The emergence of angle-resolved photoemission spectroscopy (ARPES) made it possible to observe electronic dispersion directly as a spectral function map. On the other hand, a spectral function map can be obtained theoretically, for example, in the LDA+DMFT method. The electronic band on such a map is characterized not only by its energy position at a given k point, but also by its width and intensity. To illustrate a way of quantitative comparison of theoretical spectral functions and ARPES data, spectral functions obtained by the LDA+DMFT method are chosen. It is shown that the theoretical spectral functions should take into account a number of experimental features: the photoionization cross section, the experimental energy and angular resolution, as well as the effects of the lifetime of the photo-hole arising in the process of photoemission. In this article, we present a robust procedure for taking into account these experimental features by the example of iron-based high-temperature superconductors systems: NaFeAs and FeSe on a SrTiO\textsubscript{3} substrate.

DOI: 10.1134/S0021364021020089

1. INTRODUCTION

In the last few decades, the intensive development of angle-resolved photoemission spectroscopy (ARPES), in particular, associated with the discovery of copper high-temperature superconductors (HTSCs) due to their quasi-two-dimensionality, made it possible to observe experimentally the electron band structure for various classes of materials with a fairly good instrumental resolution and in a quite wide range of binding energies [1], including weakly correlated three-dimensional systems (see, e.g., [2]). The corresponding ARPES data are maps on which the electronic states at a given point in reciprocal space are characterized by energy position, width and intensity.

On the other hand, the improvement of theoretical methods for calculating electronic states, for example, density functional theory (DFT) and its combination with methods that take into account electronic interactions (e.g., LDA+DMFT [3]), also makes it possible to obtain the electronic band structure in the form of spectral function maps. This has caused an urgent need for a quantitative comparison of theoretical and experimental electronic bands. For this, in the theoretical and experimental data, it is necessary to compare not only the qualitative energy position of the electronic bands, but also their relative intensities and widths.

In this work, it is shown that an important factor, influencing the width and intensity of the experimentally observed electron bands, to a large extent is the conditions under which an experiment was carried out: the incident beam energy and the instrumental resolution. In addition, there are certainly temperature broadening and damping associated with electron-electron (or some other) interactions in the system under study. The incident beam energy determines the relative intensity of a given electronic state to be excited, i.e., the photoionization cross section [1, 4], which significantly affects the relative intensity of various branches of the electronic spectrum. Furthermore, the instrumental resolution of detectors used in the experiment (angle and energy resolutions) provide a significant contribution to the width of the electron bands [4]. Another remarkable contribution to the width and intensity of the electronic spectrum (which is not directly related to the experimental setup) is the finite lifetime of a photo-hole arising in the process of photoemission [1].

Here, we propose how to introduce into theoretical spectral function map a number of experimental features: the photoionization cross section, experimental energy and angular resolutions, as well as the effects of the lifetime of the photo-hole. By the example of iron based HTSC (NaFeAs and FeSe on a SrTiO\textsubscript{3} substrate), it is shown that a significant contribution to the broadening of quasiparticle bands is associated precisely with taking into account these experimental...
details within the theory. It is also shown that the choice of the parameters of the broadening of the initial theoretical bands can lead to a change in the position of the maxima of the spectral function. In addition, the issue of the need to introduce some alphanumeric standard for the designation of the intensity scale is discussed when publishing both experimental and theoretical spectral function maps, which is necessary for quantitative analysis of data from various sources.

2. RESULTS

To study the effect of the inclusion of experimental features on the spectral function map, we used the data obtained earlier in LDA+DMFT(CT-QMC) calculations for superconductors NaFeAs [5] and FeSe on a SrTiO₃ substrate [6] (for details of calculations and description of methods, see the above works). Figure 1a shows the LDA+DMFT spectral function map in the high symmetry M–Γ–M direction for the NaFeAs superconductor.

The LDA+DMFT spectral function with the photoionization cross section included is plotted in Fig. 1b. To obtain the valence band, the LDA+DMFT spectra were convoluted with the Fermi distribution function at the experimental temperature 20 K. In this ARPES experiment (Fig. 1f) [7], the incident beam energy was 80 eV, which corresponds to the relative values of the photoionization cross section in the atomic limit (Fe 3d : As 4p) = 6.181 : 0.0877 [8, 9]. At the given incident beam energies, due to the photoionization cross section, the intensity of the Fe 3d states significantly increases in comparison with As 4p.

Then, to take into account the experimental energy resolution of 20 meV, the convolution of the spectral function (Fig. 1b) with the Gaussian function was performed. To this end, the so-called energy distribution curves (EDCs) are used here for convolution (Fig. 1c). The effect of the inclusion of the energy resolution is hardly noticeable in the LDA+DMFT spectral function map, since the electron–electron correlations themselves give rise to broadening and suppression of the intensity of quasiparticle bands, comparable in magnitude with the experimental resolution.

In our previous work [10], it was shown that taking into account the dependence of the lifetime of the photo-hole, arising in the process of photoemission, on the binding energy for the total density of states gives better agreement with experimental photoemission spectrum. In this work, we have applied this approach to the spectral function by performing the convolution with a Gaussian function with a width at half maximum, which is linearly dependent on the binding energy: \( C \varepsilon_B + \Gamma_{\text{exp}} \). Here, \( \varepsilon_B \) is the binding energy, \( \Gamma_{\text{exp}} \) is the experimental energy resolution, and \( C \) characterizes the decrease in the lifetime of the photo-hole when moving away from the Fermi level deep into the valence band (see [10–12]). The maximum value of the half-width of the Gaussian function was chosen 0.5 eV at energy \(-1\) eV, and below it remains constant. The spectral function map thus obtained is shown in Fig. 1d. The inclusion of the finite lifetime of a photo-hole leads to a serious suppression and broadening of quasiparticle bands, making them practically indistinguishable. The maximum intensity value on the spectral function map has been reduced from six to four in order to highlight its structure (see intensity color scale).

The final step for a quantitative comparison with ARPES was the inclusion of an experimental angular resolution of 0.5° (correspondingly, 0.04 Å⁻¹ in the \( k \) space). It was implemented via the convolution of the spectral function with the Gaussian function.
called *momentum distribution curves* (MDC) are used here for convolution (Fig. 1e).

The above analysis makes it possible to distinguish the broadening and damping of quasiparticle bands, caused by electron correlations (or other interactions) in the system, from the broadening and damping of the spectral function associated with the experimental setup and the process of photoemission itself.

We see that introduction of the experimental features for the LDA+DMFT spectral function leads to good agreement with the experimental data (Figs. 1e, 1f). In particular, for NaFeAs electron-electron correlations are moderately manifested (mass renormalization at the Fermi level is about 3) and damping of the LDA+DMFT spectral function is insignificant (Fig. 1a). While in the experiment (Fig. 1e), a rather diffuse intense formation is observed near the Fermi level. Taking into account the above-mentioned experimental features, the damping of the LDA+DMFT spectral function significantly increases, which is in good agreement with experiment. It is also worth noting that the LDA+DMFT spectral function below −2 eV, formed mainly with As $4p$ states, together with the experimental features also better agrees with the ARPES data in terms of structure and intensity.

The next system considered in this work is the FeSe superconductor on the SrTiO$_3$ substrate (FeSe/STO). A distinctive feature of this system is the presence in the ARPES spectra of the so-called “shallow” and twin bands around 50 meV below the Fermi level near the M point [13, 14]. Thus, using the FeSe/STO system as an example, one can see the influence of the inclusion of experimental features on a small energy scale.

![Figure 2](image.png)

**Fig. 2.** (Color online) (a, f) LDA+DMFT spectral function for FeSe/STO in the M–Γ–M and Γ–M–Γ directions [6]. (b, e) Experimental features indicated in the text are taken into account. (c, d) ARPES from [13]. The energy is measured from the Fermi level (white dotted line).

It can be noted that taking into account the experimental features gives a quantitatively similar structure of the LDA+DMFT and ARPES data except for the bands at the Fermi level near the Γ point. Thus, LDA+DMFT quasiparticle bands become less pronounced and much more diffuse. In this case, the “shallow” band (~50 meV) near the M point, obtained in the LDA+DMFT calculation, acquires a quantitatively similar structure (like a “tank-top”) in comparison with ARPES (see Figs. 2d, 2e).

Especially we would like to discuss shift of the intensity maxima of the spectral function depending on how fast the lifetime of the photo-hole grows with binding energy increase. This shift can be of the order of 100 meV. It is interesting that in this case the initial LDA+DMFT bands do not change its energy position. The position of the quasiparticle bands is determined experimentally by the intensity maximum of the spectral function. Thus, energy position of experimental quasiparticle band may differ from its true position, since the speed of growth of the lifetime of the photo-hole with binding energy is not known in practice. This can especially strongly affect the inter-
The shift of the most intense region near the \( \Gamma \) point for different values of speed of growth of the lifetime of the photo-hole from 0 (Fig. 3a) to \( \sim 0.5 \) (Fig. 3d) is shown in Fig. 3. For the bands near \(-0.22\) and \(-0.06\) eV, the shifts are about 50 and 15 meV, respectively. This shift of the intense region might be important for the analysis of ARPES data on such small scales, especially for superconducting systems. Since the effects of the lifetime of the photo-hole are always present, we can conclude that the energy position of the quasiparticle bands in ARPES is determined with an accuracy up to the speed of growth of the lifetime of the photo-hole with binding energy increase. For the experimental data analyzed in this work, the magnitude of the shift can be greater than the instrumental resolution (8 and 20 meV, respectively). This fact should be borne in mind when analyzing and interpreting ARPES spectra.

An important parameter that affects the visual perception of the spectral function and the analysis of its structure is the intensity of the spectral function map and the choice of the method to display it. The intensity scale is often shown by changing a certain set of colors, where a certain intensity value corresponds to a certain color from the palette. Thus, the display of the intensity scale of the spectral function map can vary in the maximum and minimum cutoff values and in the “distance” between adjacent colors, which allows one to emphasize the necessary ARPES data details. However, for a quantitative comparison of ARPES with theoretical spectra, it would be good to have the same or similar in color and magnitude scale of the intensity of the spectral function map. To do this, it is necessary to know the color scale of ARPES spectra, which is often given, and the value of the spectral function corresponding to a given color, which is almost never presented by both experimentalists and theorists.

Another “arbitrary parameter” is the choice of the linear or logarithmic intensity scale. The latter is usually used to highlight the low-intensity parts of the spectral function map. Figures 2b and 3d show the same spectral function in one color scale, but in different intensity scales: linear and logarithmic.

For convenience of quantitative comparison of data from different sources, one can designate the corresponding scale in some alphanumeric way, for example, lin0N3T4.5G7Y8Br10W (see Fig. 3a), which means a linear scale, 0—Navy, 3—Turquoise, 4.5—Green, 7—Yellow, 8—Brown, 10—White, or simply describe it in the text of the article.

3. CONCLUSIONS

In this work, using the example of LDA+DMFT spectral functions, it has been shown that for a quantitative comparison of theoretical spectral function maps with ARPES data, it is necessary to take into account experimental features: the photoemission cross section, experimental energy and angular resolution, as well as the effects of the lifetime of the photo-hole associated with the process of photoemission itself. Note that the inclusion of these experimental features is not related to the model concept of photoemission and is necessary in the analysis of theoretical results. It is also shown that the interpretation of ARPES spectra is complicated by the presence of a lifetime of the photo-hole depending on the binding energy (the explicit form of which is not known for a particular material), which leads to a shift in the intensity maxima of spectral functions relative to the true position of the quasiparticle band. The importance of a detailed description of the color intensity scale for...
the quantitative comparison of spectral maps from different sources is shown.

ACKNOWLEDGMENTS

The calculations were performed on the URAN supercomputer, Institute of Mechanics and Mathematics, Ural Branch, Russian Academy of Sciences.

FUNDING

This work was supported in part by the Russian Foundation for Basic Research (project no. 20-02-00011). N.S. Pavlov acknowledges the partial support of the Council of the President of the Russian Federation for State Support of Young Scientists and Leading Scientific Schools (project no. MK-1683.2019.2).

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