ON POSSIBLE SCALING OF THE NORMAL-STATE IN-PLANE RESISTIVITY AND ASPECTS OF THE PSEUDO-GAP PROBLEM IN $Ba(Fe_{1-x}Co_x)As_2$

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Abstract

The zero field in-plane normal-state resistivity of the $Ba(Fe_{1-x}Co_x)As_2$ (x = 0.0–0.3) single crystal above T_c can be reproduced among other possibilities by a very simple expression $\rho(T) = \rho_0 + aT \exp\left(-\frac{2\Delta}{T}\right)$ and scaled thereby using the temperature independent energy scale Δ, resistivity ρ_Δ, and residual resistivity ρ_0 as scaling parameters (E. Arushanov, *et. al.* Supercond. Sci. Technol., 24, 105004 (2011)). We show that this Δ is related to the inflection point T_{ip} of $d\rho/dT$, $\Delta/T_{ip} = 1.5$.

1. Introduction

Recently, transition-metal oxypnictides composed by an alternate stacking of Ln_2O_2 layers and T_2Pn_2 layers (Ln:La, Pr, Ce, Sm, Nd; T: Fe, Co, Ni, Ru; Pn: P or As) have been identified as novel high-T_c materials [1–5]. The discovery of superconducting transition temperatures up to T_c = 26 K in $LaFeAsO_{1-x}F_x$ with x = 0.11 [1] with a primitive tetragonal ZrCuSiAs-type (1111-type) structure has captured the imaginations of physicists and chemists worldwide. It has been found that the replacement of the nonmagnetic La by magnetic rare earth elements substantially increases T_c to its current record of 56.3 K [6] for this structure class. Subsequent works have led to the identification of superconductors with similar FeAs layers in the body-centered-tetragonal ThCr2Si$_2$-type (122-type) structure. To date, the maximum T_c value achieved for this structure class is 38 K for $Ba_{0.6}K_{0.4}Fe_2As_2$ [7].

Attention has largely shifted from the 1111 to the 122- and 11-type compounds, even though they have lower T_c, mainly because of the possibility of growing large single crystals of the latter compounds providing more definitive characterizations of the properties, especially by neutron scattering [5].

The electronic phase diagrams of $Ba(Fe_{1-x}Co_x)As_2$ (x = 0.0–0.3) pnictide superconductors in the normal state based on the analysis of electrical resistivity have been reported for a wide range of doping [8–10]. Despite the similarity of the phase diagrams of cuprates and iron based pnictides, it has been well established that the underlying physics of these compounds is different. Cuprates are doped charge transfer insulators with properties tightly related to strong

electron correlations, while iron pnictides are less correlated metallic systems with a spin density wave (SDW) state at low doping [9] for most of the so-called parent compounds under certain circumstances (ignoring special pressure or strain effects as well as the special case of the so-called codoping of electrons and holes). All $Ba(Fe_{1-x}Co_x)As_2$ phase diagrams [8-10] show an asymmetric shape of the superconducting dome with, however, some difference in compositions corresponding to maximum T_c and to the phase boundary (T_c vanishes at $x \leq 0.16$ [9] or at $x \leq 0.18–0.2$ [8, 10]). Thus, the shape of the superconducting dome is really different from that of the cuprates.

It has been shown that the temperature-dependent resistivity $\rho(T)$ of several members of the iron-pnictide superconductor family including $Ba(Fe_{1-x}Co_x)As_2$ can be scaled using energy scale Δ, resistivity ρ_Δ, and residual resistivity ρ_0 as scaling parameters [11–16]. In this study, based on our previous $Ba(Fe_{1-x}Co_x)As_2$ scaling data [13, 14], we show that Δ is related to inflection point T_{ip} of $d\rho/dT$, namely, $\Delta/T_{ip} = 1.5$ and $T_{sdw} \sim T_{ip}$ in the underdoped regime.

2. Results and discussion

The scaling behavior of the normal state resistivity for $Ba(Fe_{1-x}Co_x)As_2$ (x = 0.00–0.30) was analyzed using the scaling methods reported in [17–19] and experimental data presented in [9, 10]. Using the following astonishing simple expression for the scaling function of ρ

$$\rho(T) = \rho_0 + aT \exp\left(-\frac{2\Delta}{T}\right), \quad (1)$$

(where ρ_0 is the residual resistivity and 2Δ defines the energy scale controlling the linear and superlinear behavior) proposed by Moshchalkov [17] we have obtained a good fit for $\rho(T)$ of $Ba(Fe_{1-x}Co_x)As_2$ samples with x ranging from 0.0 to 0.3 in a broad temperature region (see Fig. 1) and the obtained nearly "universal" scaling-law for

$$r(t) = (\rho-\rho_o)/(\rho_\Delta-\rho_o) \quad \text{with} \quad t = T/2\Delta, \quad (2)$$

for all Co concentrations (see Fig. 2, note that ρ_Δ is the resistivity at $t = 1$, i.e. at $T = 2\Delta$).

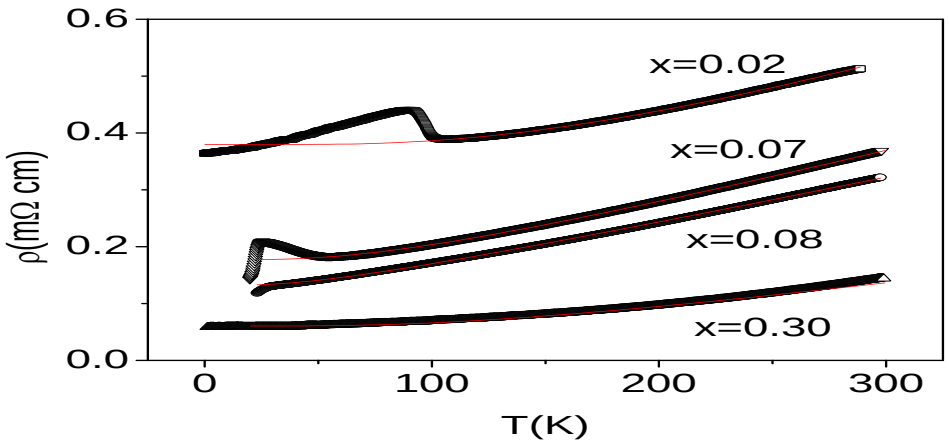

Fig. 1. Temperature dependence of resistivity for $Ba(Fe_{1-x}Co_x)_2As_2$ (x = 0.02, 0.075, and 0.30). The solid lines represent a fit using Eq. (1) (the figure is taken from [13]).

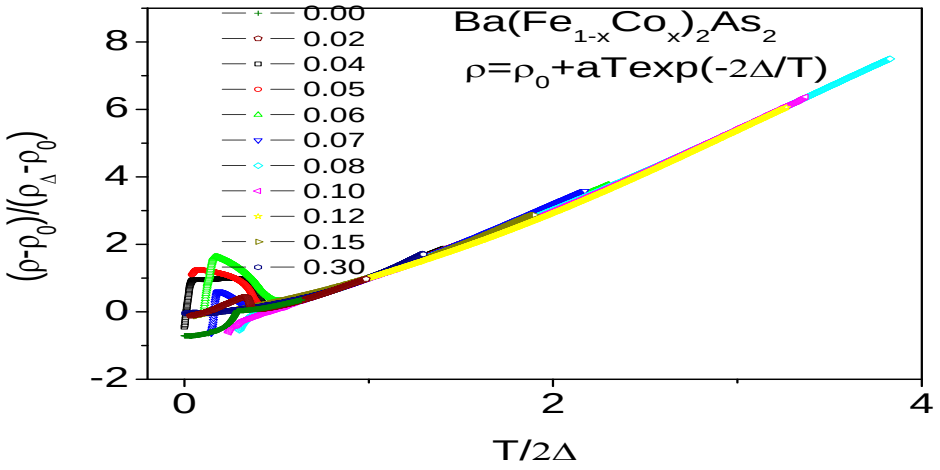

Fig. 2. Scaling analysis on the temperature dependence of the resistivity of various $Ba(Fe_{1-x}Co_x)_2As_2$ samples ($0 \le x \le 0.3$). The temperature is rescaled with Δ (an energy scale) and the resistivity is given by $\frac{\rho - \rho_0}{\rho_\Delta - \rho_0}$ in which the extrapolated residual resistivity ρ_0 has been subtracted and ρ_Δ is the resistivity at $T = 2\Delta$. (the figure is taken from [13]).

Thereby adopting the validity of Eq. (1), one arrives approximately at a "universal" quasi-linear "scaling" function for a wide temperature region of $1.5 < t < 7$, if the off-set --1.8 is ignored:

$$r(t) = t \exp(1-1/t) \approx -1.8 + 2.6\, t\,, \qquad (3)$$

(see also Fig. 2). Empirically, we obtained a slightly different expression:

$$r(t) \approx -1.8 + 2.426\, t\,. \qquad (4)$$

Thus, the two material and sample dependent parameters ρ_0 and a that still appear in Eq. (1) are almost eliminated in Eqs. (3) and (4).

It should be noted that, in many cases, an alternative power-law fit

$$\rho(T) = \rho_o + AT + BT^2\,, \qquad (5)$$

including both a non-Fermi liquid linear term and a standard Fermi-liquid quadratic temperature term due to electron–electron interaction applied in [26] yields although a slightly worse but, in principle, quite similar accuracy compared to Eq. (1). In [26], this behavior was dubbed as an argument for a "lacking" pseudo-gap. Anyhow, the weak point of both approaches ((1) and (5)) is the broad temperature region up to $T = 300$ K and above included in the fit because this way the improper inclusion of a region above T^* into the fit might strongly affect/falsify the analysis. This is especially dangerous in the overdoped region where the pseudo-gap phase is believed to vanish. Therefore, rigorously speaking, both approaches should be considered simply as a more or less convenient formal description of available resistivity data including only a few parameters.

Within a consequent microscopic description of a pseudo-gap scenario, one would expect a dominant contribution to the total conductivity by the non-gapped fraction of "normal" quasi-particles and a strongly temperature dependent one from the pseudo-gapped subsystem. Then, for a monotonously increasing or constant pseudo-gap at low-temperatures, the observed (fitted) residual and low-temperature resistivity should be determined, at first glance, only by the

"normal" quasi-particles. (In case of a non-Fermi liquid for the "normal" subsystem, the situation becomes even more unclear with respect to the origin of ρ_0 !). In this context, the success of both expressions is very surprising. Alternatively, the total conductivity should be determined by a small number of highly mobile quasi-particles in the pseudo-gap phase. To the best of our knowledge, a similar situation can take place only in an anisotropic nodal gapped phase.

The obtained 2Δ values presented in Table 1 show a minimum at about $x = 0.07–0.08$ which corresponds to the highest T_c value, a strong enhancement with x decreasing down to 0, and a weaker one with increasing x in the optimal doped–overdoped regimes ($x = 0.08–0.3$). It should be noted that, in the underdoped regime, the characteristic energy Δ almost linearly drops with increasing doping [13]. A similar variation of Δ and/or the characteristic temperature is observed in $YBa_2Cu_3O_x$ [17] and $La_{2-x}Sr_xCuO_4$ [20] as well as in other members of the cuprate family (see, e.g., Fig. 11 in [19]); this is qualitatively consistent with the doping dependence of their pseudo-gap-values reported in the interpretations of ARPES, tunnelling, and other measurements [19]. In general, pseudogap related features have attracted considerable attention for several unconventional superconductors and correlated compounds including also reports for several iron pnictide superconductors studied by various experimental techniques, such as Knight-shift, anisotropic transport, NMR, and ARPES. Qualitatively, the pseudo-gap is generally understood as a partial gapping of the Fermi surface, while other parts remain metallic.

Table 1. Scaling parameter Δ and deflection temperature T_{ip} for $Ba(Fe_{1-x}Co_x)_2As_2$ derived from the resistance and superconducting transition temperatures T_c data reported by Rollier-Albenque et al. [9] and Fang et al. [10] . Superconducting transition temperatures T_c are also taken from [9, 10]

$Ba(Fe_{1-x}Co_x)_2As_2$ [10]	2Δ (K)	T_c (K)	T_{ip} (K)	$Ba(Fe_{1-x}Co_x)_2As_2$ [9]	2Δ (K)	T_c (K)	T_{ip} (K)
$x = 0.00$	469	-	156.3	$x = 0$	450		128.3
$x = 0.02$	303	-	101	$x = 0.014$	326		108.7
$x = 0.04$	212	8	70.7	$x = 0.02$	289		96.3
$x = 0.05$	195	11	65	$x = 0.03$	223	2	74.3
$x = 0.06$	130	19	43.3	$x = 0.04$	173	8	57.7
$x = 0.07$	137	22.5	45,7	$x = 0.045$	157	12	52.2
$x = 0.08$	78	25	26	$x = 0.055$	134	19	44.7
$x = 0.10$	89	24	29.7	$x = 0.06$	106	21	35.3
$x = 0.12$	92	20	30.7	$x = 0.07$	72	25	23.9
$x = 0.15$	156	11	52	$x = 0.08$	70	23	23.3
$x = 0.30$	231		77	$x = 0.12$	101	16	33.6
				$x = 0.14$	125	11	
				$x = 0.20$	208		69.3

Thus, the electronic density of states at the Fermi level decreases at low temperatures. However, on a quantitative level, there is a considerable scattering for various methods; in particular, this concerns energy scale Δ or 2Δ introduced above for the scaling of the resistivity

(see also some remarks given below). However, in spite of a still missing proper microscopic understanding, there are several serious physical problems related to the pseudo-gap even on a phenomenological level. If the pseudo-gap characterizes the order parameter of a special thermodynamic phase competing or sometimes coexisting with superconductivity, there should be a sizable temperature dependence at least in the vicinity of the corresponding phase boundary, in particular, at least close to its onset temperature usually denoted as T^*. In cases of anisotropic pseudo-gaps, phases with nodes, such a temperature dependence, cannot be ignored at all! Only in isotropic nodeless cases at $T << T^*$, this scenario might be meaningful for the interpretation of experimental data. For a first estimate, ignoring strong coupling effects, the evaluation of T^* by adopting the well-known BCS-relation $2\Delta = 3.52\ k_B T^*$ might be useful. Thus, for a derived pseudo-gap as small as 100 K, only a low-temperature fit of any quantity below 50 K makes sense. In the following, we will adopt this isotropic and temperature independent scenario for the sake of simplicity. A detailed comparison with other approaches and analysis of other physical properties will be given elsewhere. Thereby, it should be borne in mind that, starting from a semi-microscopic model for the pseudo-gapped and remaining unaffected electrons at the complex Fermi surfaces, one will come up with different pseudo-gap values because the weight of each point at the Fermi surface is certainly different for different physical properties affected, for instance, in the case of transport properties by the local Fermi velocities and the impurity dependent intra- and interband scattering rates. All these subtle points are ignored in a formal comparison of different measurements without adopting a certain microscopic model for the underlying multiband electronic structure.

It should be noted that, in cuprates, both Δ and scaling parameter T^* show a strong decrease with increasing x in the underdoped regime [18, 20] and almost constant values in overdoped regime ($La_{2-x}Sr_x CuO_4$, x = 0.22–0.34) [20]. The observed compositional dependence of Δ in $Ba(Fe_{1-x}Co_x)As_2$ (x = 0.0–0.3) in the overdoped regime is different from that reported for cuprates.

The first and second derivatives of the temperature dependence of resistivity for the $Ba(Fe_{1-x}Co_x)As_2$ system reported by Rullier-Albenque et al. [9] and Fang et al. [10] were analyzed, and the value of inflection point T_{ip} for $d\rho/dT$ was determined (see Fig. 3 and Table 1).

It is shown in Fig. 3 for a representative $\rho(T)$ curve that inflection point T_{ip} for $d\rho/dT$ is closely related to Δ, namely, Δ/T_{ip} =1.5 for that scaling function $\rho(T)$ (Eq. 1). It is noteworthy that, in a formal sense, this is close to the well-known prediction of the BCS theory: Δ/T^*=1.76, where the superconducting gap and the transition temperature have been replaced by their pseudo-gap related counter parts. To avoid possible misunderstandings, we emphasize that, in the present context, there is no direct and obvious relation of the former to the corresponding "real" superconducting gap and/or the superconducting transition temperature T_c for the compounds under examination. The $Ba(Fe_{1-x}Co_x)As_2$ phase diagram is presented in Fig. 4.

We can see a reasonable correlation between the T_{SDW} values reported in [10] and our T_{ip} data with $T_{sdw} \sim T_{ip.}$in the underdoped regime. According to [21], the Ba-, Sr-, and Ca-122 magnetic parent compounds with $2\Delta_{SDW}/T_N \approx 5.3$, 8.7, and even 12 exhibit large deviations from the BCS relation as observed in recent optical measurements. In our opinion, this observation indicates the importance of strong coupling and retardation effects well beyond the validity of a weak coupling BCS-type description. The above suggests that, within our approach, a connection between the magnetic SDW-gap and the pseudo-gap is unlikely and/or the inflection point temperature T_{ip} mentioned above might be of some other origin.

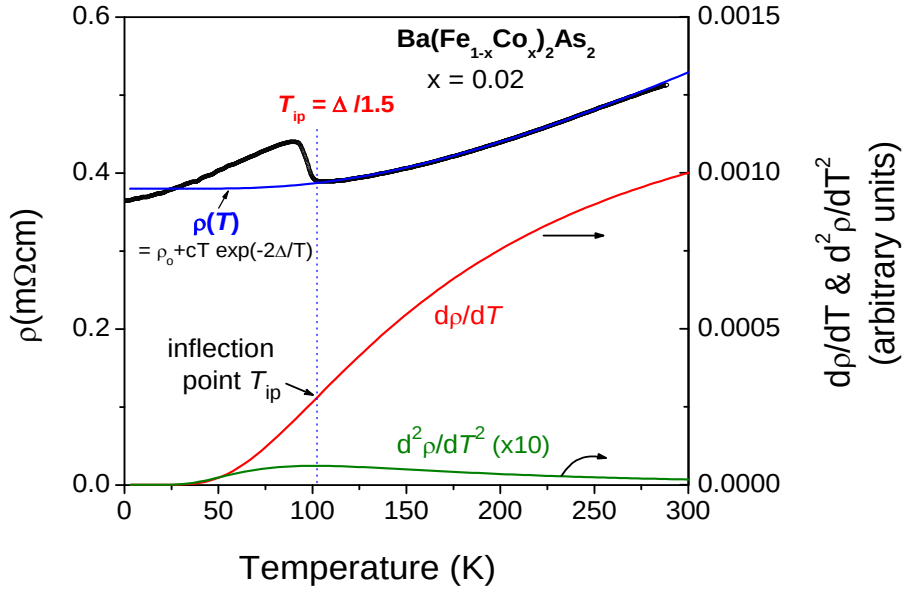

Fig. 3. Temperature dependence of the resistivity of $Ba(Fe_{1-x}Co_x)_2As_2$ for x = 0.02 (black solid line). The data were fitted by $\rho(T)$ according to Eq. (1) (blue line). The first derivative $d\rho/dT$ (red line) with the inflection point at $T = T_{ip}$ and $d^2\rho/dT^2$ (green line) which is 10 times magnified are shown.

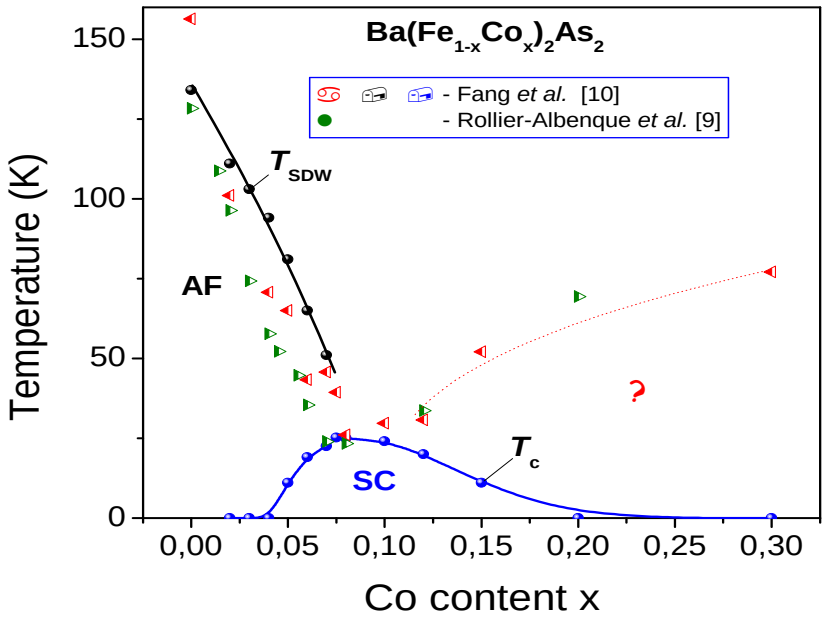

Fig. 4. Phase diagram of $Ba(Fe_{1-x}Co_x)_2As_2$ systems ($0 \le x \le 0.3$). The T_{ip} values were calculated using the resistivity data reported by Rullier-Albenque et al. [9] and Fang et al. [10]. The T_{sdw} and T_c values were taken from [10].

Following [22], we could say that our observation of a doping independent scaling law in the normal state of pnictide superconductors could be probably used as an indication that a pseudogap-like behavior is the reason for a predominant energy scale which controls the low energy excitations. The possible existence of a pseudo-gap in $LaO_{1-x}F_xFeAs$ and $SmFeAsO_{1-x}F_x$ compounds has been reported by Liu et al. [23], Jia et al. [24], and Ou et al. [25] on the base of high resolution photoemission measurements as well as for isomorphic $Ca(Fe_{1-x}Co_x)As_2$ [27] on the basis of NQR measurements with the electric field gradient along the *c*-axis. The reported pseudogap for $x = 0$ .063 of (88 ± 6) K is comparable with that for $x = 0.08$ and 0.1 for the Ba counter part (see Table 1) with the data of [10] and $x = 0.07$ of [9]. However, the temperature dependent spin-latice relaxation rate $1/T_1T$ cannot be attributed to an isotropic pseudo-gap. For the isovalently doped $BaFe_2(As_{0.45}P_{0.55})_2$ system [28], a similar value has been reported. However, at variance with our analysis, nothing could be observed in the overdoped regions. A pseudo-gap like behavior has been also derived from NMR spin relaxation rates and Co Knight-shift as well as for interlayer resistivity measurements for $Ba(Fe_{1-x}Co_x)As_2$ [26] but not for the intralayer one. For completeness, note that no pseudo-gap behavior could be derived from STM-measurements for the title compounds [29]. This lacking observation might be ascribed to specific surface properties, whereas bulk sensitive specific heat data for $Ba(Fe_{1-x}Co_x)As_2$ for the linear electronic specific heat (Sommerfeld coefficient) [30] are in conflict by a factor of two with the presence of both usual high-energy and low-energy mass renormalizations and compatible with a reduced electronic density of states which might be caused by a pseudo-gap for a subgroup of electrons. Similar problems for the empirical mass enhancement arise also for overdoped $BaFe_2(As_{0.45}P_{0.55})_2$ samples if the pure band mass scaling shown in Fig. 5 of [31] is adopted. In the context of the transport data reported here, one might suppose that only a subgroup of fast electrons is mainly affected by the pseudo-gap. Comparison of the Δ values for the two samples shown in Table 1 reveals some scattering for the latter. This might be ascribed to different amounts of disorder. Therefore, a systematic study of possible correlations and the amount of disorder as measured by the residual resistivity is of considerable general interest for the elucidation of the microscopic mechanism behind the pseudo-gap.

The microscopic interpretation of the observed gap-like feature Δ is rather unclear at present. One option in connection with the pseudo-gap-like feature more pronounced in the interlayer direction at a significantly larger energy scale would be given by an extremely anisotropic pseudogap observed by our sensitive scaling method for the first time also in the planar direction. Alternatively, it might be related to a slight misorientation in the studied resistivity data taken from the literature and our scaling method could be used as an additional technique to detect it by measuring an angular-dependent admixed *c*-axis contribution. The presence of an inflection point might be also related to a starting saturation phenomena pointing to a lower limit of the mean free path like in the well-known Joffe-Regel scenario given by the interatomic distance.

Among other possibilities for a pseudo-gap like scenario in general, at least three scenarios are worth studying theoretically in more detail: (i) a long-range Coulomb interaction disorder related feature; (ii) a pairing mechanism related pseudo-gap as discussed for the cuprates, and (iii) a band structure related feature from a band slightly below the Fermi energy whose excitations provide additional charge carriers at higher temperatures. A thermal delocalization of localized electrons would also add charge carriers In general, a corresponding systematic study of other FeAs-based pnictides is of considerable interest and might be useful in discriminating between the proposed scenarios and elucidating the unclear nature of the pseudo-gap.

3. Conclusions

The zero-field normal-state resistivity for various levels of doping for $Ba(Fe_{1-x}Co_x)As_2$ (x = 0.05–0.30) can be scaled onto a single universal curve. Energy scale Δ, resistivity ρ_Δ, and residual resistivity ρ_0 are suitable scaling parameters for $Ba(Fe_{1-x}Co_x)As_2$ (x = 0.05–0.30). The existence of a universal metallic $\rho(T)$ curve is interpreted as an indication of a single mechanism which dominates the scattering of the charge carriers in $Ba(Fe_{1-x}Co_x)As_2$ (x = 0.05–0.30) and/or changes in the number of available charge carriers due to a specific electronic structure. We have shown that Δ is related to inflection point T_{ip} of $d\rho/dT$, Δ/T_{ip}=1.5 with $T_{SDW} \sim T_{ip}$ in the underdoped regime. Further comprehensive studies are required to clarify the microscopic nature of the observed Δ and its possible relation to the pseudo-gap reported in numerous recent studies based on other experimental techniques. Regardless of the final applicability of certain pseudo-gap scenarios to iron pnictides and related compounds, the empirical findings presented in this study are expected to be useful for any sophisticated microscopic description hopefully achieved in the near future.

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