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Fermi surface shrinking, band shifts and interband coupling in iron-based pnictides

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ABSTRACT

Band shifts are systematically observed in pnictides using de Hass-van Alphen and ARPES techniques. Most interesting, such shifts result to be band-sensitive, so that hole-like bands are shifted downwards while electron-like ones are shifted upwards. In this contribution we present a comprehensive explanation for the origin of such band shifts. Using a four band Eliashberg analysis, we show that they are a natural consequence of the multiband character of these systems and of the strong particle-hole asymmetry of the bands. We also show that the relative sign of such shifts provides a direct experimental evidence of a dominant interband scattering. A quantitative analysis in LaFePO yields a spin-mediated interband coupling of the order $V \approx 0.46$ eV which corresponds to a mass enhancement $Z \approx 1.5$.

The discovery of high-T_c superconductivity in iron-based pnictides gives rise to new interesting challenges in the field of condensed matter [1]. The main object of investigation in this context is as usual the assessment of the microscopic origin of the superconducting pairing. Due to the closeness of a long-range SDW phase, promising candidates in pnictides are the interband spin-fluctuations, connecting electron-like and hole-like bands with a vector $\mathbf{Q} = (\pi, \pi)$. Such spin-fluctuations are in addition expected to give rise to a $s_\pm$ gap symmetry for the superconducting order parameter, where the gap on the electron Fermi sheets has opposite sign than on the hole-like bands [2]. Unfortunately, no direct measurement of the relative sign of the superconducting order parameter is nowadays available, and a definitive proof of a dominant role of interband (spin-mediated) interactions is still lacking.

Another puzzling feature of these materials is the systematic experimental observation, by using ARPES [3–6] and de Haas-van Alphen (dHvA) [7–9] probes, of relative band shifts when compared with DFT calculations. Quite interesting, such shifts are *band selective*, so that electron-like bands result to be shifted upwards while hole bands are shifted downwards. In this contribution we show that presence itself of such shift reveals the strong particle-hole asymmetry of each band whereas the particular sign of the band shift of the hole and electronic sheets provides a direct evidence of a dominant *interband* scattering [10].

To this aim we employ a multiband analysis where the self-energy can be written as

$$\Sigma_\alpha(i\omega_n) = -T \sum_{m,\beta} V_{\alpha,\beta} D(\omega_n - \omega_m) G_\beta(i\omega_m). \tag{1}$$

Here α, β are band indexes, $V_{\alpha,\beta} (V_{\alpha,\beta} = V_{\beta,\alpha})$ is the multiband interaction, $G_\alpha(z)$ is the local Green's function for the α band, namely:

$$G_\alpha(i\omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n - \epsilon_{\mathbf{k},\alpha} - \Sigma_\alpha(i\omega_n) + \mu}, \tag{2}$$

and $D(\omega_l)$ is the boson mediator propagator with a characteristic energy scale ω_0.

Eqs. (1) and (2) can be solved numerically in a self-consistent way. The imaginary part of the self-energy is related to the renormalization function $Z_\alpha(i\omega_n) = 1 - \mathrm{Im}\Sigma_\alpha(i\omega_n)/\omega_n$, whereas the low energy limit of the real part $\chi_\alpha = \mathrm{Re}\Sigma_\alpha(i\omega_{n=0})$ gives rise to a *band-selective* shift. This contribution is neglected in the standard Eliashberg theory, where, as we show below, the infinite bandwidth approximation enforces the particle-hole symmetry.

In order to gain a qualitative insight on the physical origin of such shift, it is instructive to consider the lowest order perturbation theory where the Green's function in Eq. (1) is taken to be the non-interacting. We consider for simplicity two-dimensional parabolic bands with $\epsilon_{\mathbf{k},\alpha} \in [E_{\mathrm{min},\alpha} : E_{\mathrm{max},\alpha}]$ which for pnictides is a good approximation, and in the adiabatic limit $\omega_0 \ll |E_{\mathrm{max},\alpha}|, |E_{\mathrm{min},\alpha}|$ we can write:

$$\chi_\alpha \approx -\frac{\omega_0}{2} \sum_\beta V_{\alpha,\beta} N_\beta \ln \left| \frac{E_{\mathrm{max},\beta} - \mu}{E_{\mathrm{min},\beta} - \mu} \right|, \tag{3}$$

where $N_\alpha = 1/(E_{\mathrm{max},\alpha} - E_{\mathrm{min},\alpha})$.

It is now easy to see that in the infinite bandwidth approximation, as well as in any case where particle-hole symmetry is pres-

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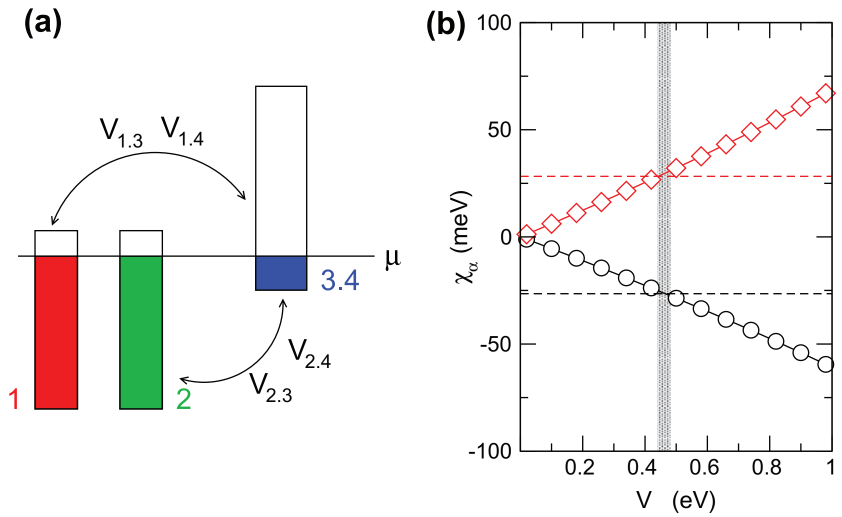

Fig. 1. (a) Sketch of our band structure model and (b) bands shift $\chi_{0,\alpha}$ as function of the interband coupling V. The horizontal dashed lines mark the average band shift as evaluated in Ref. [7,8], the vertical grey region the estimate coupling $V \simeq 0.46$ eV.

ent, $|E_{\max,\alpha} - \mu| = |E_{\min,\alpha} - \mu|$ so that χ_α. Eq. (3) shows also another interesting result, namely that the *sign* of the band shift χ_α depends on the overall electron-like or hole-like character of the bands β coupled to the band α. This is particularly important in iron-based pnictides where, due to the nesting properties, the dominant coupling is thought to be the spin-mediated interband interaction. In such a situation, the particle-hole asymmetry of the electron bands is responsible for the downward shift of the hole-like bands which, vice versa, give rise to the upward shift of the electron ones. In full generality we can say thus *the simple observation of a upward shift of the electron bands and the downward shift of the hole-like ones is a direct experimental evidence in these compounds of the dominance of the interband coupling on the intraband one, which would produce the opposite scenario.*

We can employ this analysis to get a more quantitative insight on LaFePO where detailed measurements of the band shifts by means of dHvA techniques have been reported. Following Ref. [11] we consider four bands and we assume, because of the nesting properties, a purely interband scattering connecting hole-like and electron-like bands, as depicted in Fig. 1a.

Since in LaFePO all the Fermi areas are roughly comparable, we assume as a first approximation $V_{1,3} = V_{1,4} = V_{2,3} = V_{3,4} = V$. To account for a spin-mediated interaction mechanism we use the Lorentzian spectrum typical of spin-fluctuations [12] $B(\Omega) \propto \Omega\omega_0/\pi(\omega_0^2 + \Omega_2)$, with the characteristic energy scale $\omega_0 = 20$ meV [13–16]. We model each band with a purely two-dimensional parabolic dispersion. We extract the band parameters from the LDA calculations [17], and we renormalize the electronic energy scales by a factor 2 to take into account the high-energy narrowing of the band-structure observed by ARPES [18]. All the estimated values are reported in Table 1.

Table 1
Microscopic band parameters extracted from LDA calculations [17] after a band structure renormalization by a factor 2. Also shown, in the last two columns on the right, the calculated band shifts $\chi_{0,\alpha}$ and the renormalized mass m^*_α for $V = 1.55$ eV and $V = 0.46$ eV, respectively. m_e is the free electron mass.

Band index	$E_{\max,\alpha}$ (eV)	$E_{\min,\alpha}$ (eV)	N_α (eV^{-1})	χ_α (meV)	m^*_α/m_e
1	0.102	−2.516	0.382	−26.5	1.6
2	0.102	−1.231	0.750	−26.5	3.2
3,4	1.776	−0.147	0.520	31	2.3

In Fig. 1b we show the band shifts $\chi_{\alpha,0}$ evaluated from the numerical solution of Eqs. (1) and (2) as a function of V. Note that, since we are considering $V_{\alpha,\beta} = V$, the band shift of the two different hole bands is equal $\chi_1 = \chi_2$, as well as for the two electron bands. From Fig. 1b we get an estimate $V \approx 0.46$ eV to account for the hole band shift $\Delta_{1,2} \approx -26.5$ meV needed to reproduce the experimental Fermi area with the renormalized band-structure [10]. With these values we obtain a multiband coupling matrix $\lambda_{\alpha\beta} = V_{\alpha\beta}N_\beta$

$$\hat{\lambda} = \begin{pmatrix} 0 & 0 & 0.24 & 0.24 \\ 0 & 0 & 0.24 & 0.24 \\ 0.18 & 0.34 & 0 & 0 \\ 0.18 & 0.34 & 0 & 0 \end{pmatrix}, \tag{4}$$

which gives $T_c \approx 9$ K in good agreement with the experimental value $T_c^{\rm exp} \approx 6$ K. The total coupling per band is roughly isotropic $\lambda_\alpha = \sum_\beta \lambda_{\alpha\beta} \approx 0.48$–$0.52$, in the weak coupling regime. With these values we can compute the mass renormalization factor $Z_\alpha \approx 1.5$ and the specific heat per unit cell $\gamma = \sum_\alpha (\pi/3\hbar^2) m_\alpha Z_\alpha k_B^2 a^2 N_A$, where k_B is the Boltzmann constant, N_A the Avogadro number and $a = 3.9$ Å. We obtain thus $\gamma = 14.1$ mJ/mol K^2 also in good agreement with experimental estimates $\gamma^{\rm exp} \approx 11$–$14$ mJ/mol K^2 [19–21].

In conclusion, we showed that the band shifts reported in pnictides when comparing the experimentally measured Fermi surfaces and band dispersions with LDA calculations are a direct consequence of the coupling to a bosonic mode, once that the strong particle-hole asymmetry and the multiband character of these systems are properly taken into account. Moreover, we showed that the sign of the measured shifts provide a direct evidence of the predominance of the *interband* scattering, suggesting spin-fluctuations as a natural candidate for such kind of interband coupling.

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