ANOMALIES IN THE TEMPERATURE DEPENDENCE OF COEFFICIENTS IN LAYERED STRUCTURES WITH INTRODUCED IMPURITIES

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Abstract

The temperature dependence of specific resistance ρ and thermoelectric coefficient α is studied in terms of the Mott and Davis theory for electronic processes in quasi-two-dimensional disordered systems. The existence of a peak in the electron state density defined by the two-dimensionality of the system and narrow energy bands makes it possible to describe the anomalies in the temperature dependence of α and ρ values in high-temperature superconducting cuprates obtained on the basis of *FeAs*.

1. Introduction

Intensive researches on HTSC iron-based compounds (ferropnictides) have been conducted in recent years. Great interest in these compounds is determined, first of all, by the possibility of obtaining a high-temperature of superconducting transition $(T_c \sim 55K)$ [1]. A detailed description of this class of materials obtained on the basis of *FeAs* is given in [2–4].

Note that, from the point of view of electronic properties, the above mentioned materials are quasi-two-dimensional (layered) systems. This fact allows neglecting the existence of a direction perpendicular to layers in some cases [5].

First, it is necessary to know the physical properties in the normal state of layered system. In this sense, the determination of kinetic coefficients and their temperature dependence is of special interest. In particular, in compounds $YBa_2Cu_3O_4$ and $La_{2-x}(SrBa)_xCuO_4$, a number of anomalies in the temperature dependence of thermoelectric coefficient α and electrical resistivity ρ are observed. In some works [5–7], these anomalies in the first compound are explained in terms of phenomenological models, which assume that a peak exists on the Fermi surface and the energy bands are narrow.

From our point of view is interesting to determinate the above mentioned quantities α and ρ without assuming the existence of a peak on Fermi surface of any origin. These quantities should be determined considering the real electron state density, which is inherent in quasi-two-dimensional systems. It will give us the possibility to compare the results obtained in a phenomenological approach [5–7], temperature dependence of α and ρ in cuprates and in new materials based on *FeAs*. The application of the same approach to cuprates and new *FeAs* materials is justified because they both are quasi-two-dimensional and, from our point of view, the peculiarities in the electron state density which are characteristic of two-dimensional systems must manifest themselves in the properties of kinetic coefficients of both classes of materials.

Thermoelectric coefficient α and electrical resistivity ρ are calculated in this study. We proceed from the determination of these coefficients on the basis of the Mott and Davis theory of electronic processes in two-dimensional disordered systems with an anisotropic energy spectrum [8, 9].

2. Determination of conductivity σ and thermoelectric coefficient α

We use the Mott and Davis theory [8, 9] for electronic processes in no crystalline state. According to this theory, in the case of strong dispersion $\frac{\hbar}{\tau} \approx \varepsilon_F$, quantities σ and α will be represented in the form:

$$\sigma = \int \sigma(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon , \tag{1}$$

$$\alpha = \frac{k_B}{e\sigma} \int \sigma(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon}\right) \frac{\varepsilon - \mu}{k_B T} \, d\varepsilon, \tag{2}$$

Here the conductivity σ(ε) is described by the Kubo-Greenwood formula:

$$\sigma(\varepsilon) = M \, |D(\varepsilon)|^2_{av} \, g^2(\varepsilon), \tag{3}$$

where *M* is a constant, $D(\varepsilon)$ is the matrix element of electron interaction in an acyclic field, $f=1/\{1+\exp[\beta(\varepsilon - \mu)]\}$ is the function of Fermi distribution, $g(\varepsilon)$ is the electron state density. Further we choose the approximation $|D(\varepsilon)|_{av} = const$, which corresponds to the approximation with constant relaxation time τ. Along with (1) and (2), we introduce the condition defining the chemical potential:

$$n = \int f(\varepsilon) g(\varepsilon) d\varepsilon \Big/ \int g(\varepsilon) d\varepsilon, \tag{4}$$

where *n* is the degree of filling of the energy band by quasiparticles.

3. Density of electronic states

We examine quasi two-dimensional systems. In this case, it possible to represent the dispersion law for the energy of quasi-particles (see for example [10, 11]) in the form:

$$\varepsilon(\vec{k}) = \varepsilon_1 - W_1 \cos(k_x \alpha) - W_2 \cos(k_y b), \tag{5}$$

where $(W_1 + W_2)$ - half breadth of energy band: *a* ,*b* are the lattice constants.

This formula is obtained in the strong bound approximation of the band theory, which would describe the properties of electrons near the Fermi surface in a semiquantitative way. In order to simplify the task, we considered only the nearest neighbors in (5).

The electron state density is defined by the expression

$$g(\varepsilon) = \sum_{k_x, k_y} \delta\left[\varepsilon - \varepsilon(\vec{k})\right]. \tag{6}$$

Substituting (5) in (6) and integrating over k_x and k_y, we transform the density of electron states $g(\varepsilon)$ (see [12], [13]) to the following form:

$$g(\varepsilon) = \frac{1}{\pi^2 ab}\left\{ \frac{\theta\,[(\varepsilon - \varepsilon_1)^2 - (W_1 - W_2)^2]}{\sqrt{W_1 W_2}}\, K(k_1) + \frac{2\theta\,[(W_1 - W_2)^2 - (\varepsilon - \varepsilon_1)^2]}{\sqrt{(W_1 + W_2)^2 - (\varepsilon - \varepsilon_1)^2}}\, K(k_2) \right\}. \qquad (7)$$

where

$$\Theta(x) = \begin{cases} 1 & for \quad x > 0 \\ 0 & for \quad x < 0 \end{cases};$$

$$k_1^2 = \frac{(W_1 + W_2)^2 - (\varepsilon - \varepsilon_1)^2}{4W_1 W_2}; \quad k_2^2 = \frac{4W_1 W_2}{(W_1 + W_2)^2 - (\varepsilon - \varepsilon_1)^2}, \qquad (8)$$

$K(k)$ is the first kind elliptic integral. At $W_1 = W_2$ we will obtain an expression for two-dimensional isotropic system:

$$g_{is}(\varepsilon) = \lim_{W_1 \to W_2} g\,(\varepsilon) = \frac{1}{\pi^2 ab}\, \frac{K\,(k_1)}{\sqrt{W_1 W_2}}. \qquad (9)$$

In a limiting case at $W_2 = 0$ we obtain the electron state density for quasi-one-dimensional system with a root peculiarity:

$$g_{one}(\varepsilon) = \frac{1}{\pi a}\, \frac{1}{\sqrt{W_1^2 - (\varepsilon - \varepsilon_1)^2}}. \qquad (10)$$

In a two-dimensional case, formula (7) has a logarithmic peculiarity, as follows:

$$K\,(k) \underset{k \to 1}{\to} \ln \frac{4}{\sqrt{1 - k^2}}. \qquad (11)$$

Substituting expression (7) in formulas (1), (2), and (4), we will transform these functions in a form convenient for calculation. To this end, we will analyze electron state density $g(\varepsilon)$. There are three features in the calculated quantity $g(\varepsilon)$ that appears in (7):

(i) $g(\varepsilon)$ limits the definition domain of ε with two finite limits [ε_a, ε_b], where $\begin{Bmatrix} \varepsilon_a \\ \varepsilon_b \end{Bmatrix} = \varepsilon_1 \mp (W_1 + W_2)$;

(ii) $g(\varepsilon)$ has a logarithmic divergence at points [ε_c ,ε_d], where $\begin{Bmatrix} \varepsilon_c \\ \varepsilon_d \end{Bmatrix} = \varepsilon_1 \mp (W_1 - W_2)$;

(iii) the first term in (7) is nonzero on segments [ε_α, ε_c] and [ε_d, ε_b]; the second term, on segment [ε_c, ε_d].

We represent quantities $\sigma(T)$, $\alpha(T)$, and $n(\delta)$ through the integrals of the type

$$C_\gamma^{(\beta)} = \int_{\varepsilon_\alpha}^{\varepsilon_b} F_\gamma(\varepsilon)\, g^\beta\,(\varepsilon)\, d\varepsilon, \qquad (12)$$

$$\bar{\sigma} = C_1^{(2)} \qquad \text{where} \qquad F_1\,(\varepsilon) = \frac{1}{4\,k_B T}\, \frac{1}{ch^2 \frac{\varepsilon - \mu}{2k_B T}} \qquad (13)$$

$$\alpha = \frac{k_B}{e}\ \frac{C_2^{(2)}}{C_1^{(2)}}, \qquad \text{where} \qquad F_2(\varepsilon) = \frac{1}{4\,k_B T}\ \frac{\frac{\varepsilon-\mu}{k_Б T}}{ch^2\frac{\varepsilon-\mu}{2k_B T}} \tag{14}$$

$$n(\delta) = \frac{C_3^{(1)}}{C_4^{(1)}}, \qquad \text{where} \qquad F_3(\varepsilon) = \frac{1}{1+\exp\frac{\varepsilon-\mu}{k_B T}}\ ;\ F_4(\varepsilon) = 1. \tag{15}$$

On the basis of expressions (12)–(15) taking into account properties of density of electronic states, having executed a number of mathematical transformations, we transform the expression for the above quantities σ, α and *n* to the form:

$$\bar{\sigma} = \sigma\,\frac{\pi^4 a^2 b^2 W_1^2}{MD} = \frac{1}{\bar{T}}\left\{\int_0^1 \frac{K^2(x)x dx}{\varphi(\eta,x)}\left[\frac{1}{ch^2\dfrac{\delta-\varphi(\eta,x)}{2\bar{T}}}+\frac{1}{ch^2\dfrac{\delta+\varphi(\eta,x)}{2\bar{T}}}\right]+\right.$$
$$\left.+\int_{\frac{2\sqrt{\eta}}{1+\eta}}^1 \frac{K^2(x)dx}{x\varphi(\eta,1/x)}\left[\frac{1}{ch^2\dfrac{\delta-\varphi(\eta,1/x)}{2\bar{T}}}+\frac{1}{ch^2\dfrac{\delta+\varphi(\eta,1/x)}{2\bar{T}}}\right]\right\}; \tag{16}$$

$$\alpha = \frac{k_Б}{e\,\bar{\sigma}\,\bar{T}}\left\{\int_0^1 \frac{K^2(x)x\,dx}{\varphi(\eta,x)}\left[\frac{\delta-\varphi(\eta,x)}{\bar{T}ch^2\,\dfrac{\delta-\varphi(\eta,x)}{2\,\bar{T}}}+\frac{\delta+\varphi(\eta,x)}{\bar{T}ch^2\,\dfrac{\delta+\varphi(\eta,x)}{2\,\bar{T}}}\right]+\right.$$
$$\left.+\int_{\frac{2\sqrt{\eta}}{1+\eta}}^1 \frac{K^2(x)dx}{x\varphi(\eta,1/x)}\left[\frac{\delta-\varphi(\eta,1/x)}{\bar{T}ch^2\dfrac{\delta-\varphi(\eta,1/x)}{2\bar{T}}}+\frac{\delta+\varphi(\eta,1/x)}{\bar{T}ch^2\dfrac{\delta+\varphi(\eta,1/x)}{2\bar{T}}}\right]\right\}; \tag{17}$$

$$n = \left\{\int_0^1 \frac{K^2(x)xdx}{\varphi(\eta,x)}\left[\frac{1}{1+exp\dfrac{\delta-\varphi(\eta,x)}{\bar{T}}}+\frac{1}{1+exp\dfrac{\delta+\varphi(\eta,x)}{\bar{T}}}\right]+\right.$$
$$\left.+\int_{\frac{2\sqrt{\eta}}{1+\eta}}^1 \frac{K(x)dx}{x^2\varphi(\eta,1/x)}\left[\frac{1}{1+exp\dfrac{\delta-\varphi(\eta,1/x)}{\bar{T}}}+\frac{1}{1+exp\dfrac{\delta+\varphi(\eta,1/x)}{\bar{T}}}\right]\right\}\times$$
$$\times\left\{\int_0^1 \frac{K(x)dx}{\varphi(\eta,x)}+\int_{\frac{2\sqrt{\eta}}{1+\eta}}^1 \frac{K(x)dx}{x^2\varphi(\eta,1/x)}\right\}^{-1}. \tag{18}$$

where

$$\delta = \frac{\varepsilon_1-\mu}{W_1}\ ; \qquad \bar{T} = \frac{k_Б T}{W_1}; \quad \frac{W_2}{W_1} = \eta \le 1;$$
$$\varphi(\eta,x) = \sqrt{(1+\eta)^2 - 4\eta x^2};\ |D(\varepsilon)|_{av}^2 = D = const. \tag{19}$$

The system of equations (16)–(17) describes the temperature dependence of the quantities in question: thermoelectric coefficient α and electric resistivity ρ. In the presented form, this system of equations is more convenient for numerical calculations.

4. Numerical calculations and discussion of the results

Note that electron state density $g(\varepsilon)$ plays an important role in the obtained formulas. Expression (7) can be transformed into the form:

$$\frac{g(\varepsilon)}{g_0} = \frac{\theta(1+\eta)^2 - \lambda^2}{\sqrt{\eta}} \left\{ \theta\ (\lambda^2 - (\eta-1)^2)\, K(k) + \frac{\Theta((\eta-1)^2 - \lambda^2)}{k} K\left(\frac{1}{k}\right) \right\}, \qquad (20)$$

where

$$\lambda = \frac{\varepsilon}{W_1},\quad K = \frac{\sqrt{(1+\eta)^2 - \lambda^2}}{(2\sqrt{\eta})},\quad \eta = \frac{W_1}{W_2}, \qquad (21)$$

The dependence of $g(\varepsilon)/g_0$ on λ for different values of parameter η is given in Fig. 1. The calculations were conducted on the base of formula (20), which requires the consideration of logarithmic peculiarity of the elliptic function $K(k)$ [11]. This approach in the calculation of electron state density is adequate and can be used for the calculation of the kinetic coefficients of quasi two-dimensional systems. This conclusion results from the comparison of Fig. 1 with the results obtained earlier [13], where the elliptic function was calculated precisely.

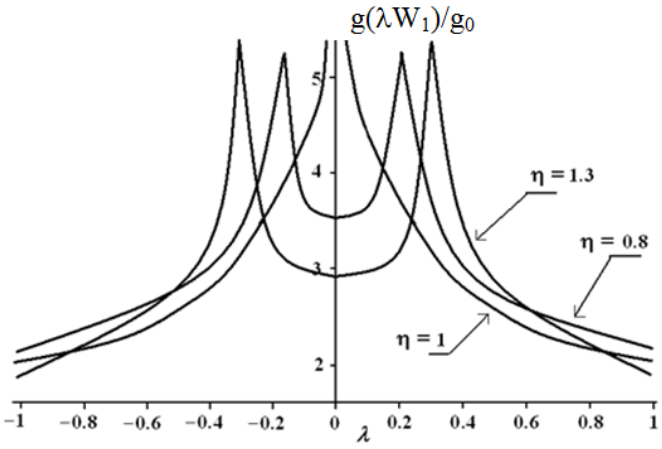

Fig. 1. Electron states density $g(\varepsilon)$ as function of $\lambda = \varepsilon/W_1$ in the approach taking into account the logarithmic peculiarity of function $K(\kappa)$.

According to this, the values of theory parameters play an important role, especially, the energy band width. The examined compounds based on *FeAs* are metals; at the first sight, the energy bands cannot be narrow. However, there is a lot of works stating that the energy bands are narrow at strong and medium electron correlation (see [2]).

The question about the role of inter-electron correlations in the new superconductors remains debatable. The most probable is that the correlations in these systems are intermediary between typical metals and Mott-type dielectrics. Thus, we deal with the state of a correlated metal. Here, we examine a simple model of strong electron interaction in a layered system. However, this approach does not forbid us to consider the band width taking into account these correlations. As was specified above, this band width can be very narrow in the new *FeAs* materials.

The calculations of quantities α and ρ are performed based on the system of equations (11)−(19) within the above mentioned approach for electron state density, which has a peak on the Fermi surface and narrow energy bands.

The temperature dependence of thermoelectric coefficient α and electrical resistivity ρ are presented in Figs. 2a and 2b, respectively. The theoretical dependences are shown by continuous lines, and the experimental data for the $YBa_2Cu_3O_4$ compound are shown by small circles and shaded numbers. Theory parameters n and η are chosen so that the theoretical and the experimental dependences gave qualitative conformity. Case 1a (the dependence of α on T) corresponds to cases (1,1′), (2,2′), and (4,4′).

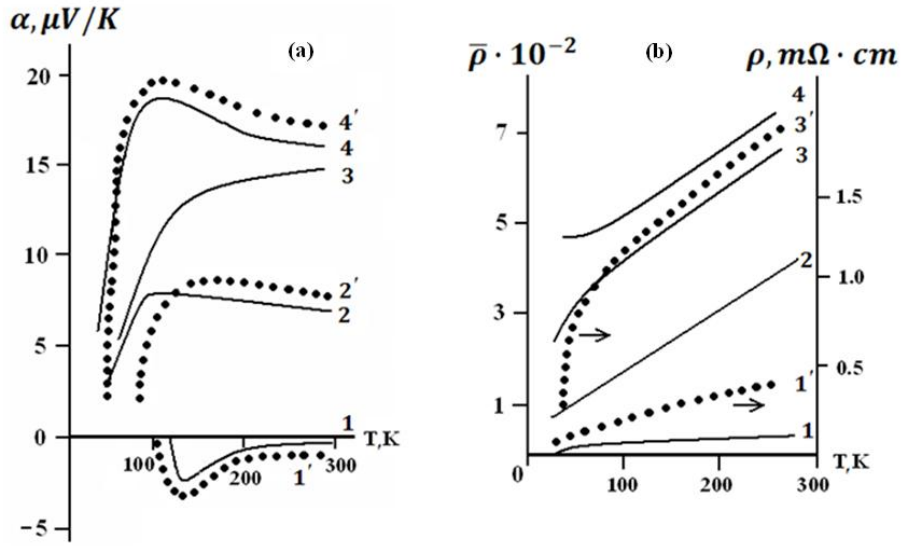

Fig. 2. Temperature dependence of (a) thermoelectric coefficient α and (b) electrical resistivity ρ. Continuous and dashed curves correspond to theoretical results and experimental data, respectively. Case (a): continuous curves *1−4* correspond to parameters $n = 0.513$, $\eta = 0.9$, $n = 0.481$, $\eta = 0.9$; $n = 0.457$, and $\eta = 0.9$, respectively. Curves *1′* and *2′* denote the experimental data for $YBa_2Cu_3O_x$ with oxygen content $x = 7.02$; $x = 6.88$ [7]; curve *4′* stands for $x = 5.34$ [6]. Case (b): curves *1−4* stand for parameter $n = 0.499$ and various values of $\eta = 1, 0.9, 0.4, 0.6$, respectively. Curves *1′* and *3′* denote the experimental data for $x = 0.12$ and $x = 0.53$, respectively [6].

Hereinafter, the values of theory parameters n and η and the content of oxygen or the impurity in the examined compounds [6, 7, 22, 23] are given in the explanations to the figures. Figure 2b shows quantities ρ and $\bar{\rho}$ as a function of temperature. The curves are marked similarly to the ones from Fig. 2a. Here, we emphasize the conformity of our theoretical results with the experimental data on compound YBa_2Cu_3Ox (*1, 1′)* and (*3, 3′*).

Thus, for both quantities $\alpha(T)$ and $\rho(T)$ we have qualitative conformity between the theory developed by us and experimental data. We emphasize that this conformity takes place in the case of narrow energy bands $(W_1 \sim 0.08\ eV)$. Note that the same order of band width was chosen

in [5−7], where the abnormal behavior of kinetic coefficients is explained on the basis of a phenomenological model with a peak in the electron state density of unknown origin.

As follows from Fig. 2a and 2b, the temperature dependence of coefficients α and ρ is quite various and defined by the values of chemical potential (filling degree numbers n) and parameter $\eta = W_2/W_1$. Thermoelectric factor α rapidly increases and forms a maximum in the region of low temperatures and slowly decreases as the temperature increases. Resistivity $\bar{\rho}$ linearly increases with increasing temperature.

The temperature dependences of thermoelectric coefficient α and electrical resistivity ρ are shown in Figs. 3a and 3b. In this case, the values of theory parameters n and η are different from the ones in Figs. 2a and 2b. This was done in order to describe the behavior of these quantities in the case of new materials based on *FeAs*. Dependence $\alpha(T)$ in the case of compound $Ba(Fe_{1-x}Co_x)As_2$ is given in Fig. 3a, and the dependence of $\bar{\rho}$ on T is given in Fig. 3b for the same compound.

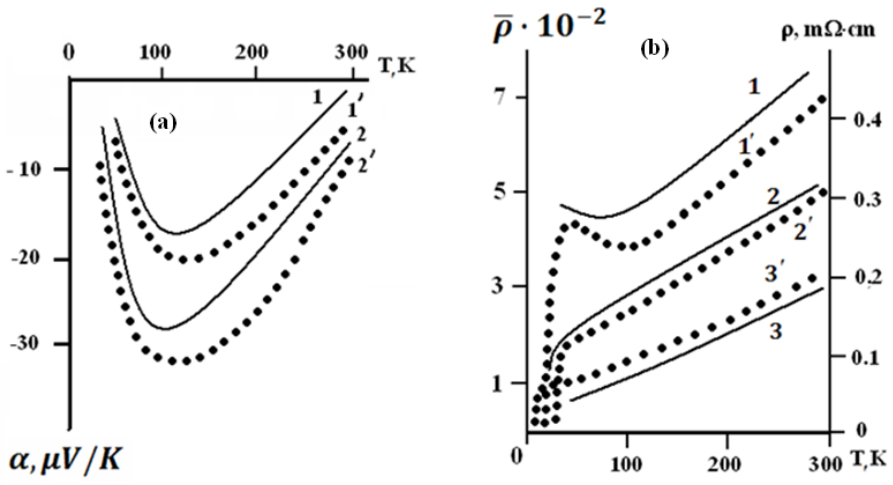

Fig. 3. (a) Temperature dependence of thermoelectric coefficient α: curve *1* corresponds to *n=0. 523, η=0.9*, curve *2*, to *n=0.545, η=0.9*. Curves *1′* and *2′* correspond to the experimental data for compound $Ba(Fe_{1-x}Co_x)As_2$ at $x = 0.4$ and $x = 0.3$ respectively [22]. (b) Temperature dependence of electric resistivity ρ: curves *1−3* are for parameter $n = 0.499$ and various values of η (η*=0.38, 0.7, and 0.85,* respectively). Curves *1′–3′* correspond to the experimental data for $Ba(Fe_{1-x}Co_x)As_2$ at *x=0.06, 0.08,* and *0.15*, respectively [23].

Figures 3a and 3b show a quality coincidence of the proposed theory with the experimental data for both $\alpha(T)$ and $\rho(T)$. In the two figures, we have the following compliance: (*1*, *1′*), (*2*, *2′*), (*3*, *3′*). As in the case of cuprates, this consistency between theory and experiment takes places in the presence of narrow energy bands. We emphasize that, in the case of a more careful selection of theory parameters, it is possible to achieve closer values for theoretical and experimental dependences for the examined quantities α and ρ.

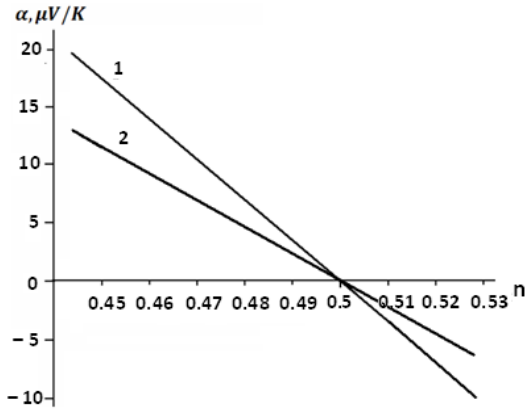

Fig. 4. Dependence of thermoelectric coefficient α on the degree of filling of the energy band (n). Curve *1* corresponds to $\eta = 1$ *and* $T = 120$ *K*; curve *2*, to $\eta = 0.8$ and $T = 140$ *K*.

5. Conclusions

(i) Based on the Mott–Davis theory of electron processes in disordered quasi two-dimensional systems, the experimentally observed behavior of electrical resistance $\rho(T)$ and thermoelectric coefficient $\alpha(T)$ can be described qualitatively owing to the existence of a peak in the electron state density and narrow energy bands in quasi two-dimensional systems, as observed earlier in cuprates and recently in compounds based on *FeAs* [2].

(ii) The nature of the temperature dependence of thermoelectric coefficient α and electrical resistance ρ is quite various and determined by the value of chemical potential (parameter n, which defines the degree of filling of the energy band) and the parameter of the anisotropy of energy spectrum $\eta = W_1/W_2$. Selecting these parameters in a proper way we can achieve consistency between theoretical dependences $\alpha(T)$ and $\rho(T)$ and the experimental data. Based on the application of theory [10] to quasi two-dimensional systems, the behavior of quantities α and ρ in cuprates and in new *FeAs* materials is described using the example of $YBa_2Cu_3O_x$ and $Ba(Fe_{1-x}Co_x)As_2$.

(iii) The above results suggest that the proposed model allows qualitatively describing the behavior of kinetic coefficients α and ρ as a function of temperature in a normal phase of quasi-two-dimensional systems, such as high-temperature copper materials and compounds based on FeAs. Thus, it is important to consider the existence of peaks in the density of electronic states characteristic of these systems and narrowness of the energy bands. In our opinion, there is no need to artificially introduce the existence of a peak in the density of electronic states (as it occurs in [5−7]). The variation in parameters n and η has a more essential impact on $\alpha(T)$ than on $\rho(T)$. In particular, we obtain $\alpha(T) > 0$ for all temperatures $0 < T < 300$ *K* at $n < 0.5$ and $\alpha(T) > 0$ at $n > 0.5$ (Fig. 4). As noted earlier, in the above calculations we assume that the energy bands are very narrow due to strong and medium electron correlations. However, the question about the energy band width in the materials based on *FeAs* remains debatable. We believe that these materials with a medium electron correlation are close to the state of Mott dielectrics and this fact makes them similar to HTSC cuprates [24].

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