\text{top}}$ angle is 102.8°). Here As$^{\text{top}}$ refers to an As atom placed above the Fe plane. In the 1111 family, the tetrahedron is squashed and the $\text{As}^{\text{top}}$–Fe–As$^{\text{top}}$ or P$^{\text{top}}$–Fe–P$^{\text{top}}$ angle depends on the specific composition, being equal to 113.7° in LaFeAsO [1] and 120.6° in LaFePO [7]. Differences in the electronic properties of these compounds have been attributed to the different distortion of the tetrahedra [15]. The As–Fe–As angle is also sensitive to doping [16]–[20] and can be deeply modified under pressure [21]. An example of the latter is the collapsed tetragonal phase found in CaFe$_2$As$_2$ under pressure [21]. In [16, 17], a possible correlation between the superconducting critical temperature and the As–Fe–As angle has been suggested with deviations within a family from the regular tetrahedron being detrimental for superconductivity. In Ba$_{1-x}$K$_x$Fe$_2$As$_2$, at optimal doping the tetrahedron changes from squashed (in underdoped) to elongated (in overdoped) [20]. It has been argued [16, 17] that there is a correlation between stronger interaction and higher critical temperature in iron pnictides due to a narrower bandwidth for the regular tetrahedron. This argument seems to be supported by the lower critical temperatures and lack of structural distortion and magnetism in LiFeAs and LaFePO. An unusually large sensitivity of the iron moment [22] and the band structure [13, 23, 24] to the separation of the As atoms with respect to the plane has also been found in density functional theory calculations.

In this paper, we analyze the angle dependence of the band structure within a tight-binding model in which hopping between Fe atoms is assumed to be mediated by As and its magnitude is calculated within the Slater–Koster framework [25]. We show that the two-orbital model which only includes $d_{xz}$ and $d_{yz}$ is extremely sensitive to changes in the angle formed by the As–Fe bonds. Such a sensitivity originates from the appearance of flat bands in the $(0, 0)$–$(\pm \pi, 0)$ and $(0, 0)$–$(0, \pm \pi)$ directions for the regular tetrahedron case. The corresponding peak in the density of states (DOS) is found at the Fermi level at half-filling. The flat bands disappear when the tetrahedron is distorted. Within the present model this result is independent of any fitting parameter. Inclusion of the $d_{xy}$ orbital modifies this picture but maintains the dependence of the DOS and band structure on the angle.
Figure 1. Lattice structure of the FeAs layers with each Fe atom surrounded by four As atoms in a distorted tetrahedral geometry. The Fe atoms form a square lattice. At the center of each square, above and below in a checkerboard form, lie the As atoms. $\alpha$, the angle formed by the Fe–As bond and the Fe plane, is related to the $\text{As}^{\text{top}}$–Fe–$\text{As}^{\text{top}}$ (or Fe–As–Fe, with the Fe atoms being next-nearest neighbors) angle $\eta$ as $2\alpha = 180^\circ - \eta$. For instance, for a regular tetrahedron $\eta = 109.47^\circ$ and $\alpha = 35.26^\circ$.

2. Two-orbital model

We construct a tight-binding model to describe the band structure of the FeAs layers around the Fermi level in the tetragonal phase. We describe the distortion of the tetrahedron in terms of the angle $\alpha$ formed by the Fe–As bond direction with the Fe plane, see figure 1. The advantage of using this angle, instead of the more common Fe–As–Fe or As–Fe–As ones, is that it is defined uniquely. On the contrary, there are two different Fe–As–Fe angles (depending on whether the Fe atoms are nearest or next-nearest neighbors) and, for non-regular tetrahedra, there are also two different As–Fe–As angles (between top As and between top and down As). The correspondence between $\alpha$ and the Fe–As–Fe or As–Fe–As angles is straightforward (see the caption to figure 1).

According to first-principles calculations, several bands cross the Fermi level and the DOS at the Fermi level is dominated by Fe-d orbitals with little weight of pnictogen p-orbitals [10, 23, 26]. We work with the Fe-square lattice and take the $x$- and $y$-axes along the Fe–Fe bonds. Only the Fe-orbitals are included in the tight binding. The As atoms only enter the model indirectly via the Fe–Fe hopping amplitudes. Under these assumptions the Hamiltonian for the two orbital ($d_{xz}$, $d_{yz}$) model is given by

$$H = \sum_{i,j,\beta,\gamma,\sigma} \left( t^x_{\beta,\gamma} c^\dagger_{i,j,\beta,\sigma} c_{i+1,j,\gamma,\sigma} + t^y_{\beta,\gamma} c^\dagger_{i,j,\beta,\sigma} c_{i,j+1,\gamma,\sigma} + t'_{\beta,\gamma} c^\dagger_{i,j,\beta,\sigma} c_{i+1,j+1,\gamma,\sigma} + t''_{\beta,\gamma} c^\dagger_{i,j,\beta,\sigma} c_{i+1,j-1,\gamma,\sigma} + \text{h.c.} \right)$$

$$+ \sum_{i,j,\beta,\sigma} \epsilon_\beta c^\dagger_{i,j,\beta,\sigma} c_{i,j,\beta,\sigma} - \mu. \tag{1}$$

Here $i, j$ and $\sigma$ label the sites in the two-dimensional (2D) lattice and the spin, respectively, while $\beta$ and $\gamma$ refer to the Fe-d orbitals included in the tight binding. $\epsilon$ is the on-site energy and $\mu$ is the chemical potential. We first restrict ourselves to two degenerate $d_{xz}$ and $d_{yz}$ orbitals, as in other minimum models recently discussed [14, 27, 28]. Due to the degeneracy of $d_{xz}$ and $d_{yz}$
orbs, the on-site energies $\epsilon_{xz} = \epsilon_{yz}$ only shift the bottom of the bands and, for simplicity, we take them to be equal to zero. The hopping amplitudes $t$ are calculated from orbital overlap integrals within the Slater–Koster framework [25]. This formalism was used before in [27] and captures the correct symmetry of the energy bands. It differs from the first two-band model proposed in the literature [14] where hopping parameters are chosen to fit the bands. In our model, direct Fe–Fe hopping is neglected, i.e. we assume that all hopping takes place via As atoms. Neglecting the energy splitting between As p$_{x,y}$ and p$_z$ orbitals and to second order in perturbation theory:

$$t'_{xz,xz} = 2 \left[ (t_{xz,xz})^2 - (t_{y,xz})^2 - (t_{z,xz})^2 \right] / (\epsilon_d - \epsilon_p),$$  

(2)

$$t'_{yz,xz} = 2 \left[ (t_{xz,xz})^2 - (t_{y,xz})^2 + (t_{z,xz})^2 \right] / (\epsilon_d - \epsilon_p)$$  

(3)

and $t'_{yz,yz} = t'_{xz,xz}$, $t'_{yz,yz} = t'_{xz,xe}$. Hopping to nearest neighbors between $xz$ and $yz$ vanishes. Next-nearest neighbor hopping amplitudes satisfy $t''_{xz,yz} = -t'_{xz,yz}$, $t''_{xz,xz} = t'_{xz,xz}$, $t''_{yz,yz} = t'_{yz,yz}$ and $t''_{yz,xz} = t'_{xz,xz}$ with

$$t''_{xz,xz} = \left[ (t_{xz,xz})^2 + (t_{y,xz})^2 - (t_{z,xz})^2 \right] / (\epsilon_d - \epsilon_p),$$  

(4)

$$t''_{yz,yz} = \left[ -t_{xz,xz} t_{y,xz} - t_{y,xz} t_{y,yz} - t_{x,xz} t_{z,yz} \right] / (\epsilon_d - \epsilon_p)$$  

(5)

with $\epsilon_p$ and $\epsilon_d$ the on-site energies of the pnictogen-p and Fe-d orbitals, and $t_\delta, \beta$, where $\delta = x, y, x$ and $\beta = xz, yz$, the overlap between As-p$_\delta$ and Fe-d$_\beta$ orbitals. These expressions take into account that two As atoms mediate the hopping between nearest neighbors, while only one As atom is involved in the hopping between next-nearest neighbors. Overlap between As-p orbitals and Fe-d orbitals is given in terms of two integrals, taken as disposable constants, $pd_\sigma$ and $pd_\pi$, where as usual $\sigma$ and $\pi$ refer to the component of angular momentum around the axis [25]. The sign of $pd_\sigma$ is taken to be opposite to that of $pd_\pi$ [29]. The angle dependence is evident in the Fe–As overlaps:

$$t_{x,xz} = \sin \alpha \left( -\frac{\sqrt{3}}{2} \cos^2 \alpha (pd_\sigma) + \sin^2 \alpha (pd_\pi) \right),$$  

(6)

$$t_{y,xz} = \frac{1}{2} \sin \alpha \cos \alpha \left( \sqrt{3} (pd_\sigma) - 2 (pd_\pi) \right),$$  

(7)

$$t_{z,xz} = \frac{\cos \alpha}{\sqrt{2}} \left( \sqrt{3} \sin^2 \alpha (pd_\sigma) + (1 - 2 \sin^2 \alpha) (pd_\pi) \right)$$  

(8)

and $t_{x,yz} = t_{x,xz}$, $t_{y,yz} = t_{y,xz}$ and $t_{z,yz} = t_{z,xz}$. The angle dependence of the hopping parameters that enter equation (1) and of the Fe–As overlaps are shown in figure 2. A strong dependence is seen, especially in the Fe–Fe hopping, for the angles found experimentally (shaded area in figure 2). In this figure, Fe–Fe hopping parameters and Fe–As overlaps are given in units of $(pd_\sigma)^2 / (\epsilon_p - \epsilon_d)$ and $pd_\sigma$, respectively. In these units, all the hopping amplitudes and orbital integrals depend on a unique free parameter, $pd_\sigma$.

Diagonalization of the Hamiltonian results in two bands

$$E^\pm(k) = \epsilon_\cdot(k) - \mu \pm \sqrt{\epsilon_-\cdot(k)^2 + \epsilon_{xy}^2(k)}$$  

(9)

with

$$\epsilon_\cdot(k) = (t^x_{xz,xz} + t^y_{xz,xz}) (\cos k_x + \cos k_y) + 4t'_{xz,xz} \cos k_x \cos k_y,$$  

(10)
Figure 2. Angle dependence of the Fe–Fe hopping parameters (left) and Fe–As overlap integrals (right) that enter the two-orbital model. Fe–As overlap integrals and Fe–Fe hopping parameters are in units of $pd_\sigma$ and $pd_\pi/(\epsilon_d - \epsilon_p)$, respectively. $pd_\pi = -0.2$. Shaded areas correspond to the experimentally relevant angles.

$$
\epsilon_-(\mathbf{k}) = (t_{xz,xz}^\prime - t_{xz,xz}^\prime)\cos k_x - \cos k_y),
$$

$$
\epsilon_{xy}(\mathbf{k}) = 4t_{yz,xz}^\prime \sin k_x \sin k_y.
$$

The DOS for a squashed ($\alpha = 32.71^\circ$), a regular ($\alpha = 35.26^\circ$) and an elongated tetrahedron ($\alpha = 39.13^\circ$), corresponding to As$^{\text{top}}$–Fe–As$^{\text{top}}$ angles of 114.58°, 109.47° and 101.74°, respectively, and $pd_\pi = -0.2$ is plotted in figure 3 (top panels). In this figure, the chemical potential is at $\omega = 0$, assuming half-filling. Two peaks are observed in the DOS for the three angles. The DOS of each of the two bands $E^\pm$ (equation (9)) is also plotted in these figures. It can be seen that each of the peaks comes from one of the two bands. The height of the high-energy peak is very strongly sensitive to $\alpha$. In particular, the intensity of this peak is much higher for a regular tetrahedron. Inspection of the band structure in the lower plots of figure 3 reveals the existence of a flat band along $(0, 0) - (\pi, 0)$ in this case. By symmetry, the band is flat also along the $(0, 0) - (0, \pm \pi)$ and $(0, 0) - (-\pi, 0)$ directions. The flat bands in the regular tetrahedron geometry ($\alpha = 35.26^\circ$) appear for any value of $pd_\sigma$ and $pd_\pi$. From the expressions for the hopping amplitudes given above, for this $\alpha$ it can be shown that $t_{xz,xz}^\prime + 2t_{xz,xz}^\prime = 0$, which cancels the $k_x$ dependence of the band structure for $k_y = 0$ (alternatively, it cancels the $k_y$-dispersion for $k_x = 0$). This equality for the regular tetrahedron comes from $t_{x,z} = t_{z,x}$, see equations (6) and (8) and the right panel of figure 2. The topology of the energy contours and, therefore, that of the Fermi surface, is also strongly sensitive to $\alpha$ as shown in figure 4 for the same parameters used in figure 3.

Due to the change in the energy contour (and the Fermi surface topology), and the very high peak in the DOS, if interactions were included, the magnetic and superconducting properties of this two-orbital model would be extremely sensitive to the angle $\alpha$. This is particularly evident.
Figure 3. Top (bottom) figures: DOS (band structure) for the two-orbital model corresponding to the squashed (left), regular (middle) and elongated (right) tetrahedra. The corresponding angles are $\alpha = 32.71^\circ$, $35.26^\circ$ and $39.13^\circ$, respectively. In the top figures, the green (light) lines show the total DOS. Black and red lines give the DOS corresponding to the $E^-$ and $E^+$ bands (equation (9)), respectively. The DOS is smoothed by a Lorentzian of width 0.02. Energies are in units of $pd^2/\sigma/(\epsilon_d - \epsilon_p)$.

in a picture that ascribes the magnetic transition to a spin density wave due to nesting. As shown in figure 4, this two-band model predicts a hole pocket around the (0, 0) point of the Brillouin zone and another around ($\pi$, $\pi$), while band structure calculations yield both hole pockets around (0, 0). We now show that including a third orbital maintains some angle dependence in the electronic properties although when the hybridization with the third orbital is strong the conditions for the flat band are not fulfilled.

3. Three-orbital model

According to LDA [10, 23, 26] the $d_{xy}$ orbital contributes to the Fermi surface and it is expected to be relevant in any description of iron pnictides [30]. Hamiltonian (1) can be straightforwardly generalized to include the $d_{xy}$ or any of the $e_g$ orbitals [25]. In the case of the regular tetrahedron, including only the crystal field due to the arsenic environment, the three $t_{2g}$ orbitals ($d_{xy}$, $d_{yz}$ and $d_{xz}$) are degenerate [23]. The inclusion of the crystal field produced by the Fe environment and/or the distortion of the tetrahedra breaks this degeneracy. As the As atom approaches the Fe plane, the $d_{xy}$ orbital becomes higher in energy as compared with the (still degenerate) $d_{xz}$ and $d_{yz}$ orbitals. The level splitting $\epsilon_{xy} - \epsilon_{xz,yz}$ introduces a new parameter in the calculation. When both Fe and As crystal field effects are included, $\epsilon_{xy} - \epsilon_{xz,yz}$ is slightly larger for the squashed tetrahedron than for the regular or elongated one. Expansion of the hopping parameters to second order in perturbation theory also contributes to the renormalization of the on-site energies $\epsilon_{xy}$ and $\epsilon_{xz,yz}$.

New Journal of Physics 11 (2009) 013051 (http://www.njp.org/)
Figure 4. Energy contour plots for the squashed (top), regular (middle) and elongated (bottom) tetrahedral geometries for the same parameters as in figure 3. Left figures correspond to $E^-$ and right figures to $E^+$, see equation (9). The Fermi surface is in black (darker lines). The topology of the Fermi surface changes with the angle.

For large level splittings $\epsilon_{xy} - \epsilon_{xz,yz} \gtrsim W$, with $W$ being the bandwidth of the two-orbital model, the hybridization between $d_{xy}$ and the bands $E^+$ and $E^-$ of the two-orbital model is weak and the picture described above remains. However, in real materials the level splitting is expected to be smaller [23]. Figure 5 shows the DOS of the three-orbital model for the same geometries as in figure 3 and with $\epsilon_{xy} - \epsilon_{xz,yz} = 0.15$ and $pd_y = -0.2$. For simplicity, we neglect the angle dependence of the level splitting. Figure 5 reveals that a clear dependence of the DOS on the angle $\alpha$ still prevails within the three-orbital model. Note that the Fermi level is expected to be around the center of the band where the effect of changing the angle is very strong [31]. However, the origin of the dependence of the DOS on the angle $\alpha$ is qualitatively different from the one found in the two-orbital model: due to the hybridization with the $d_{xy}$ orbital, the flat band that appeared in the regular tetrahedron geometry within the two-orbital model is partially destroyed in the three-band model.
In conclusion, we have analyzed the angle dependence of the band structure within a Slater–Koster-based tight-binding model for iron pnictides. In both two- and three-orbital models, the DOS and therefore the Fermi surface are strongly sensitive to changes in the angle formed between the Fe–As bonds. This result is relevant for both weak coupling theories based on the nesting mechanism, which is very sensitive to the shape of the Fermi surface, and for strong coupling theories, since superexchange also depends on orbital overlaps. In the two-orbital model a flat band is formed when the As-tetrahedron is regular, which results in a strong peak in the DOS. This result is robust against changes in the fitting parameters. Hybridization with a third orbital modifies this picture although the dependence on the angle remains, in particular for low energies. In our description, the bandwidth does not seem to depend very strongly on the angle, though it seems to be slightly narrower for a more elongated tetrahedron.

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