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# Anisotropy of the optical conductivity of a pnictide superconductor from the undoped three-orbital Hubbard model

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The resistivity anisotropy unveiled in the study of detwinned single crystals of the undoped 122 pnictides is here studied using the two-dimensional three-orbital Hubbard model in the mean-field approximation. Calculating the Drude weight in the  $x$  and  $y$  directions at zero temperature for a  $\mathbf{Q}=(\pi,0)$  magnetically ordered state, the conductance along the antiferromagnetic direction is shown to be larger than along the ferromagnetic direction. This effect is caused by the suppression of the  $d_{yz}$  orbital at the Fermi surface, but additional insight based on the momentum dependence of the transitions induced by the current operator is provided. It is shown that the effective suppression of the inter-orbital hopping  $d_{xy}$  and  $d_{yz}$  along the  $y$  direction is the main cause of the anisotropy.

PACS numbers:

## I. INTRODUCTION

One of the most intriguing puzzles in the study of the Fe-based high temperature superconductors<sup>1</sup> is the discovery of unexpected transport anisotropies in detwinned single crystals of doped and undoped  $\text{AFe}_2\text{Sr}_2$  ( $\text{A} = \text{Ba}, \text{Sr}, \text{Ca}$ ).<sup>2-5</sup> Studies of the in-plane resistivity<sup>6</sup> showed that the effect is the largest at low doping  $x \sim 2-4\%$  in  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ , but it is present even in the undoped limit  $x=0$  at low temperatures, i.e. in the magnetically ordered state with wavevector  $(\pi,0)$ . Recent studies<sup>7</sup> for the undoped 122 materials have revealed a low-temperature anisotropy (defined as  $R = \rho_b/\rho_a - 1$ )  $R \sim 0.4, 0.35$ , and  $0.09$ , for  $\text{A} = \text{Ba}, \text{Sr}$ , and  $\text{Ca}$ , respectively. This anisotropy is counter-intuitive because along the  $a$ -axis the spins order in an antiferromagnetic (AFM) arrangement, while along the  $b$ -axis they are ferromagnetic (FM). Intuition based on, e.g., double-exchange mechanisms for manganites would suggest that the FM direction should be less resistive than the AFM one. Optical conductivity measurements concluded that this unexpected anisotropy is caused by changes in the populations of the orbitals  $d_{xz}$  and  $d_{yz}$  at the Fermi surface (FS).<sup>8</sup> This is in agreement with early mean-field studies where the unbalanced FS orbital population, without long-range orbital order, led to results compatible with photoemission techniques.<sup>9</sup>

Several calculations have recently addressed the experimentally observed transport anisotropy. Using a five-orbital Hubbard model treated in a mean-field approximation, and calculating the Drude weights via the Fermi velocities at the FS, results compatible with experiments were reported.<sup>10</sup> This agreement was observed in regimes where long-range orbital order is not present, and indeed the FS redistribution of spectral weight among the  $d_{xz}$  and  $d_{yz}$  orbitals caused by the  $(\pi,0)$  magnetic order<sup>9</sup> is needed to understand the experimental results. Other calculations also for the five-orbital Hubbard model arrived to similar conclusions.<sup>11-14</sup>

In this publication, the transport anisotropy found in experiments is revisited from the perspective of a simpler three-orbital Hubbard model.<sup>15</sup> Our goal is to refine the intuitive explanations given in Refs. 10,11, by focusing on the three orbitals widely believed to be the most important in pnictides, namely  $d_{xz}$ ,  $d_{yz}$ , and  $d_{xy}$ , and also by identifying the electronic hopping amplitudes that cause the anisotropy. Our main results are that the experimentally observed anisotropy clearly appears in the three-orbital model, in a state that is  $(\pi,0)$  magnetically ordered, and it is mainly caused by the suppression of *inter*-hopping  $d_{xz}$ - $d_{yz}$  processes along the FM direction.

## II. MODELS AND METHODS

In this manuscript, the three-orbital Hubbard model for the pnictides at overall electronic density  $n=4/3$  (per site and per orbital) will be used.<sup>15</sup> The hopping amplitudes that reproduce the FS in the paramagnetic state, with hole and electron pockets, were already provided and discussed in detail in Ref. 15. However, to help the readers in the understanding of our results, in Table I these intra- and inter-hopping amplitudes (in eV units) are provided again. From Table I note that the hoppings involving the  $d_{xy}$  orbital, both intra-orbital and also inter-orbital with  $d_{xz}$  and  $d_{yz}$ , are the largest in value, inducing a large Fermi velocity in the regions of the FS where the  $d_{xy}$  orbital dominates. This suggests that the  $d_{xy}$  may play an important role in the anisotropy. The full three-orbital Hubbard model also contains a Coulombic on-site interaction (see Eq. (11) of Ref. 15), involving an intra-orbital Hubbard repulsion  $U$ , an inter-orbital repulsion  $U'$ , and a Hund coupling  $J$ , with the constraint  $U'=U-2J$ . The Hartree mean-field approximation used here has also been much discussed in previous literature and the reader is referred to Refs. 15–18 for details. The mean-field order parameters are the three electronic densities of each orbital, i.e.  $n_{xz}$ ,  $n_{yz}$ , and  $n_{xy}$ , and the three magnetic moments  $m_{xz}$ ,  $m_{yz}$ , and  $m_{xy}$ , and they are all

$t_{\mathbf{il}}^{\alpha\beta}$	$\mathbf{l} = \mathbf{x}$	$\mathbf{l} = \mathbf{y}$	$\mathbf{l} = \mathbf{x} + \mathbf{y}$	$\mathbf{l} = \mathbf{x} - \mathbf{y}$
$\alpha\beta = 11$	-0.06	-0.02	-0.03	-0.03
$\alpha\beta = 22$	-0.02	-0.06	-0.03	-0.03
$\alpha\beta = 33$	0.2	0.2	-0.3	-0.3
$\alpha\beta = 12$	0.0	0.0	-0.01	0.01
$\alpha\beta = 13$	0.2	0.0	-0.1	-0.1
$\alpha\beta = 23$	0.0	0.2	-0.1	0.1

TABLE I: Tight-binding (TB) hopping parameters of the three-orbital Hubbard model used in this manuscript. The energy unit is eV. The labeling convention is  $1=d_{xz}$ ,  $2=d_{yz}$ ,  $3=d_{xy}$ . The 13 and 23 hoppings are all affected by a factor  $(-1)^{|\mathbf{z}|} = (-1)^{i_x+i_y}$ , with  $\mathbf{i}=(i_x, i_y)$  being the label of the Fe sites of a two-dimensional lattice. This modulation takes into account the two-Fe unit cell of the original FeAs layers.<sup>15</sup> The TB Hamiltonian is defined as  $H_{\text{HT}} = \sum_{\mathbf{il}\alpha\beta\sigma} t_{\mathbf{il}}^{\alpha\beta} (c_{\mathbf{i},\alpha,\sigma}^\dagger c_{\mathbf{i}+\mathbf{l},\beta,\sigma} + h.c.)$ , where  $c_{\mathbf{i},\alpha,\sigma}^\dagger$  creates an electron at orbital  $\alpha$  of site  $\mathbf{i}$  with spin projection  $\sigma$ .  $\mathbf{i} + \mathbf{l}$  denotes nearest and next-nearest neighbor sites to  $\mathbf{i}$ .

determined via the minimization of the Hartree mean-field energy. In the mean-field equations, the wavevector  $\mathbf{Q} = (\pi, 0)$  is assumed.

Let us focus now on the optical conductivity  $\sigma(\omega)$ . Following well-known computational studies of  $\sigma(\omega)$  in the context of the cuprates,<sup>19</sup> let us define first the paramagnetic current operators in the two directions as

$$\begin{aligned} \hat{j}_x &= \sum_{\langle \mathbf{i}, \mathbf{l} = \hat{\mathbf{x}}, \hat{\mathbf{x}} + \hat{\mathbf{y}}, \hat{\mathbf{x}} - \hat{\mathbf{y}} \rangle} \sum_{\alpha, \beta, \sigma} -it_{\mathbf{il}}^{\alpha\beta} (c_{\mathbf{i},\alpha,\sigma}^\dagger c_{\mathbf{i}+\mathbf{l},\beta,\sigma} - h.c.), \\ \hat{j}_y &= \sum_{\langle \mathbf{i}, \mathbf{l} = \hat{\mathbf{y}}, \hat{\mathbf{x}} + \hat{\mathbf{y}}, -\hat{\mathbf{x}} + \hat{\mathbf{y}} \rangle} \sum_{\alpha, \beta, \sigma} -it_{\mathbf{il}}^{\alpha\beta} (c_{\mathbf{i},\alpha,\sigma}^\dagger c_{\mathbf{i}+\mathbf{l},\beta,\sigma} - h.c.), \end{aligned} \quad (1)$$

while the kinetic energy operators are

$$\begin{aligned} \hat{T}_x &= \sum_{\langle \mathbf{i}, \mathbf{l} = \hat{\mathbf{x}}, \hat{\mathbf{x}} + \hat{\mathbf{y}}, \hat{\mathbf{x}} - \hat{\mathbf{y}} \rangle} \sum_{\alpha, \beta, \sigma} t_{\mathbf{il}}^{\alpha\beta} (c_{\mathbf{i},\alpha,\sigma}^\dagger c_{\mathbf{i}+\mathbf{l},\beta,\sigma} + h.c.), \\ \hat{T}_y &= \sum_{\langle \mathbf{i}, \mathbf{l} = \hat{\mathbf{y}}, \hat{\mathbf{x}} + \hat{\mathbf{y}}, -\hat{\mathbf{x}} + \hat{\mathbf{y}} \rangle} \sum_{\alpha, \beta, \sigma} t_{\mathbf{il}}^{\alpha\beta} (c_{\mathbf{i},\alpha,\sigma}^\dagger c_{\mathbf{i}+\mathbf{l},\beta,\sigma} + h.c.). \end{aligned} \quad (2)$$

The total current, up to the first order term in the external field  $\mathbf{A}=(A_x, A_y)$ , can be written as  $\hat{J}_x=(\hat{j}_x + \hat{T}_x A_x)/N$  and  $\hat{J}_y=(\hat{j}_y + \hat{T}_y A_y)/N$ . The real part of the optical conductivity in the  $x$  direction is given by:<sup>19</sup>

$$\begin{aligned} \text{Re}\sigma_{xx}(\omega) &= D_x \delta(\omega) \\ &+ \frac{\pi}{N} \sum_{n \neq 0} \frac{|\langle \phi_0 | \hat{j}_x | \phi_n \rangle|^2}{E_n - E_0} \delta(\omega - (E_n - E_0)), \end{aligned} \quad (3)$$

and from the  $\sigma(\omega)$  sum-rule, it can be shown that the Drude weight in the  $x$  direction  $D_x$  is<sup>19</sup>

$$\frac{D_x}{2\pi} = \frac{\langle \phi_0 | -\hat{T}_x | \phi_0 \rangle}{2N} - \frac{1}{N} \sum_{n \neq 0} \frac{|\langle \phi_0 | \hat{j}_x | \phi_n \rangle|^2}{E_n - E_0}, \quad (4)$$

where  $\phi_0$  is the many-body ground state (in this case the mean-field  $\mathbf{Q}=(\pi, 0)$  state), and  $\phi_n$  represents the many-body excited states, also produced in the mean-field calculation, with  $E_0$  and  $E_n$  their corresponding energies. The optical conductivity and Drude weight in the  $y$  direction can be obtained and expressed similarly.  $N$  is the number of sites. In our calculation, the Dirac  $\delta$  functions are regularized as a Lorentzian  $\delta(\omega) \approx (1/\pi) \epsilon / (\omega^2 + \epsilon^2)$  with a small but finite broadening parameter  $\epsilon$ .

### III. RESULTS

One of the main results found in our study is shown in Fig. 1 where  $\sigma(\omega)$  in the two directions is shown for a state with magnetic order  $(\pi, 0)$ . The values of the couplings  $U$  and  $J$  are representative of the so-called “physical region” that was previously unveiled for the same three-orbital model.<sup>16</sup> In other words, by a comparison between neutron scattering and photoemission experiments against mean-field results, in previous studies it was concluded that the three-orbital model has a “physical region” (where theory matches experiments) in the range  $U \sim [0.7, 1.3]$  and  $J/U \sim [0.15, 0.33]$ ,<sup>16</sup> where the state is simultaneously magnetic and metallic as in pnictide parent compounds. Our  $\sigma(\omega)$  study is restricted to that “physical region”. A recent publication<sup>20</sup> includes a summary of values of the couplings  $U$  and  $J$  from a variety of calculations and comparisons with experiments, and the ratio  $J/U=1/4$  appears to be in the middle of the accepted range. For this reason,  $J/U$  will be fixed to  $1/4$  in the present study.

Figure 1 shows that  $\sigma(\omega)$  for the three-orbital model is found to be in good qualitative agreement with experiments, namely at small frequency  $\omega$ , where the Drude peak is located, the weight of this peak is larger along the AFM direction (the  $x$  direction) than along the FM direction.<sup>2</sup> Similar results were obtained in the entire “physical region”, see Fig. 2. In addition, the finite frequency peak in the FM direction was found to scale with  $J$ . The ratio  $D_{\text{AFM}}/D_{\text{FM}}$  (i.e.  $D_x/D_y$ ) in the range of  $U$  shown in Fig. 2 varies approximately between 1.6 and 2.2, in qualitative agreement with results for the five-orbital model.<sup>10,11</sup> Thus, it is here concluded that the three-orbital model<sup>15</sup> is sufficient to reproduce the d.c. conductivity anisotropy found in experiments.<sup>2</sup> While a five-orbital model description will be more accurate, the difficulty in handling five orbitals can be avoided if simpler models that capture the essence of the problem are unveiled.

For completeness, in Fig. 3(a) the population of the three orbitals is shown in the range of  $U$ 's studied. From this figure, it is clear that there is no long-range orbital

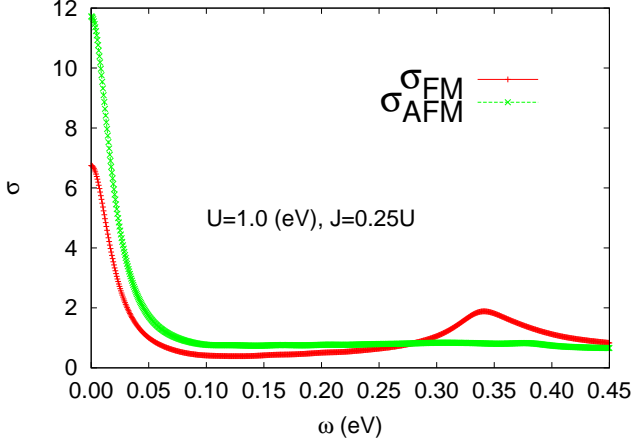


FIG. 1: (color online) Example showing  $\sigma(\omega)$  in the “physical region”<sup>16</sup> of the three-orbital model ( $\epsilon=0.02$ ). The unit of  $\sigma(\omega)$  is  $e^2/\hbar$ . The couplings are  $U = 1.0$  eV and  $J=U/4$ . The AFM direction (i.e. the  $x$  direction for magnetic wavevector  $(\pi, 0)$ ) has a larger zero frequency conductivity than the FM direction, as in experiments. The FM direction also has a peak at a finite frequency  $\sim J$ .

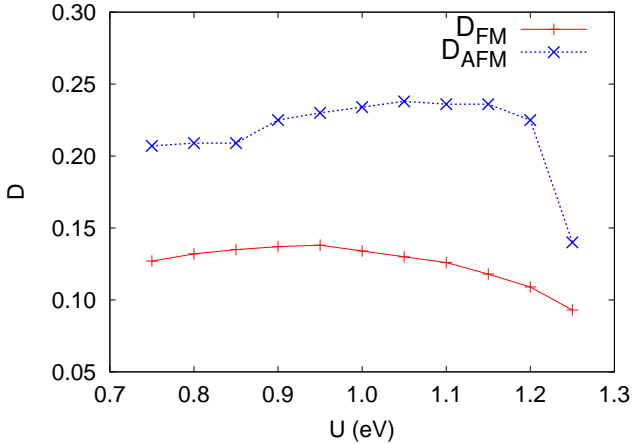


FIG. 2: (color online) Drude weight/ $\pi$  vs.  $U$  in the “physical region” of the three-orbital model, at  $J=U/4$ . In this regime, the inequality  $D_{\text{AFM}} > D_{\text{FM}}$  holds. As  $U$  increases toward the upper limit shown, the Drude weights in both directions are reduced due to increasing insulating tendencies.<sup>16</sup>

order since the orbitals  $d_{xz}$  and  $d_{yz}$  are nearly identically populated. Further increasing  $U$  eventually leads to a regime of orbital-order,<sup>15</sup> but the opening of a gap renders the system insulating. It is important to note that Fig. 3(a) contains results obtained by integrating the orbital-selective density-of-states over all frequencies, while if the focus is only the vicinity of the FS, the orbital-weight redistribution phenomenon is observed.<sup>15</sup> As shown below, this redistribution is important to understand the anisotropy.

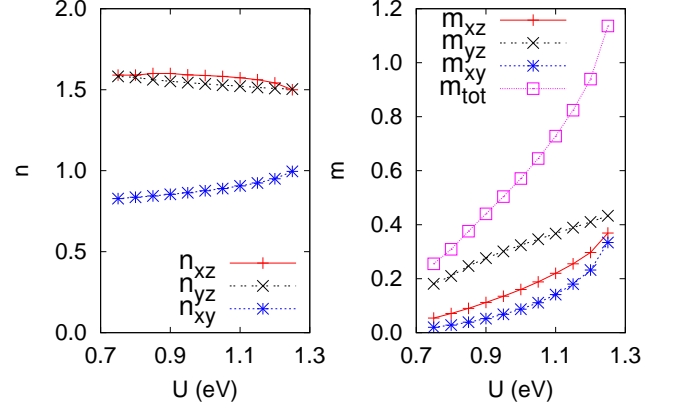


FIG. 3: (color online) (a) Charge density of each orbital vs.  $U$  in the “physical region” of the three-orbital model, at  $J=U/4$ , and for spin order  $(\pi, 0)$ . (b)  $m_\alpha$  vs.  $U$  in the same  $U$  range, at  $J=U/4$ , and for spin order  $(\pi, 0)$ .

In addition, Fig. 3(b) shows that the magnetic moment in the range investigated is compatible with pnictides neutron experiments, ranging from  $\sim 0.25$  Bohr magnetons ( $\mu_B$ ) for the 1111 to  $\sim 1 \mu_B$  for the 122 compounds.<sup>16</sup>

#### IV. INTUITIVE ORIGIN OF THE ANISOTROPY

While the notion of an orbital weight redistribution at the FS is well established,<sup>9,10</sup> with the  $d_{yz}$  orbital suppressed for  $\mathbf{Q}=(\pi, 0)$ , it is desirable to develop a more intuitive understanding of its influence on transport properties. For this purpose, the kinetic energy and current operators will be expressed in momentum space as:

$$\begin{aligned} \hat{T}_a &= \sum_{\mathbf{k}} \sum_{\alpha, \beta, \sigma} t_a^{\alpha\beta}(\mathbf{k}) c_{\mathbf{k}, \alpha, \sigma}^\dagger c_{\mathbf{k}, \beta, \sigma} = \sum_{\mathbf{k}} \hat{T}_a(\mathbf{k}), \\ \hat{j}_a &= \sum_{\mathbf{k}} \sum_{\alpha, \beta, \sigma} j_a^{\alpha\beta}(\mathbf{k}) c_{\mathbf{k}, \alpha, \sigma}^\dagger c_{\mathbf{k}, \beta, \sigma} = \sum_{\mathbf{k}} \hat{j}_a(\mathbf{k}), \end{aligned} \quad (5)$$

where  $a$  is the direction index ( $x, y$ ). From Eq.(4), the  $\mathbf{k}$  contribution (unfolded first Brillouin zone) to the Drude weight is defined as  $D_a(\mathbf{k}) = D_{1,a}(\mathbf{k}) - D_{2,a}(\mathbf{k})$ , where

$$\begin{aligned} \frac{D_{1,a}(\mathbf{k})}{2\pi} &= \frac{\langle \phi_0 | -\hat{T}_a(\mathbf{k}) | \phi_0 \rangle}{2N}, \\ \frac{D_{2,a}(\mathbf{k})}{2\pi} &= \frac{1}{N} \sum_{n \neq 0} \text{Re} \frac{\langle \phi_0 | \hat{j}_a(\mathbf{k}) | \phi_n \rangle \times \langle \phi_n | \hat{j}_a | \phi_0 \rangle}{E_n - E_0}, \end{aligned} \quad (6)$$

since summing over  $\mathbf{k}$  leads to Eq. (4).

From Fig. 4(b) it is clear that the  $(\pi, 0)$  pocket contributes significantly to  $D_{2,y}$  since this wavevector region has sizable intensity. However, the contribution of the

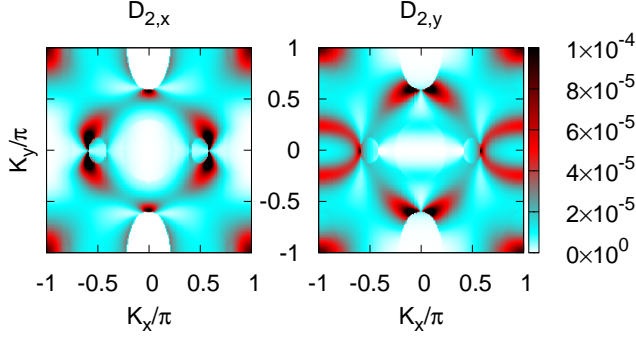


FIG. 4: (color online)  $D_{2,a}(\mathbf{k})/\pi$  in the “physical region”<sup>16</sup> of the three-orbital model ( $U=1.0$  eV,  $J=U/4$ ) and with spin order  $(\pi, 0)$ . For a discussion of the results see text.

$(0, \pi)$  pocket to  $D_{2,x}$  is negligible, thus inducing the significant anisotropy observed in the overall Drude weight (note that the rest of the highly intense features in  $D_{2,y}$  are  $\pi/2$ -rotated those of  $D_{2,x}$  and thus do not contribute to the anisotropy). The reason is the orbital weight redistribution at the FS: according to nesting scenarios, the  $(0, 0)$  pocket (with mainly  $d_{xz}$  and  $d_{yz}$  character), interacts with the  $(\pi, 0)$  pocket (mainly  $d_{xy}$  and  $d_{yz}$ ) when the magnetic wavevector is  $\mathbf{Q}=(\pi, 0)$ . This interaction needs to be intra-orbital,<sup>21</sup> hence the  $d_{yz}$  states at the  $(\pi, 0)$  pocket are raised above the FS, while the  $d_{xy}$  states are not. On the other hand, the  $(0, \pi)$  states are not moved above the FS if  $\mathbf{Q}=(\pi, 0)$ , and hence this phenomenon does not occur for  $D_{2,x}$ . Note that the results of Fig. 4 based on the Drude weights directly address the anisotropy in transport, and complements the analysis based on the orbital-weight redistribution.<sup>9,10</sup> Also note that a similar analysis of  $D_{1,y}$  and  $D_{1,x}$  (not shown) does not lead to the same clear anisotropy that  $D_{2,a}$  provides.

To further simplify the understanding of the anisotropy evident in Fig. 4 let us now focus on the most relevant electronic hopping processes. Analyzing the values of the hopping amplitudes (Table 1), it is clear that those involving the  $d_{xy}$  orbital (both inter- and intra-orbital) should be the most relevant since the other hoppings are much smaller in magnitude. The direct intra-orbital hopping  $d_{xy}-d_{xy}$  ( $t_{11}^{33}$  in Table 1) is not suppressed at the FS and should equally contribute to charge transport in both directions. Thus, the conductance should not drop to zero in any of the two directions due to this intra-orbital contribution. However, the inter-orbital hopping  $d_{xy}-d_{yz}$  is suppressed at the FS in a magnetic state  $(\pi, 0)$ . This hopping occurs *only* along the  $y$  direction, as previously discussed.<sup>15</sup> On the other hand, the hopping  $d_{xy}-d_{xz}$  is *not* suppressed and can contribute to electronic hopping along the  $x$  direction. For these reasons, an asymmetry

is expected between the  $x$  and  $y$  directions in transport, as found in Fig. 1. In addition, for  $\mathbf{k}$  close to the  $(\pi, 0)$  pocket the inter-orbital  $d_{xy}-d_{yz}$  hopping, which only exists along the  $y$  direction, needs an excitation to contribute to  $\sigma(\omega)$  along the FM direction ( $y$ -axis) because  $d_{yz}$  is suppressed at the FS. This observation justifies the presence of a peak scaling with  $J$  in  $\sigma_{\text{FM}}$  (Fig. 1).

To transform the intuition developed above based on hopping amplitudes into actual transport properties, the Drude weight will also be decomposed according to the hoppings corresponding to the different orbitals, via the following definitions:

$$\frac{D_a^{\alpha\beta}}{2\pi} = \frac{\langle \phi_0 | -\hat{T}_a^{\alpha\beta} - \hat{T}_a^{\beta\alpha} | \phi_0 \rangle}{2N} - \frac{1}{N} \sum_{n \neq 0} \text{Re} \frac{\langle \phi_0 | \hat{j}_a^{\alpha\beta} + \hat{j}_a^{\beta\alpha} | \phi_n \rangle \langle \phi_n | \hat{j}_a | \phi_0 \rangle}{E_n - E_0}, \quad (7)$$

for inter-orbital hopping ( $\alpha \neq \beta$ ) ( $a=x, y$ ). The operators in Eq. (7) arise from Eq. (2) via  $\hat{T}_a = \sum_{\alpha, \beta} \hat{T}_a^{\alpha\beta}$  and  $\hat{j}_a = \sum_{\alpha, \beta} \hat{j}_a^{\alpha\beta}$ . For the case of intra-orbital, the diagonal Drude weight  $D_a^{\alpha\alpha}$  is obtained from Eq. (7) by replacing  $\hat{T}_a^{\alpha\beta} + \hat{T}_a^{\beta\alpha}$  by  $\hat{T}_a^{\alpha\alpha}$  and  $\hat{j}_a^{\alpha\beta} + \hat{j}_a^{\beta\alpha}$  by  $\hat{j}_a^{\alpha\alpha}$ . The several Drude components obtained by this procedure are in Table II. From this Table, it can be seen that the main anisotropy arises from the fact that  $D_x^{13} \sim 0.125$  is an order of magnitude larger than  $D_y^{23} \sim 0.011$ , due to the FS suppression of the  $d_{yz}$  orbital. The rest of the contributions in Table II that are unrelated to the inter-orbital hopping involving  $d_{xy}$  are similar in both directions and are not relevant to understand the anisotropy. Actually, for the largest of those, the naive intuition suggesting a better conductance along the FM direction *is* satisfied since  $D_y^{33} > D_x^{33}$ .

## V. SUMMARY

A mean-field study of  $\sigma(\omega)$  employing a three-orbital Hubbard model for the magnetically ordered parent compounds of the pnictides has been here reported. In agreement with experiments, the conductance along the AFM direction is shown to be larger than along the FM direction. The simplicity of this model allowed us to reduce this effect to an intuitive picture: (i) The AFM conductance behaves normally with a suppression of its value as compared with the non-interacting limit due to spin scattering, in agreement with intuition. (ii) However, along the FM direction the drastic reduction in the weight of the  $d_{yz}$  orbital at the FS leads to an even larger effective *suppression* of the  $d_{xy}-d_{yz}$  hopping and associated conductance along that FM direction, causing the anisotropy found experimentally.

$\alpha\beta$	11	22	33	12	13	23
$D_x^{\alpha\beta}$	0.019	-0.003	0.073	0.013	0.125	0.005
$D_y^{\alpha\beta}$	0.020	0.002	0.087	0.014	-0.01	0.011

TABLE II: Drude weight/ $\pi$  decomposed into the different orbitals ( $1=d_{xz}$ ,  $2=d_{yz}$ ,  $3=d_{xy}$ ) of the three-orbital model working at  $U=1.0$  eV and  $J=U/4$ . Finding small negative Drude weights in some cases is a well-known spurious effect<sup>19</sup> arising from differences of two large numbers in Eq. (4).

## VI. ACKNOWLEDGMENTS

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- <sup>1</sup> D. C. Johnston, *Adv. Phys.* **59**, 803 (2010), and references therein.
  - <sup>2</sup> For a recent review see I. R. Fisher, L. Degiorgi, and Z. X. Shen, *Rep. Prog. Phys.* **74**, 124506 (2011).
  - <sup>3</sup> Jiun-Haw Chu, James G. Analytis, David Press, Kristiaan De Greve, Thaddeus D. Ladd, Yoshihisa Yamamoto, and Ian R. Fisher, *Phys. Rev. B* **81**, 214502 (2010).
  - <sup>4</sup> M. A. Tanatar, E. C. Blomberg, A. Kreyssig, M. G. Kim, N. Ni, A. Thaler, S. L. Bud'ko, P. C. Canfield, A. I. Goldman, I. I. Mazin, and R. Prozorov, *Phys. Rev. B* **81**, 184508 (2010).
  - <sup>5</sup> Early experimental studies of the optical conductivity can be found in W. Z. Hu, J. Dong, G. Li, Z. Li, P. Zheng, G. F. Chen, J. L. Luo, and N. L. Wang, *Phys. Rev. Lett.* **101**, 257005 (2008); D. Wu, N. Barisić, N. Drichko, S. Kaiser, A. Faridian, M. Dressel, S. Jiang, Z. Ren, L. J. Li, G. H. Cao, Z. A. Xu, H. S. Jeevan, and P. Gegenwart, *Phys. Rev. B* **79**, 155103 (2009); A. V. Boris, N. N. Kovaleva, S. S. A. Seo, J. S. Kim, P. Popovich, Y. Matiks, R. K. Kremer, and B. Keimer, *Phys. Rev. Lett.* **102**, 027001 (2009); M. Nakajima, S. Ishida, K. Kihou, Y. Tomioka, T. Ito, Y. Yoshida, C. H. Lee, H. Kito, A. Iyo, H. Eisaki, K. M. Kojima, and S. Uchida, *Phys. Rev. B* **81**, 104528 (2010).
  - <sup>6</sup> J-H. Chu, Jiun-Haw Chu, James G. Analytis, Kristiaan De Greve, Peter L. McMahon, Zahirul Islam, Yoshihisa Yamamoto, and Ian R. Fisher, *Science* **329**, 824 (2010).
  - <sup>7</sup> E. C. Blomberg, M. A. Tanatar, A. Kreyssig, N. Ni, A. Thaler, Rongwei Hu, S. L. Budko, P. C. Canfield, A. I. Goldman, and R. Prozorov, *Phys. Rev. B* **83**, 134505 (2011); and references therein.
  - <sup>8</sup> A. Duszka, A. Lucarelli, A. Sanna, S. Massidda, J.-H. Chu, I.R. Fisher, and L. Degiorgi, *EPL* **93**, 37002 (2011).
  - <sup>9</sup> M. Daghofer, Q.-L. Luo, R. Yu, D. X. Yao, A. Moreo, and E. Dagotto, *Phys. Rev. B* **81**, 180514(R) (2010).
  - <sup>10</sup> B. Valenzuela, E. Bascones, and M. J. Calderón, *Phys. Rev. Lett.* **105**, 207202 (2010).
  - <sup>11</sup> K. Sugimoto, E. Kaneshita, and T. Tohyama, *J. Phys. Soc. Jpn.* **80**, 033706 (2011). See also E. Kaneshita, T. Morinari, and T. Tohyama, *Phys. Rev. Lett.* **103**, 247202 (2009).
  - <sup>12</sup> Density functional results, in the spin-polarized generalized gradient approximation, are also compatible with experiments (J. Ferber, Johannes Ferber, Yu-Zhong Zhang, Harald O. Jeschke, and Roser Valenti *Phys. Rev. B* **82**, 165102 (2010)).
  - <sup>13</sup> For other DFT results in this context see A. Sanna, F. Bernardini, G. Profeta, S. Sharma, J. K. Dewhurst, A. Lucarelli, L. Degiorgi, E. K. U. Gross, and S. Massidda, *Phys. Rev. B* **83**, 054502 (2011).
  - <sup>14</sup> For a study of the optical conductivity using the DFT+DMFT approximation see Z. P. Yin, K. Haule, and G. Kotliar, *Nature Physics* **7**, 294 (2011).
  - <sup>15</sup> Maria Daghofer, Andrew Nicholson, Adriana Moreo, and Elbio Dagotto, *Phys. Rev. B* **81**, 014511 (2010).
  - <sup>16</sup> Qinlong Luo, George Martins, Dao-Xin Yao, Maria Daghofer, Rong Yu, Adriana Moreo, and Elbio Dagotto, *Phys. Rev. B* **82**, 104508 (2010).
  - <sup>17</sup> Rong Yu, Kien T. Trinh, Adriana Moreo, Maria Daghofer, Jose Riera, Stephan Haas, and Elbio Dagotto, *Phys. Rev. B* **79**, 104510 (2009).
  - <sup>18</sup> A. Moreo, M. Daghofer, J. A. Riera, and E. Dagotto, *Phys. Rev. B* **79**, 134502 (2009).
  - <sup>19</sup> E. Dagotto, *Rev. Mod. Phys.* **66**, 763 (1994).
  - <sup>20</sup> A. A. Schafgans, S. J. Moon, B. C. Pursley, A. D. LaForge, M. M. Qazilbash, A. S. Sefat, D. Mandrus, K. Haule, G. Kotliar, and D. N. Basov, *arXiv:1106.3114*.
  - <sup>21</sup> A. Nicholson, Qinlong Luo, Weihao Ge, José Riera, Maria Daghofer, George B. Martins, Adriana Moreo, and Elbio Dagotto, *Phys. Rev. B* **84**, 094519 (2011).
  - <sup>22</sup> For the case of doped systems other effects, such as charge stripes (Qinlong Luo, Dao-Xin Yao, Adriana Moreo, and Elbio Dagotto, *Phys. Rev. B* **83**, 174513 (2011)), may be needed to quantitatively understand the transport anisotropy which is larger than for the undoped case.