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Temperature and doping dependence of normal state spectral properties in a two-orbital model for ferropnictides

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ABSTRACT

Using a second-order perturbative Green's functions approach we determined the normal state spectral function $A(\vec{k},\omega)$ employing a minimal model for ferropnictides. Used before to study magnetic fluctuations and superconducting properties, it includes the two effective bands related to Fe-3d orbitals proposed by S. Raghu et al. [Phys. Rev. B 77 (2008) 220503(R)], and local intra- and inter-orbital correlations for the effective orbitals. Here, we focus on the normal state electronic properties, in particular the temperature and doping dependence of the total density of states, $A(\omega)$, and of $A(\vec{k},\omega)$ in different Brillouin zone regions, comparing them with existing angle resolved photoemission spectroscopy (ARPES) and theoretical results. We obtain an asymmetric effect of electron and hole doping, quantitative agreement with the experimental chemical potential shifts, as well as spectral weight redistributions near the Fermi level with temperature consistent with the available experiments. In addition, we predict a non-trivial dependence of $A(\omega)$ with temperature, exhibiting clear renormalization effects by correlations. Interestingly, investigating the origin of this predicted behavior by analyzing the evolution with temperature of the k-dependent self-energy obtained in our approach, we could identify a number of Brillouin zone points, not probed by ARPES yet, where the largest non-trivial effects of temperature on the renormalization are predicted for the parent compounds.

1. Introduction

In 2008, the discovery of superconductivity in $LaFeAsO_{1-x}F_x$, with transition temperature $T_c = 26$ K at $x \gtrsim 0.05$ doping [1], prompted great interest in the experimental and theoretical study of iron-based superconductors. LaOFeAs-like compounds, denoted as the 1111-ferropnictide family, served as starting point and were followed rapidly by the discovery of similar electronic properties in a series of other iron-based families of compounds. In the meantime many new superconductors have been found, all of them including quasi-two dimensional(2D) layers with a square-lattice array of Fe ions [2,3]. A vast amount of experimental and theoretical effort has been devoted to explore this family of compounds, evidenced by more than 15,000 articles published since 2008 according to the latest reviews, see e.g. Refs. [4–7] and references therein. Therefore, in the following we will focus on the previous research work most relevant to provide a proper context for the discussion of the open problem which we have addressed, and the new results on the normal state spectral properties we obtained.

It is generally recognized that the ground state properties of the ferropnictide parent compounds are mostly well described by first principles density functional theory (DFT) calculations, indicating that the low energy excitations are mainly due to electrons in the Fe-3d orbitals [8,9]. For LaOFeAs, calculations were carried out almost simultaneously in a number of works [10–14]. The Fermi surface topology and band structure are rather similar for the 11 (e.g. FeSe), 111 (e.g. LiFeAs, NaFeAs), 122 (e.g. $BaFe_2As_2$, $CaFe_2As_2$, $EuFe_2As_2$), 1111 (e.g. LaOFeAs, LaFePO, SmFeAsO, CeFeAsO) series of iron-based superconductors [15–19]. However, as a function of doping the agreement between DFT calculations and ARPES experiments in materials like LaOFeAs diminishes [12], and unexpected Fermi surface topology changes were found as a function of temperature and doping [20–23].

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Theoretical predictions showed that the 1111 compounds consist of two quasi-2D Fermi cylinders at the zone center (Γ) and a massive 3D hole pocket at the Z-point [10,24]. This behavior was observed by ARPES and quantum oscillation measurements [25]. On the other hand, in the case of 122 compounds, observations related to the dimensionality of the electronic structure revealed quite different behavior, i.e. a more 3D nature of the electronic structure was found in electron doped $BaFe_2As_2$ [26,27] whereas a quasi-2D electronic structure was derived for the case of K-doped $BaFe_2As_2$ [28]. Interestingly, Lui et al. [29] showed a transformation of the nature of the electronic structure of $CaFe_2As_2$ from quasi-2D to more 3D as a function of temperature, going from the high-temperature tetragonal to the low-temperature orthorhombic phases.

Many aspects of the temperature dependence of the normal state spectral properties remain largely unstudied in ferropnictides, which motivated our present work. Here, we present our study of the changes with temperature and doping of the normal state electronic structure, throughout the Brillouin zone (BZ). We compare our results with ARPES experimental and previous theoretical results, where feasible, and have been able to predict interesting non-trivial temperature dependent effects at Brillouin zone points, yet unexplored by ARPES. To do this, we employed a minimal microscopic model, which includes two effective bands [30] to describe the low energy band structure, as well as intra- and inter-orbital local Coulomb interactions, as detailed in next section. Similar effective two-orbital models have been studied before, focusing on other aspects of the problem, mostly on the superconducting properties. For example, investigations of pairing mechanisms and gap symmetry were reported [31–38], studies of spin fluctuations [31,32,34] and a spin-density wave phase [39], Mott transition for strong electron correlations [40–42], lattice and orbital properties [42–45], etc. In our case, we studied the minimal microscopic two-orbital model using analytical perturbative techniques to take into account the effect of electron correlations, in order to determine the relevant normal state Green's functions and the corresponding temperature-dependent electronic spectral density. We would like to highlight the fact that, in contrast to other analytical techniques, in our approach a k-dependent self-energy is obtained, also dependent on temperature and doping, enabling us to explore normal state physical properties throughout the Brillouin zone, and thus address new problems.

Our perturbative treatment for the electronic correlations in ferropnictides is justified by previous estimations of intermediate values for them, both from numerical calculations and experimental results. For example, a combination of local density approximation for DFT and dynamical mean field theory (DMFT) calculations for REOFeAs (RE = La, Ce, Pr, and Nd) [46], estimated a Hubbard local intra-orbital correlation value: $U \sim 3.69$ eV. Refs. [11,47] estimated that with $U = 4$ eV, width of Fe-bands $W_{Fe} = 3$ eV from LDA, and a Hund's coupling energy $J = 0.7$ eV, taking for the inter-orbital correlation $V = U - 2J$ as in most Refs. [46,48–53], in this case yielding $V = 2.6$ eV, the available normal state ARPES results could be described, while the same parameters were also adopted for studying the superconducting state in Ref. [48]. Furthermore, it was concluded [47] that $U = 4.5$ eV would transform the system into a Mott-insulator, in contrast to other LDA + DMFT predictions [49–52], reporting that the system remains metallic and does not transform into a Mott-insulator even increasing U up to 5 eV, with $W_{Fe} = 4$ eV and $J = 0.7$ eV; while for $J = 0$ an electronic structure characteristic of much weaker correlations is obtained, with a quasiparticle weight renormalization factor $Z \sim 0.8$ [52]. From ARPES, mass renormalization factors between 1.5 and 2.5 were estimated in 122 compounds of the form $Sr_{1-x}K_xFe_2As_2$, depending on the Fermi surface sheet [54–57], with similar reports of 1.3–2.1 for 1111 and other 122 compounds [25,58,59]. X-ray absorption spectroscopy estimations of U, placed it below ∼4 eV [60,61]. To describe the smaller experimental Fermi-surface areas reported in de Haas–van Alphen experiments in $SrFe_2As_2$ [58], a renormalization of the LDA band structure was suggested in 2009 [62], estimating an interband scattering of magnitude ~ 0.46 eV between hole and electron bands to explain the reported experimental band shifts [25]. Regarding the minimal two-orbital model by Raghu et al. of Ref. [30], the full bandwidth of the non-interacting band structure is about 12 eV, and local intra-orbital correlation values $U/W = 0.2$–0.5 have been used previously [31,32]. Adding Hund's coupling J and local Coulomb correlations, a Mott transition in the two-orbital model [30] was predicted at a critical interaction $U_c/W \sim 2.66/(1 + J/U)$ [41], if $J/U < 0.01$, with a decrease of U_c for larger J: deducing that the effect of increasing Hund's coupling on critical U_c is similar to the effect of having more degenerate orbitals in a multiorbital Hubbard model [41], effectively weakening the effect of correlations [52] and stabilizing a metallic state [41].

In addition to effective two-orbital models for ferropnictides, other multiorbital effective models were proposed [4]. A three-orbital Hamiltonian was constructed involving the 3d orbital xz, yz and xy for Fe [63], and compared with the two-orbital model of Ref. [30]. Improvement of two shortcomings of the latter were reported, related to the relative weights of each orbital on the Fermi surface. Also effective four-orbital [41] and five-orbital models [4,11,32,48,53,64] were studied. Nevertheless, the effective two-orbital model of Ref. [30] is still recognized as a useful minimal model to describe the main features of the low-energy physics of ferropnictides [31–37,41,42,66].

Our paper is organized as follows. In Section 2.1 we present the microscopic correlated two-orbital model adopted for our study of the normal state of Fe-based superconductors, and describe the analytical Green's function approach we used to calculate the electronic spectral density function and the total density of states including the correlations in second-order of perturbations (further details of our analytical calculations appear in Supplementary Appendix A). In Section 3 we present and discuss electronic structure results obtained at different temperature and doping values along the Brillouin zone, and compare them with available theoretical and experimental ARPES results for the normal state spectral properties of ferropnictides. To understand the origin of the non-trivial temperature dependence we predict for the density of states, in Supplementary Appendix B we analyze the k-dependent electron self-energies obtained in our approach, having identified a number of specific Brillouin zone points, not probed by ARPES experiments yet, where we find the largest non-trivial effects of temperature on the renormalization. We conclude in Section 4, summarizing our main findings with the minimal model for pnictides and analytical treatment used, prompting for new ARPES experiments which could test our predictions, and mentioning possible extensions and applications of our work.

2. Microscopic model and analytical approach

2.1. Correlated effective two-orbital model

To describe analytically the properties of ferropnictides, we will consider a simplified model which contains the minimum number of degrees of freedom preserving the essential physics of the problem in 1111 and 122 compounds, as mentioned in previous section. In particular, a minimal two-orbital model suitable to describe the Fermi surface topology of ferropnictides was proposed by Raghu et al. in Ref. [30]. The model consists of a two-dimensional square lattice, with each site having two degenerate orbitals. Raghu et al. in Ref. [30] fitted the bare-band tight-binding