Weakness of correlation effects in BaNi$_2$As$_2$: ARPES and LDA+DMFT study

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Abstract. The BaNi$_2$As$_2$ compound is investigated using both the angle-resolved photoemission spectroscopy (ARPES) in a wide binding energy range and combined computational scheme of local density approximation together with dynamical mean-field theory (LDA+DMFT). For more realistic comparison of LDA+DMFT spectral functions with ARPES data we take into account several experimental features: the photoemission cross-section, the experimental energy and angular resolutions and the photo-hole lifetime effects. In contrast to isostructural iron arsenides the BaNi$_2$As$_2$ within LDA+DMFT appears to be weakly correlated (effective mass enhancement about 1.2). This dramatic reduction of the correlation strength comes from the increase of 3d-orbital filling, when going from Fe to Ni, together with rather large bare Ni-3d LDA bandwidth. Nevertheless, even weakened electron correlations cause remarkable reconstruction of the bare BaNi$_2$As$_2$ LDA band structure and corresponding LDA+DMFT calculations provide better agreement with ARPES than just renormalized LDA results.

Keywords: Angle-resolved photoemission spectroscopy, Iron-based superconductors, Electronic structure

1. Introduction

At present, for more than ten years, new high-temperature iron-based superconductors have been intensively studied both experimentally and theoretically (cf. reviews [1, 2, 3, 4, 5, 6]). The discovery of these new iron-based superconductors gave rise to two large groups of materials: pnictides [1, 2] and chalcogenides [7]. Electronic band structures of these superconductors, as well as some related systems, were compared in Refs. [8, 9].

One of these related systems is BaNi$_2$As$_2$ – compound isostructural to well studied BaFe$_2$As$_2$ high temperature superconductor. In the BaNi$_2$As$_2$ there is no spin density
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wave (SDW) type of magnetic ordering in contrast to iron arsenides [10]. The low-
temperature evolution of thermal conductivity and specific heat in BaNi$_2$As$_2$ is quite
similar to the conventional BCS superconductors [11]. It corresponds to a weak coupling
regime with $T_c = 0.7$ K [12], which is in good agreement with the simple BSC-like $T_c$
estimation based on DFT/LDA calculated density of states (DOS) on the Fermi level [13]
done in Refs. [8, 14]. In case of phosphorus doping of BaNi$_2$As$_2$ the $T_c$ abruptly increases
from 0.7 to 3.3 K [15]. The enhanced superconductivity is accompanied by the triclinic-
to-tetragonal phase transition [16] and change of the phonon spectrum [15]. A number
of LDA calculations were done for BaNi$_2$As$_2$ [10, 17, 18, 19]. However, to our knowledge,
electron correlation effects in BaNi$_2$As$_2$ were not investigated yet. Thus, there is an open
question why manifestation of the correlations in BaNi$_2$As$_2$ is rather weak [10], while
for iron arsenides, the correlations are significant ($m^*/m \sim 3$) and for chalcogenides,
e.g. KFe$_2$Se$_2$, can be even stronger ($m^*/m \sim 5$) [9].

In this paper we present joint study of BaNi$_2$As$_2$ within the angle-resolved
photoemission spectroscopy (ARPES) and combined computational scheme of local
density approximation and dynamical mean-field theory (LDA+DMFT) [20, 21]. The
high resolution ARPES measurements were done in a wide binding energy range
and include both Ni-3d, As-4p states completely. To provide better comparison of
LDA+DMFT spectral functions with ARPES data the photoemission cross-section,
the experimental energy and angular resolutions and the photo-hole lifetime effects
are included into consideration. Here using LDA+DMFT calculations we explicitly
demonstrate that correlation effects are rather weak in BaNi$_2$As$_2$ because of almost
occupied Ni-3d states. However correlation effects in BaNi$_2$As$_2$ remarkably reconstruct
bare LDA bands and give good, almost quantitative agreement with experimental
ARPES data.

2. Computational details

The crystal structure of BaNi$_2$As$_2$ above $T = 131$ K has the tetragonal symmetry
with I4/mmm space group. Lattice constants are $a = b = 4.112$ and $c = 11.542$
Å. The atomic positions in the elementary unit cell are following: Ba – 2a(0, 0, 0),
Ni – 4d(0, 0.5, 0.25), As – 4e(0, 0, 0.3476) [12]. The LDA calculations were performed
within the Elk full-potential linearized augmented plane-wave (FP-LAPW) code [22].
We employed the CT-QMC impurity solver [23, 24, 25, 26, 27, 28] for the DMFT
part of LDA+DMFT calculations. To define the DMFT lattice problem for BaNi$_2$As$_2$
compound we used the LDA Hamiltonian projected to Ni-3d, As-4p and Ba-5d Wannier
functions.

The DMFT(CT-QMC) computations were done at the inverse temperature $\beta = 40$
($\sim 290$ K) with about $10^8$ Monte-Carlo sweeps. The interaction parameters of the
Hubbard model were taken as $U = 4.5$ eV and $J = 0.85$ eV. These values are slightly
larger [29] than typical values for iron arsenides [30, 31, 32]. We employed the self-
consistent fully-localized limit definition of the double-counting correction ($E_{dc}$) [33, 34].
Thus computed values of the Ni-3d occupancies and the corresponding double-counting energies are $n_d = 9.21$, $E_{dc} = 35.69$ eV. The LDA+DMFT spectral function maps were obtained after an analytic continuation of the local self-energy $\Sigma(\omega)$ from the Matsubara frequencies to the real ones. To this end we have applied the Pade approximant algorithm [35] and checked the results with the maximum entropy method [36] for the Green’s function $G(\tau)$.

3. Experimental details

The ARPES experiments were performed at the I05 beamline of the Diamond Light Source [37]. The single crystalline samples were cleaved in ultra high vacuum (better than $2^{-10}$ mbar). The photoemission spectra with total energy resolution of 20 meV and angular resolution of 0.5° were measured at 7 K, using photons with the energy 120 eV of various polarizations.

4. Results and discussion

In Fig. 1 LDA calculated total, Ni-3d and As-4p densities of states (left) and band dispersions (right) for the BaNi$_2$As$_2$ are shown. Band structure of BaNi$_2$As$_2$ is quite different to a typical one of iron arsenides. There are three bands crossing the Fermi level in the Γ-X direction instead of five in BaFe$_2$As$_2$ [38] or NaFeAs [39] and four instead of two in the P-N direction. Let us point out that the Fermi level is located on the Ni-3d high energy band edge since BaNi$_2$As$_2$ is significantly electron doped with respect to BaFe$_2$As$_2$ or NaFeAs. The Fermi level is about 1.5 eV higher in BaNi$_2$As$_2$ than in the
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BaFe$_2$As$_2$. However the shape of densities of states is quite similar to iron arsenides up to a shift in energy.

Figure 2. Comparison of ARPES data second derivatives for horizontal and vertical polarizations with LDA+DMFT quasiparticle bands (white lines) with $k_z = 0$ (panels a,b), $k_z = 0.5 \pi/c$ (panels c,d) and $k_z = 0.95 \pi/c$ (panels e,f).

In Fig. 2 we present the LDA+DMFT results compared with the ARPES data. It is well known that by varying a beam energy in ARPES experiments one can access different values of $k_z$ component of the momenta [40]. However to obtain a precise value of $k_z$ one should know an exact geometry of ARPES experiment [40], the work function and the inner potential for this particular material [41]. Since it’s difficult to find latter ones (e.g. inner potential), we compare the second derivatives of ARPES data and the theoretical LDA+DMFT calculated spectral function maps at different $k_z$ values. In Fig. 2 we plotted only three of them: $k_z = 0$ (panels a,b), $k_z = 0.5 \pi/c$ (panels c,d) and $k_z = 0.95 \pi/c$ (panels e,f). Here $c$ is the lattice constant along the z-axis mentioned above.

In the LDA+DMFT calculated data (white lines on Fig. 2) the quasiparticle band near Γ-point around $-0.5$ eV is present only at $k_z \approx \pi/c$ (panels e,f). At $k_z = 0.9 \pi/c$ this band changes shape and looses similarity to the ARPES quasiparticle band. At $k_z = \pi/c$ the band lays slightly above the experimental one. Therefore for all following figures of this paper we chose $k_z = 0.95 \pi/c$ and thus the notation of the Γ-point is $(0,0,0.95 \pi/c)$ and of the X-point is $(\pi/a, \pi/a, 0.95 \pi/c)$.

In Fig. 3 on panels (a) and (f) LDA bands and LDA+DMFT spectral function map are presented in X-Γ-X high symmetry direction. Next to them on panels (b) and (g) LDA and LDA+DMFT spectral function maps including photoemission cross-section ratio are shown. For the given experimental photon energy 120 eV corresponding cross-section ratios can be interpolated in the atomic limit as Ni-3d : As-4p : Ba-5d = 5.28 : 0.06 : 0.98.
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Figure 3. LDA (upper line) and LDA+DMFT (lower line) spectral function maps, with the photoemission cross-section contributions (panels b,g). On panels (c,h) in addition to (b,g), the energy resolution is taken into account. Then on (d,i) panels the energy resolution and the photo-hole lifetime effects are considered. Finally on panels (e,j) the k-space resolution is introduced. Corresponding LDA and LDA+DMFT spectral functions have the same intensity scale. The Fermi level is at zero energy.

(see Ref. [42]). Also theoretical spectra were multiplied with the Fermi function at experimental temperature 7 K thus cutting off quasiparticle bands above the Fermi level. Because of photoemission cross-section relative amplification the Ni-3d states become more bright especially in (−3; −2) eV energy interval. Then the theoretical spectra obtained above are convoluted with the Gaussian function to take into account
the experimental energy resolution of 20 meV for LDA (panel c) and LDA+DMFT (panel h). The effect of the bare LDA band broadening due to experimental resolution is quite noticeable (Fig. 3(c)). But for the LDA+DMFT bands broadening due to experimental resolution is hardly observable because electron correlations themselves produce significant band damping.

In our earlier work Ref. [43] it was demonstrated that an energy dependent broadening of the theoretical spectral functions gives better agreement with the experimental data. To this end theoretical quasiparticle bands were convoluted with a Gaussian with a full width at half maximum increasing as $C \cdot \epsilon_B + \Gamma_{exp}$. Here $\epsilon_B$ is the binding energy, $\Gamma_{exp}$ is the experimental resolution, and $C$ characterizes the increase of the broadening with energy upon moving away from Fermi level due to photo-hole lifetime effects (for more details see Refs. [43, 44, 45]). The maximum allowable broadening was limited to 0.5 eV for the energy lower than -1 eV. Corresponding broadened LDA and LDA+DMFT spectral function maps are drawn on panels (d) and (i) in Fig. 3. The photo-hole lifetime effects provide rather strong damping of the quasiparticle bands making them nearly indistinguishable. Maximum value of the spectral function between panels c and d (h and i) drops down about 5 times. Thus to keep quasiparticle bands visible enough we change corresponding intensity scales (see color scale tick labels). Finally to complete realistic comparison of the theory with ARPES we consider the experimental angular resolution of 0.5 degrees (k-space resolution 0.04 Å⁻¹) by the Gaussian function for LDA (panel e) and LDA+DMFT (panel j). At first glance LDA spectral function map on Fig. 3(e) is very similar to LDA+DMFT one on Fig. 3(j). So one can conclude that consideration of all described above experimental features masks bare LDA bands in a manner similar to correlation effects.

Let’s compare LDA and LDA+DMFT experimental-like broadened spectral functions with ARPES on Fig. 4. Total quasiparticle bandwidth is almost the same for the theory (panels (b) for LDA and (e) for LDA+DMFT) and ARPES data (panels (a), (c) or (d), (f)). It means that for rather strong Coulomb interaction $U=4.5$ eV and $J=0.9$ eV LDA+DMFT gives weak mass renormalization of only 1.2. Since the LDA and LDA+DMFT spectral function maps are so similar to each other and agree well with the ARPES experiment one can conclude that correlations have little effect on the electronic structure in BaNi$_2$As$_2$ system. Nevertheless, despite the weakness of correlation effects in BaNi$_2$As$_2$ the LDA+DMFT calculations show considerable reconstruction of bare LDA bands which gives better agreement with experimental ARPES data. The presence of correlations shifts the bright region near Γ-point from $-3.5$ eV (LDA) to $-3$ eV (LDA+DMFT). The region around $-3$ eV corresponds to Ni-3d$_{x^2-y^2}$ and Ni-3d$_z^2$ states (see Fig. 5 panels (a), (b), (c) and (d)). Thus we find out that LDA+DMFT spectral function map with weak manifestation of correlation effects almost quantitatively describes ARPES data. Here we primarily discuss the behavior of the self energy on the large scales, comparable to the width of the whole 3d band, the effects of the structural transition on the band positions do not alter the conclusions.
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Figure 4. Comparison of ARPES (a,b panels, same on d,f), LDA (b panel) and LDA+DMFT (e panel) experimental-like broadened spectral function maps in the XΓX high symmetry direction for BaNi$_2$As$_2$. On the (b) and (e) panels the LDA and LDA+DMFT spectral function maps are shown as obtained on panels (e) and (f) of Fig. 3. The Fermi level is at zero energy.

Now it is time to discuss the origin of the weakness of these correlation effects. Corresponding 5-band model calculations were done e.g. in the work of L. Medici and co-authors in Ref. [46]. There it was shown that iron arsenide superconductors with about 6 electrons per Fe atom and Coulomb interaction about 4.5 eV should have quasiparticle mass renormalization $m^*/m \sim 3$. For the case of BaNi$_2$As$_2$ our LDA+DMFT results give Ni-3d state occupancy $\sim 9.2$ electrons which is far away from Fe-3d states occupancy in iron arsenides. Following model calculations of L. Medici and co-authors from [46] for such high filling and approximately the same Coulomb interaction the corresponding mass renormalization should be slightly above one. The same mass renormalization is obtained in our material specific LDA+DMFT calculations for BaNi$_2$As$_2$.

Another reason of small mass enhancement is that the Ni-3d state bandwidth ($W$) is about 4.75 eV (see Fig. 1). This is perhaps the largest $W$ value among iron arsenides or chalcogenides: KFe$_2$Se$_2$ – 3.5 eV [47], in NaFeAs – 4.5 eV [30]. Correspondingly, the electron correlations that are proportional to $U/W$ ratio, where $U$ is Coulomb interaction are getting significantly weaker.

Let us emphasize another peculiarity of BaNi$_2$As$_2$ that differs it from regular iron arsenide superconductors. Once we plot orbital resolved LDA+DMFT spectral function maps for Ni-3d and As-4p states one can see that all these orbitals are present at the Fermi level (see Fig. 5). Also orbital resolved spectral function maps are very useful for better understanding of ARPES data. Main contribution to spectral function at the Fermi level comes from to Ni-3d$_{xy}$ and As-4p$_z$ states. The quasiparticle band at $-0.5$ eV near $\Gamma$-point corresponds to hybrid Ni-3d$_{xy}$ – As-4p$_z$ state. The quasiparticle bands
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Figure 5. Orbital resolved LDA+DMFT spectral function maps for Ni-3d (a,c,g,i) and As-4p (e,k) states in the XIX high symmetry direction for BaNi$_2$As$_2$. Same with taking into account the experimental resolution and the photo-hole lifetime effects (b,d,f,h,j,l). The Fermi level is at zero energy.

located below $-2.0\text{ eV}$ for horizontal polarization ARPES data (Fig. 4(d)) represent Ni-3d$_{x^2-y^2}$ and Ni-3d$_{z^2}$ states. For vertical polarization ARPES data (Fig. 4(f)) high intensity region around Γ-point in interval ($-1; -2\text{ eV}$) belongs to Ni-3d$_{yz,xy}$, Ni-3d$_{xy}$ and Ni-3d$_{z^2}$ states. The flat band near $-0.8\text{ eV}$ has Ni-3d$_{x^2-y^2}$ character. One can see from comparison of Fig. 5 and Fig. 4 that the As-4p states are almost not resolved due to the suppression of photoemission cross-section and photo-hole lifetime effects. Thus in the ARPES data below $-3\text{ eV}$ the As-4p states are visible as a strongly blurred background.

5. Conclusions

In this work we present realistic comparison of LDA+DMFT spectral functions with ARPES data. In our theoretical approach we include several experimental details:
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the photoemission cross-section, the experimental energy and angular resolutions and the photo-hole lifetime effects. Consideration of mentioned above experimental contributions highlight the importance of electron correlation effects for true description of the electronic structure.

The BaNi$_2$As$_2$ is a close relative of iron arsenide high temperature superconductors which are quite correlated materials (for iron arsenides $m^*/m \sim 3$ and for iron chalcogenides are even stronger $m^*/m \sim 5$ [9]). However the LDA+DMFT calculations for BaNi$_2$As$_2$ show quite weak manifestation of correlations in a very good agreement with ARPES results. Here within LDA+DMFT we have explicitly found that mass enhancement for BaNi$_2$As$_2$ $m^*/m$ is 1.2 for quite strong Coulomb interactions $U=4.5$ eV and $J=0.9$ eV. There are a couple of reasons for that: (i) almost fully occupied Ni-3d states with 9.2 electrons and (ii) quite large Ni-3d states bandwidth $W=4.75$ eV, which is perhaps the largest $W$ value among iron arsenides or chalcogenides: KFe$_2$Se$_2$ – 3.5 eV [47], in NaFeAs – 4.5 eV [30].

Despite the weak manifestation of electron correlations the LDA+DMFT calculations lead to remarkable reconstruction of bare LDA bands. As a result, Ni-3d states are significantly compressed around $-3$ eV. All these provides almost quantitative agreement of LDA+DMFT results with ARPES, and show that even small manifestation of electron correlations play significant role in establishing the electronic structure of this material. Finally we have shown why the electronic structure of Ni-based compound is so weakly renormalized, and therefore vastly improve our understanding of the physics of electron-electron correlations in iron based superconductors and related materials.

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