Bulletin of National University of Uzbekistan: Mathematics and Natural Sciences

Volume 1 | Issue 2 Article 2

9-25-2018

Electronic specific-heat anomalies in high-T_c cuprates

S. Dzhumanov
National University of Uzbekistan

E. Karimboev
National University of Uzbekistan, ekarimboev@mail.ru

B. Yavidov
Nukus State Pedagogical Institute

Recommended Citation

Dzhumanov, S.; Karimboev, E.; and Yavidov, B. (2018) "Electronic specific-heat anomalies in high-T_c cuprates," *Bulletin of National University of Uzbekistan: Mathematics and Natural Sciences*: Vol. 1 : Iss. 2 , Article 2.
Available at: https://uzjournals.edu.uz/mns_nuu/vol1/iss2/2

Bulletin of National University of Uzbekistan: Mathematics and Natural Sciences

ELECTRONIC SPECIFIC-HEAT ANOMALIES IN HIGH-T_c CUPRATES

[1]Dzhumanov S., Karimboev E. X.[1], Yavidov B. Ya.[2]
[1]*National University of Uzbekistan, Tashkent, Uzbekistan*
[2]*Nukus State Pedagogical Institute, Nukus, Uzbekistan*
e-mail: `ekarimboev@mail.ru`

Abstract

In this work, we study the electronic specific heat $C_e(T)$ of underdoped to overdoped high-T_c cuprates, and identify the nature of anomalies in $C_e(T)$ at the superconducting transition temperature T_c and at temperatures above T_c. The doped cuprate superconductor is considered as a multi-carrier model system which is composed of different types of charge carriers. The normal-state electronic specific heat $C_n(T)$ of high-T_c cuprates below a characteristic pseudogap (PG) temperature T^* is calculated taking into account three contributions coming from the excited components of Cooper pairs, the ideal Bose-gas of incoherent Cooper pairs and the unpaired carriers in the impurity band. Above T^*, two contributions to $C_n(T)$ coming from the unpaired intrinsic and extrinsic polarons are calculated within the two-component degenerate Fermi-gas model. The total electronic specific heat $C_e(T) = C_n(T) + C_s(T)$ below T_c is calculated by considering the contribution $C_n(T)$ and the contribution $C_s(T)$ coming from the superfluid bosonic carriers. We have shown that our theoretical predictions of the behaviors of $C_e(T)$ near T_c and above T_c are strikingly similar to the behaviors of the electronic specific heat observed below and above T_c in LSCO and YBCO. There is fair quantitative agreement between theoretical predictions about the anomalies in $C_e(T)$ (i.e. a λ-like anomaly near T_c and a BCS-type anomaly above T_c near T^*) and experimental data.

Keywords: cuprate superconductors, polaronic carriers, electronic specific heat properties, λ-like and BCS-like anomalies, pseudogap and impurity effects.

Physics and Astronomy Classification Scheme: 74.00.00

Introduction

The electronic properties of high-T_c cuprate superconductors are fundamentally different from those of conventional superconductors. The normal and superconducting (SC) properties of underdoped to overdoped cuprates are unusual in respect to the behaviors of standard Landau and BCS Fermi liquids [1,2,3,4,5]. Various anomalies observed in the normal state of these materials are thought to arise from a pseudogap (PG) state that, depending on the doping level, is realized below a characteristic temperature $T^* > T_c$ [2,3,4,5]. Understanding of the PG phenomena in underdoped to overdoped cuprates is believed to be the key to the elucidation of the mechanism of high-T_c superconductivity. The origin of the PG state in the cuprates is still controversial.

The important normal state properties of high-T_c cuprates closely related to the mechanism of superconductivity are their thermal properties, which are significantly different from those of conventional superconductors both in the SC state and in the normal state [2,5,6,7,8,9,10]. Measurements of the electronic specific heat $C_e(T)$ in $\mathrm{La_{2-x}Sr_xCuO_4}$ (LSCO) and $\mathrm{Yba_2Cu_3O_{7-\delta}}$ (YBCO) showed a clear λ-like anomaly at T_c [6,7,10], more or less pronounced BCS-type anomalies somewhat above T_c or even well above T_c [6,7,10] and a linear term at low temperatures [11]. It seems more likely that the linear term in the specific heat of cuprate superconductors is not intrinsic property of the SC state in high-T_c cuprates, but due to the presence of some impurity phases [12]. In addition to a clear λ-like anomaly at T_c, the other anomalous feature is the presence of jump-like anomalies above T_c in the specific heat spectrum of high-T_c cuprates [9]. It was assumed [6,11] that the BCS-type anomaly in the normal-state electronic specific heat $C_n(T)$ of the cuprate superconductors is manifested above T_c. Nevertheless, some researchers attributed the observed specific heat jump in high-T_c cuprates above T_c to some kind of phase transition other than the BCS-type phase transition or just simply ignored it. It is often misinterpreted that the λ-like anomaly in $C_n(T)$ at T_c is the BCS-type jump of the specific heat. Actually, a λ-like SC transition in cuprate superconductors occurring at T_c is quite different from a BCS-type transition corresponding to the formation of Cooper pairs above T_c. Various theoretical models have been proposed to explain the puzzling features of high-T_c cuprates (see, e.g., Refs. [2,6,7,9,10,11,12,13]). But in judging the relevance of these approaches to the problem of high-T_c cuprates, one should consider their compatibility with the observed specific heat properties of underdoped to overdoped cuprates. Many of the existing theories are not capable of accounting for the full body of experimental data. So far, the origins of the electronic specific-heat anomalies in high-T_c cuprates have not been fully understood. Many experiments indicate (see Refs. [14,15,16]) that unconventional electron-phonon interactions (including polaronic effects) may be involved in the PG phenomenon and high-T_c superconductivity in the cuprates. Another distinctive property of cuprate superconductors is that they are doped materials and the expected jumps of $C_e(T)$ at the λ-like SC transition near T_c and of $C_n(T)$ at transitions near T^* may be strongly influenced by the impurity phase and electronic inhomogeneities. Therefore, there is considerable motivation to explore the effects of these phase transitions on the electronic specific heat of underdoped to overdoped cuprates taking into account possible charge inhomogeneity and impurity effects.

In this work, we study the specific heat properties of high-T_c cuprates in the normal and SC states. We argue that the relevant charge carriers in doped cuprates are large polarons residing in the polaronic an impurity bands. We describe the underlying pairing mechanism leading to the formation of the BCS-like PG in high-T_c cuprates. The normal-state specific heat $C_n(T)$ of the LSCO and YBCO compounds below the PG formation temperature T^* is calculated by considering three contributions from the excited components of polaronic Cooper pairs, the ideal Bose-gas of incoherent (non-SC) Cooper pairs and the unpaired carriers bound to impurities. The total electronic specific heat $C_e(T)$ below T_c is calculated by considering the contribution $C_s(T)$ coming from the superfluid (SF) bosonic carrier (polaronic Cooper pairs) and the contribution $C_n(T)$. Numerical results obtained for $C_n(T)$ above T_c and for

$C_e(T)$ below T_c are compared with experimental data. For all cases considered, good quantitative agreement is found between theory and experiment.

1 Polaronic carriers, impurity centers and inherent electronic inhomogeneities

The strong electron correlations play a dominating role only in undoped cuprates and drive these systems into a charge-transfer (CT)-type Mott insulating state [17,18]. Upon hole doping, the oxygen valence band of these anisotropic three-dimensional cuprates is occupied by free holes. As the doping level is increased towards the underdoped level, the doped cuprates become unusual metals (above T_c) or superconductors (below T_c) and the importance of electron correlations diminishes [18,19,20] and other factors will dominate in these systems. The high-T_c cuprates are doped polar materials where the electron-phonon interactions are expected to be sufficiently strong and unconventional. The strong electron-phonon interactions in these materials are responsible for the self-trapping and pairing of charge carriers. Actually, in the intermediate and strong electron-phonon coupling regimes, the charge carriers are dressed by the static lattice distortions (i.e. static phonons) and these dressed carriers are polarons [21,22].

The polaronic nature of charge carriers is believed to be very important for the understanding of the anomalous electronic properties of doped high-T_c cuprates. Further, the inhomogeneous nature of these materials is another important feature and the intrinsic inhomogeneities of the charge carrier distribution are responsible for the charge segregation, which may manifest itself via local phase separation [18,20]. In cuprates the doping process inevitably introduces disorder (i.e. inhomogeneity) in the spatial distribution of dopants and charge carriers. It seems likely that the inhomogeneous spatial distribution of doped charge carriers occurs over the main CuO_2 layers (with nonzero thickness) and the impurity centers between these CuO_2 layers. It turns out that the carrier concentration is slightly higher in the outer CuO_2 layers than in the inner one and the hole distribution in some layered cuprates was highly inhomogeneous with only $\sim 10\%$ of holes in the inner CuO_2 layers (see Ref. [23]). However, the disbalance in the distribution of doped carriers among two different regions, namely, impurity-free regions (e.g., CuO_2 layers) and impurity sites may be opposite, depending on the material and doping levels. The charge carriers being placed in a polar crystal will interact both with lattice vibrations (i.e., acoustic and optical phonons) and lattice defects (e.g., dopants and impurities). Therefore, the ground states of the doped hole carriers are their intrinsic and extrinsic self-trapped (polaronic) states lying in the CT gap of the cuprates [20]. Experimental [14,22,23,24] studies show that the electron-phonon interaction is responsible for the enhanced polaron masses $m_p = (2-3)m_e$ [14,24,25] (where m_e is the free electron mass). At some doping levels the intrinsic and extrinsic large polarons can be considered as a two-component degenerate Fermi-gas. For these polaronic carriers, the degeneracy conditions $W_p >> k_BT$ and $W_I >> k_BT$ are well satisfied, where W_p and W_I are the band widths of intrinsic and extrinsic polarons, respectively. The normal state Cooper pairing of large intrinsic polarons is expected in the intermediate coupling regime and the formation of incoherent bosonic Cooper pairs becomes possible at $T^* > T_c$ in the CuO_2 layers of the cuprates. It is natural to believe that the relevant charge carriers in doped cuprates are large intrinsic polarons and preformed bosonic Cooper pairs in the CuO_2 layers and large extrinsic polarons lying between the CuO_2 layers. In fact, the doped cuprates may be viewed as a mixture of different phases and the electronic properties of these compounds are better described in terms of a multi-carrier model. One can expect that the BCS-like pairing PG, impurity phase and electronic inhomogeneity strongly affect the normal-state electronic specific heat properties of underdoped to overdoped cuprates.

2 The BCS-type Cooper pairing of carriers above T_c

It is believed that the high-T_c cuprates fall in strong and intermediate electron-phonon coupling regimes, where the polaronic effects seem to be important and the standard BCS pairing theory describing the formation of Cooper pairs at the SC transition temperature T_c does not work. Therefore, the BCS pairing theory should be modified to include polaronic effects. Actually, the BCS-based theory can be also extended to the cases of the interacting polaronic Fermi gases. In these cases, the BCS-type Cooper pairing of polaronic carriers (i.e. the carriers dressed by the static lattice distortions within the CuO_2 layers in the intermediate coupling regime) may occur in the CuO_2 layers (with nonzero thickness) at a temperature T^* higher than the T_c at which the preformed bosonic Cooper pairs condense into a SF (or SC) Bose-liquid state and the new SC order parameter appears [26,27]. The strongly polarizable lattice of the cuprates may provide a more effective pairing mechanism than the interaction of the conduction electrons with phonons in ordinary metals. In these systems, the new situation arises when the polaronic effects exist and the attractive interaction mechanism (e.g. due to exchange of static and dynamic phonons) between the polaronic carriers operating in the energy range $\{-(E_p+\hbar\omega_0),(E_p+\hbar\omega_0)\}$ is more effective than in the simple BCS picture, where E_p is the binding energy of a large polaron, $\hbar\omega_0$ is the energy of high-frequency optical phonons.

In the case of high-T_c cuprates, the unusual form of BCS theory [26,28] can describe the Cooper-like pairing of large polarons above T_c naturally. The BCS formalism, extended towards the intermediate electron-phonon coupling regime, leads to the following equation for determining the BCS-like gap or PG, Δ^* and the PG formation temperature T^*:

$$\frac{1}{\lambda^*} = \int_0^{\varepsilon_A} \frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta^{*2}(T)}} \tanh\frac{\sqrt{\varepsilon^2+\Delta^{*2}(T)}}{2k_BT}, \tag{1}$$

where $\lambda^* = D_p(\varepsilon_F)\tilde{V}_p$ is the effective BCS-like coupling constant, $D_p(\varepsilon_F) = 1/\varepsilon_F$ is the density of states (DOS) at the polaronic Fermi level for one spin orientation,

ε is the energy of large polarons measured from the polaronic Fermi energy $\varepsilon_F = \hbar^2(3\pi^2 n_p)^{2/3}/2m_p$, $n_p = N_p/\Omega$ is the concentration of intrinsic polarons in the CuO_2 layers, N_p is the number of such polarons, Ω is the crystal volume, $\tilde{V}_p = V_{ph} - \tilde{V}_c$ is the effective polaron-polaron interaction potential, V_{ph} is the phonon-mediated interaction potential between two polarons, $\tilde{V}_c = V_c/[1 + D_p(\varepsilon_F)V_c \ln(\varepsilon_c/\varepsilon_A)]$ is the screened Coulomb interaction potential, V_c is a bare Coulomb potential, $\varepsilon_A = E_p + \hbar\omega_0$ is the cutoff parameter for the unusual attractive electron-phonon interaction.

At $T = T^*$ and $\varepsilon_c > \varepsilon_A > 7k_BT^*$, we obtain from (1)

$$k_BT^* \simeq 1.134(E_p + \hbar\omega_0)exp[-\frac{1}{\lambda^*}]. \tag{2}$$

We see that the usual BCS picture ($T_c = T^*$) as the particular case is recovered in overdoped cuprates where the polaronic effect disappears ($E_p = 0$) and the prefactor in Eq. (2) is replaced by $\hbar\omega_0$.

At $E_p \neq 0$ the polaronic effects control the essential physics of underdoped to overdoped cuprates, which are bosonic (i.e. non-BCS) superconductors. The BCS-like pairing PG Δ^* gradually decreases with temperature and disappears at $T = T^* > T_c$. Therefore, in high-T_c cuprates containing dopants (impurities), the second-order phase transition at T^* should be manifested as a more or less BCS-type jump in $C_n(T)$. In the unusual BCS-like pairing picture, the disappearance of polaronic Cooper pairs does not occur at T_c as it would for conventional superconductors where $T^* = T_c$. The underdoped, optimally doped and moderately overdoped cuprates are actually non-BCS superconductors, where the separation between the two temperatures T^* (the onset of the BCS-like transition) and T_c (the onset of the λ-like SC transition) occurs due to the polaronic effects.

3 The normal-state electronic specific heat above and below the pseudogap formation temperature T^*

Charge carriers are inhomogeneously distributed in doped cuprates and possible inhomogeneities in the charge carrier distribution might be responsible for the formation of the intrinsic and extrinsic large polarons in the impurity-free regions and near the impurities. It seems likely that in underdoped and optimally doped cuprates some part of doped carriers can easily be self-trapped near the dopants (impurities) with the formation of large polarons bound to impurities and other doped carriers are self-trapped in a deformable lattice with the formation of intrinsic large polarons. Such competitive self-trapping processes lead to the redistribution of polaronic carriers among impurity-free regions and impurity sites. We believe that in the unusual metallic state of high-T_c cuprates the BCS-type Cooper pairing of large polarons would occur in the polaronic band below T^*, whereas the large polarons localized near the impurities may remain unpaired. Apparently, the contributions to $C_n(T)$

above T^*, come from these two types of large polarons and the normal-state electronic specific heat is given by

$$C_n(T > T^*) = (\gamma_1 + \gamma_2)T, \tag{3}$$

where $\gamma_i = 2\pi^2 D_p(\varepsilon_{Fi})k_B^2/3 = (\pi^2/3)k_B^2 g(\varepsilon_{Fi})$ (i=1 or 2), $g(\varepsilon_{Fi}) = 3N_i/2\varepsilon_{Fi} = 3Nf_i/2\varepsilon_{Fi}$ is the density of states at the Fermi level ε_{Fi} (including both spin orientations), N_i is the number of the i-th type of large polarons, $N = N_1 + N_2$ is the total number of polaronic carriers in the system ($N_1 = N_p$, N_2 is the number of large polarons residing in the impurity band), $f_i = N_i/N$ is the fraction of the i-th type of large polaronic carriers. For doped cuprates, the coefficient of the linear term in $C_e(T > T^*)$ is defined as

$$\gamma_e = \gamma_1 + \gamma_2 = (\frac{\pi^2}{2})k_B^2 x N_A(\frac{f_1}{\varepsilon_{F1}} + \frac{f_2}{\varepsilon_{F2}}), \tag{4}$$

where the number of CuO$_2$ formula unit (or the host lattice atoms) per unit molar volume is equal to the Avogadro number $N_A = 6.02 \times 10^{23} mole^{-1}$, $x = N/N_A$ is the dimensionless carrier concentration or doping level, $k_B N_A = 8.314 J/moleK$. The important parameters that describe the real experimental situation and the quantitative behavior of $C_n(T)$ in doped high-T_c cuprate superconductors are ε_{Fi} and f_i. Let us estimate the values of γ_e for LSCO and YBCO. Using the specific values of ε_{Fi} and f_i in the polaronic band ($\varepsilon_{F1} \simeq 0.15$ eV, $f_1 = 0.6$) and impurity band ($\varepsilon_{F2} = 0.06$ eV, $f_2 = 0.4$), we obtain $\gamma_e \simeq 5.67 mJ/moleK^2$ at $x = 0.1$ for LSCO. The experiment value of γ_e lies in the range $(4.9 - 7.3) mJ/moleK^2$ [29]. For YBa$_2$Cu$_3$O$_{7-\delta}$, the doping level can be determined from the relation [30]

$$x(\delta) = \begin{cases} (1-\delta)^3 & \text{for } 0 \le 1-\delta \le 0.5, \\ (0.5-\delta)^3 + 0.125 & \text{for } 0.5 < 1-\delta \le 1 \end{cases} \tag{5}$$

from which it follows that $x(\delta = 0.115) \simeq 0.182$. By taking $\varepsilon_{F1} = 0.20$ eV, $\varepsilon_{F2} = 0.1$ eV, $f_1 = 0.6$ and $f_2 = 0.4$ for YBCO, we find $\gamma_e \simeq 4.65 mJ/moleK^2$. This value of γ_e is well consistent with the experimental data $\gamma_e \simeq 4.3 - 4.9 mJ/moleK^2$ [31]

Below T^*, three contributions to $C_n(T)$ come from: (i) the Bogoliubov-like quasiparticles appearing at the dissociation (excitation) of Cooper pairs in the polaronic band, (ii) the unpaired polarons in the impurity band, and (iii) the ideal Bose-gas of incoherent Cooper pairs. The contribution to $C_n(T)$ coming from the Bogoliubov-like quasiparticles is determined from the relation.

$$C_{n1}(T < T^*) = \frac{g(\varepsilon_{F1})}{k_B T^2} \int_0^{\varepsilon_A} f(E)\,(1 - f(E)) \left[E^2(\varepsilon) - \frac{T}{2}\frac{d\Delta^{*2}(T)}{dT}\right] d\varepsilon, \tag{6}$$

where $g(\varepsilon_{F1}) = 3N_A x f_1/2\varepsilon_{F1}$, $f(E) = \left[e^{E/k_B T} + 1\right]^{-1}$, $E(\varepsilon) = \sqrt{\varepsilon^2 + \Delta^{*2}(T)}$.

The energy of an ideal Bose-gas below the BEC temperature T_{BEC} is given by [32]

$$U = 0.77 N_c k_B T \left(\frac{T}{T_{BEC}}\right)^{3/2}, \tag{7}$$

where N_c is the number of Bose particles. The specific heat of such a Bose-gas of incoherent Cooper pairs is determined from the relation

$$C_{n3}(T < T^*) = \frac{dU}{dT} = 1.925 k_B N_c \left(\frac{T}{T_{BEC}}\right)^{3/2}. \tag{8}$$

Then the total electronic specific heat below T^* is given by

$$C_n(T < T^*) = C_{n1}(T) + C_{n2}(T) + C_{n3}(T), \tag{9}$$

where $C_{n2}(T < T^*) = (\pi^2/3)k_B^2 g(\varepsilon_{F2})T$, $g(\varepsilon_{F2}) = 3N_A x f_2/2\varepsilon_{F2}$.

The BCS-like pairing PG, $\Delta^*(T)$ and PG temperature, T^* are determined from Eq. (1). Such a normal-state PG somewhat below T^* is determined by the formula

$$\Delta^*(T) \simeq 3.06 k_B T^* \sqrt{1 - \frac{T}{T^*}}, \tag{10}$$

which is better approximation in the temperature region $0.75T^* < T \leq T^*$. The number of incoherent Cooper pairs n_c and their BEC temperature are determined from the relations

$$n_c = \frac{1}{4} g(\varepsilon_{Fp}) \int_{-\varepsilon_A}^{\varepsilon_A} \left[1 - \frac{\varepsilon}{E}\right] \frac{e^{E/k_B T}}{e^{E/k_B T} + 1} d\varepsilon, \tag{11}$$

and

$$T_{BEC} = \frac{3.31 \hbar^2 n_c^{2/3}}{k_B m_c}, \tag{12}$$

where $m_c = 2m_p$ is the mass of polaronic Cooper pairs, $\varepsilon_{F1} > \varepsilon_A \gtrsim 0.1eV$, $m_p \simeq 2m_e$ [14].

Numerical calculations of n_c and T_{BEC} show that just below T^* the value of T_{BEC} is very close to T^* (i.e., $T_{BEC} \geq T^*$), but somewhat below T^*, $T_{BEC} >> T^*$. The calculated results for $C_n(T \leq T^*)$ and $C_n(T > T^*)$ depend sensitively on details of the distribution of polaronic carriers between the polaronic band and the impurity band through the variation of both ε_{F2} and f_2. Actually, the behavior of $C_n(T)$ is sensitive to the choice of the parameters ε_{F2}, f_2, x and self-consistent calculations which take into account changes in the distribution of charge carriers between the polaronic band and the impurity band should be used in comparing with experiment. For high-T_c cuprates, the observed temperature dependences of C_n and C_n/T can be obtained by a more appropriate choice and a careful examining of the fitting parameters. Such a fit is essential for matching the theory with the experiments on $C_n(T)$ in various high-T_c cuprates. The quantitative features of $C_n(T)$ at $T = T^*$ is basically determined by the competition between the PG and impurity effects on $C_n(T)$. This competition determines the shape and size of the possible BCS-type jumps of $C_n(T)$ above T_c in underdoped to optimally doped high-T_c cuprates. When the BCS-type contribution to $C_n(T < T^*)$ coming from the excited Fermi-components of Cooper pairs and from the bosonic Cooper pairs predominates over the contribution coming from the unpaired carriers in the impurity band, the pronounced BCS-type anomaly of $C_n(T)$ is expected at T^*. However, the situation changes markedly when the impurity contribution dominates the BCS-type contribution to $C_n(T)$. Because the jumps of $C_n(T)$ above T_c will be largely modified (i.e. strongly depressed) by the relatively large impurity contribution to the $C_n(T)$ and become weakly or less pronounced BCS-type anomalies, as observed in experiments [5,6,7,10]. Theoretical results obtained for $C_n(T \leq T^*)$, which are compared with the experimental data on the electronic specific heat of LSCO, are presented in Fig. 1 for the temperature region $0.8T^* < T \leq 1.15T^*$.

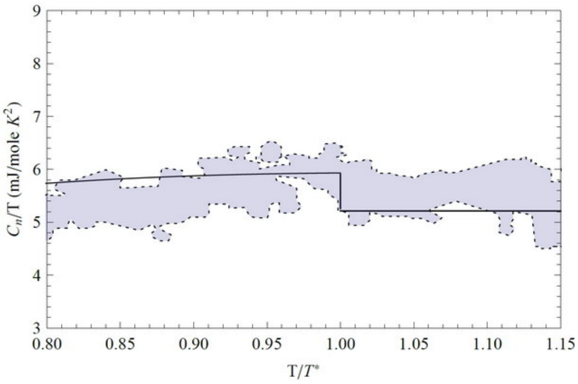

Figure 1. Electronic specific heat of LSCO with doping level $x = 0.10$ (solid line) calculated as a function of the reduced temperature T/T^* near $T^* = 98K$ using the fitting parameters $\varepsilon_{F1} \simeq 0.1665$ eV, $\varepsilon_{F2} \simeq 0.0373$ eV, $f_1 = 0.42$, $f_2 = 0.58$ and compared with experimental data for LSCO with doping level $x = 0.10$ (dotted line) [10].

One can see that the observed behaviors of $C_n(T)$ above T_c are similar to the calculated results for $C_n(T)$ at $T \leq T^*$ and $T > T^*$, as indicated by Fig. 1 (solid line). The smeared regions between dotted lines in Fig. 1 show that the spread in measured values of $C_n(T)$ are large enough. Nevertheless, there are more or less pronounced BCS-type jumps in $C_n(T)$ (see Fig. 1) close to T^* observed in LSCO above T_c [6,7,10]. The specific heat anomaly in the $200 - 240K$ temperature range, observed in an YBCO mono-crystal [7] was ascribed to some cause other than that related to the Cooper-pair formation. Perhaps this normal-state specific heat anomaly observed also near $220K$ by other authors (see Ref. [9]) in YBCO is a BCS-type anomaly of $C_n(T)$ near $T^* \simeq 220K$. The existence of a phase transition in LSCO at $T^* \approx 80K$ [5] might be associated with a BCS-type transition at T^*. While the authors of Ref. [33] argued that there is no such a phase transition in the normal state of high-T_c cuprates. However, according to Ref. [33], γ_e is insensitive to T above the characteristic PG temperature T^* and decreases rapidly below T^* just like in BCS theory.

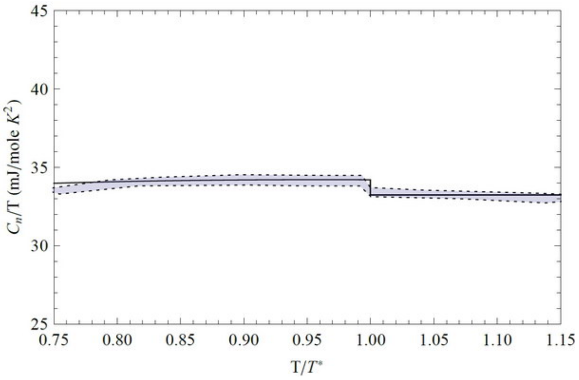

Figure 2. The electronic specific heat coefficient (C_n/T) of $YBa_2Cu_3O_{7-\delta}$ with doping level $x = 0.14$ calculated as a function of the reduced temperature T/T^* near $T^* = 167$ K using the fitting parameters, $\varepsilon_{F1} = 0.110eV$, $\varepsilon_{F2} = 0.0435eV$, $f_1 = 0.3$, $f_2 = 0.7$ and compared with experimental results for $YBa_2Cu_3O_{6.73}$ (dotted line) [33].

Thus, considering the possible noises or errors in experiments and large enough spread of experimental points in Figs. 1 and 2, our calculated results for $C_n(T)$ are in reasonable quantitative agreement with the experimental data on $C_n(T)$ for LSCO and YBCO. Our fitting curves $C_n(T)$ and $C_n(T)/T$ in Figs. 1 and 2 lie within the experimental noises and are therefore acceptable. It should be noted here that in the vicinity of T^*, the total specific heat is very large due to phonon contributions, and the observation of an anomaly due to the BCS-like PG effect is expected to be difficult, but inspection of the specific heat data of LSCO and YBCO shows that such an effect is clearly present. We argue that the expected BCS-type jumps of the electronic specific heat of high-T_c cuprate superconductors at $T^* > T_c$ are often buried within the noises and observed as the less pronounced jumps due to the impurity and sample inhomogeneity effects.

4 Electronic specific heat anomalies near superconducting transition temperature T_c

In high-T_c cuprates the polaronic carriers are bound into bosonic Cooper pairs above T_c and these Cooper pairs condense into a Bose-liquid state at T_c. The SC order parameter Δ_{SC} appearing below T_c [27,28] differs from the BCS-like pairing PG. The occurrence of superconductivity in the (bosonic) non-BCS cuprate superconductors is tied to the coherence parameter $\Delta_B = \Delta_{SC}$, which defines bond strength of all condensed bosons. Where as the BCS-like gap (or PG) defines the bond strength of the Fermi components of Cooper pairs and it may exist as the PG. For an interacting Bose gas of Cooper pairs, the chemical potential $\tilde{\mu}_B(\geqslant \Delta_B)$ and the coherence parameter $\Delta_B = \Delta_{SC}$ near T_c is given by $\tilde{\mu}_B(T) \simeq \tilde{\mu}_B(T_c)[1 + a(T_c - T)^{0.5}]$ and $\Delta_B(T) \simeq 2\tilde{\mu}_B(T_c)\sqrt{a}(T_c - T)^{0.25}$ [27], where $a = 2(c_0\gamma_B T_c)^{-0.5} \times (\varepsilon_{BA}/k_B T_c)^{0.25}$ and $c_0 = \pi^{3/2}/3.912$. We now turn to the problem of the specific heat of a SF Bose gas, which diverges as $C_{SF}(T) \sim (T_c - T)^{-0.5}$ near T_c (where $\Delta_B(T) << \tilde{\mu}_B(T) << k_B T_c$)

[14] and will exhibit a λ-like anomaly at T_c, (i.e., the behavior of $C_{SF}(T)$ is similar to that of SF ^{4}He). The temperature derivatives of $\tilde{\mu}_B$ and Δ_B entering the expression for $C_{SF}(T)$ give rise to such a λ-like divergence. By introducing the quantity of SF matter $\nu_B = N_B/N_A$ (where N_B is the number of attracting bosons (polaronic Cooper pairs) and N_A is the Avogadro number, which is equal to the number of CuO_2 formula unit per unit molar volume) and the molar fraction of the SF bosonic carriers defined by $f_s = \nu_B/\nu$ (where $\nu = N/N_A$ is the amount of doped matter), we can now write the molar specific heat of the SC Bose-gas in high-T_c cuprates as

$$C_s(T) = f_s \frac{C_{SF}(T)}{\nu_B} =$$

$$= f_s \frac{D_B k_B N_A}{4\rho_B (k_B T)^2} \int_0^{\varepsilon_{BA}} \frac{\sqrt{\varepsilon} d\varepsilon}{\sinh^2 \frac{E_B(\varepsilon)}{k_B T}} \left\{ E_B^2(\varepsilon) + \frac{a\tilde{\mu}_B(T_c)T}{2(T_c - T)^{0.5}} \left[\varepsilon - \tilde{\mu}_B(T_c)\right] \right\}. \qquad (13)$$

Here we have accounted for that $\Omega/\nu_B = N_B v_B/\nu_B = v_B N_A$ and $v_B = 1/\rho_B$. As mentioned above, the doping carriers in the cuprates are distributed between the polaronic band and the impurity band (with Fermi energy ε_{F2}) and the specific heat $C_n(T)$ of non-SC carriers below T_c is also calculated by considering three contributions from the excited components of polaronic Cooper pairs, the ideal Bose-gas of incoherent Cooper pairs and the unpaired carriers bound to impurities [34]. In this case, the fraction f_1 of doping carriers residing in the polaronic band and the other fraction f_2 of such carriers residing in the impurity band should be taken into account in comparing the specific heat $C_s(T)$ of the SC Bose-gas with experiment.

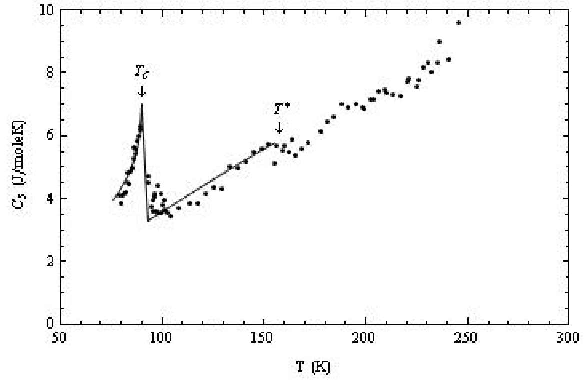

Figure 3. Temperature dependence of the electronic specific heat of $HoBa_2Cu_3O_{7-\delta}$ measured near T_c and above T_c [35]. The solid line is the calculated curve for comparing with experimental points (black circles). According to [34], $C_s(T)$ is calculated by using the parameters $\varepsilon_F = 0.12$ eV, $\varepsilon_{FI} = 0.012$ eV, $f_p = 0.3$, $f_I = 0.7$, while SC contribution $C_s(T)$ to $C_s(T)$ is calculated by using the parameters $\rho_B = 1.6 \times 10^{19} cm^{-3}$, $m_B = 2.5 m_p$, $\tilde{\mu}_B(T_c) = 1.6$ meV and $f_s = 0.03$.

Thus, the total specific heat $C_e(T) = C_s(T) + C_n(T)$ of SC and non-SC carriers below T_c is calculated and compared with the experimental data for $C_s(T)$ in high-T_c cuprates (Figs. 3 and 4).

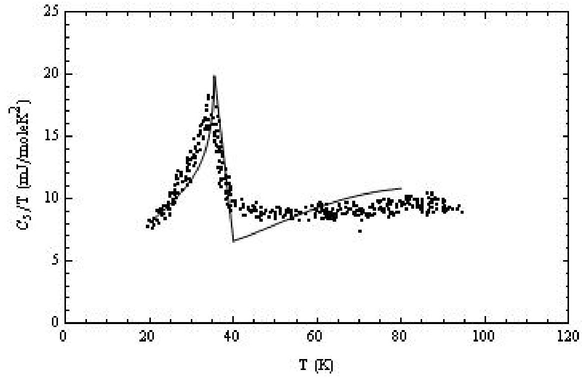

Figure 4. Temperature dependence of the electronic specific heat of LSCO measured near T_c and above T_c [10]. The solid line is the calculated curve for comparing with experimental points (black circles). According to [34], $C_s(T)$ is calculated by using the parameters $\varepsilon_F = 0.1$ eV, $\varepsilon_{FI} = 0.06$ eV, $f_p = 0.4$, $f_I = 0.6$, while SC contribution $C_s(T)$ to $C_s(T)$ is calculated by using the parameters $\rho_B = 1.4 \times 10^{19} cm^{-3}$, $m_B = 2.7 m_p$, $\tilde{\mu}_B(T_c) = 0.5$ meV and $f_s = 0.012$.

Conclusion

We have studied the electronic specific heat properties of underdoped to overdoped high-T_c cuprates and identified the nature of the anomaly in $C_n(T)$ at a characteristic temperature T^* (below which opens the BCS-like PG at the Fermi surface) above T_c and λ-like anomaly in $C_n(T)$ at the superconducting transition temperature T_c. The effects of BCS-like pairing PG and impurities on the normal-state electronic specific heat $C_n(T)$ of these high-T_c cuprate superconductors are studied within a multi-carrier model taking into account the charge carrier inhomogeneity (i.e. the possible disbalance in the distribution of doped charge carriers among two different regions, namely, impurity-free regions or CuO_2 layers and impurity sites). The relevant charge carriers in doped high-T_c cuprates are large polarons, preformed bosonic Cooper pairs in the CuO_2 layers (with nonzero thickness) and large extrinsic polarons (i.e. polaronic carriers bound to impurities) lying between the CuO_2 layers. We have considered the high-T_c cuprate superconductor above T^* as a two-carrier system and calculated two contributions to the $C_n(T)$ coming from the intrinsic and extrinsic large polarons within a two-component degenerate Fermi-gas model. We then considered the same high-T_c material below T^* as a three-carrier system and calculated three contributions to the $C_n(T)$ coming from the excited Fermi components of Cooper pairs, the ideal Bose-gas of incoherent Cooper pairs and the unpaired charge carriers in the impurity band. We have found that the jump-like anomaly of $C_n(T)$ near T^* changes strongly with the increasing of the fraction of charge carriers in the impurity band, from the sharp second-order BCS-type transition to the weakly or less pronounced BCS-type jump. The calculated results for $C_n(T)$ and $C_n(T)/T$ above T_c were compared with the experimental data obtained for $C_n(T)$ and $C_n(T)/T$ in LSCO and YBCO. The obtained results are quite similar to those found for LSCO and YBCO, although the amount of the BCS-type anomaly in the measured temperature dependences of $C_n(T)$ and $C_n(T)/T$ is weak due to the experimental noises and large spread of experimental points. The total electronic specific heat $C_e(T) = C_s(T) + C_n(T)$ near T_c is calculated by considering the contribution $C_s(T)$ coming from the superfluid bosonic carriers and the contribution $C_n(T)$ coming from exited Fermi components of Cooper pairs, the ideal Bose-gas of incoherent Cooper pairs and the unpaired charge carriers in the impurity band. The calculated results for $C_e(T)$ are in fair quantitative agreement with the experimental data for $C_e(T)$ in high-T_c cuprates. We have shown that our theoretical predictions of the behaviors of $C_n(T)$ and $C_n(T)/T$ below, at and above T^* are strikingly similar to the behaviors of the electronic specific heat properties observed above T_c in LSCO and YBCO. Our calculated results for $C_e(T)$ below T_c also closely resembles the observed λ-like behavior of $C_e(T)$.

Acknowledgments

We thank E. M. Ibragimova, P. J. Baimatov, U. T. Kurbanov and Z. S. Khudayberdiev for valuable discussions and collaborations. This work was supported by the Foundation of the Fundamental Research of Uzbek AS, Grant No Φ2-ΦA-Φ120.

References

[1] Anderson P. W., The Theory of Superconductivity in the High-T_c Cuprates. Princeton University Press, Princeton (1997).

[2] Tallon J. L. and Loram J. W. The doping dependence of T^*-what is the real high-T_c phase diagram. Physica C, 349, 53 (2001).

[3] Lee P. A., Nagaosa N., Wen X.-G. Doping a Mott insulator: Physics of high-temperature superconductivity. Rev. Mod. Phys. 78, 17 (2006).

[4] Solovjov A. L. and Tkachenko M. A. Pseudogap and local pairs in high-T_c cuprate superconductors. arXiv:1112.3812v[cond-mat,super-con].

[5] Dzhumanov S. Theory of Conventional and Unconventional Superconduтivity in the High-T_c Cuprates and Other Systems, Nova Science Publishers, New York (2013).

[6] Inderhees S. E., Salamon M. B., Goldfeld N., Rice J. P., Pazol B. G., Ginsberg D. M., Liu J. Z. and Crabtree G. W. Specific heat of single crystals of YBa_2Cu_3O7-x: Fluctuation effects in a bulk superconductor. Phys. Rev. Lett. 60, 1178 (1988).

[7] Fossheim K., Nes O. M., Legreid T., Darlington C. N. W., O'Connor D. A. and Gough C. E. Specific heat in mono-crystal YBCO: λ-like anomalys at 90 K and 229 K. Int. J. Mod. Phys. B 1, 1171 (1988).

[8] Izbizky M. A., Nunez Regueiro M., Esquinazi P. and Fainstein C. Thermal conductivity and superconductivity in $EuBa_2Cu_3O_{7-x}$. Phys. Rev. B 38, 9220 (1988).

[9] Fung P. C. W. and Kwok W. Y. T_c enhancement in superconductor-semiconductor arrays. J. Superconduct. 4, 67 (1991).

[10] Matsuzaki T., Ido M., Momono N., Dipasupil R. M., Nagata T., Sakai A. and Oda M. Superconducting gap and pseudogap behavior in high-T_c cuprates. J. Phys. Chem. Solids 62, 29 (2001).

[11] Fisher R. A., Gorden J. E. and Phillips N. E. Specific heat of the high-T_c oxide superconductors. J. Superconduct. 1, 231 (1988).

[12] Junod A. Optimization of the superconductor $YBa_2Cu_3O_{7-\delta}$: The effect of the edos, processing conditions, impurities and Fe doping on the specific heat, Meissner effect and susceptibility. Physica C 153-155, 1078 (1988).

[13] Liu F.-S., Liu W.-F., Chen W.-F. and Peng K. A possible second-order phase transition at the temperature at which a gap opens in superconductors. J. Phys.: Condens. Matter 13, 2817 (2001).

[14] Kastner M. A., Birgeneau R. J., Shirane G. and Endoh Y. Magnetic, transport, and optical properties of monolayer copper oxides. Rev. Mod. Phys. 70, 897 (1998).

[15] Kresin V. Z. and Wolf S. A. Colloquium: Electron-lattice interaction and its impact on high T_c superconductivity. Rev. Mod. Phys. 81, 481 (2009).

[16] Devreese J. T. and Alexandrov A. S. Frölich polaron and bipolaron: recent developments. Rep. Prog. Phys. 72, 066501 (2009).

[17] Zaanen J., Sawatzky G. A. and Allen J. W. Band gaps and electronic structure of transition-metal compounds. Phys. Rev. Lett. 55, 418 (1985).

[18] Zaanen J. Why high T_c is exciting. cond-mat/0103255.

[19] Lavrov A. N. and Gantmakher V. F. Low-temperature resistivity of underdoped cuprates. Phys. Usp. 41, 223 (1998).

[20] Dzhumanov S., Baimatov P. J., Ganiev O. K., Khudayberdiev Z. S. and Turimov B. V. Possible mechanisms of carrier localization, metal-insulator transitions and stripe formation in inhomogeneous hole-doped cuprates. J. Phys. Chem. Solids 73, 487 (2012).

[21] Appel J. in Polarons, edited by Firsov Ya. A., Nauka, Moscow (1975).

[22] Sugai S. Local distortion specifying the superconductor phases observed by Raman scattering. Physica C 185-189, 76 (1991).

[23] Muroi M. and Street R. Charge distribution in triple-layered copper oxide superconductors. Physica C 248, 290 (1995).

[24] Ino A., Kim C., Nakamura M., Yoshida T., Mizokawa T., Fujimori A., Shen Z.-X., Kakeshita T., Eisaki H. and Uchida S. Doping-dependent evolution of the electronic structure of $La_{2-x}Sr_xCuO_4$ in the superconducting and metallic phases. Phys. Rev. B 65, 094504 (2002).

[25] Basov D. N. and Timusk T. Electrodynamics of high-T_c superconductors. Rev. Mod. Phys. 77, 721 (2005).

[26] Dzhumanov S. and Khabibullaev P. K. Microscopic theory of single particle and pair condensation of an attracting Bose gas the basis for superfluidity and superconductivity. Pramana J. Phys. 45, 385 (1995).

[27] Dzhumanov S. The microscopic theory of superfluidity and superconductivity driven by single particle and pair condensation of attracting bosons. Int. J. Mod. Phys. B 12, 2151 (1998).

[28] Dzhumanov S. Precursor non-superconducting pairing and novel superconductivity in underdoped and optimally doped cuprates. Physica C 460-462, 1131 (2007).

[29] Kresin V. Z., Morawitz H. and Wolf S. A. Mechanisms of Conventional and High T_c Superconductivity. Oxford University Press, New-York-Oxford (1993).

[30] Muroi M. and Street R. Charge transfer, phase separation and percolative superconductivity in $YBa_2Cu_3O_{6+y}$. Physica C 246, 357 (1995).

[31] Junod A., Sanchez D., Genoud J.-Y., Graf T., Triscone G. and Muller J. Specific heat of the 95 K superconductor $YBa_2Cu_{35}O_{75}$ from 1 to 330 K. Physica C 185-189, 1399 (1991).

[32] Landau L. D. and Lifshitz E. M. Statistical Physics. Part I. Nauka, Moscow (1976).

[33] Loram J. W., Mirza K. A., Wade J. M., Cooper J. R. and Liang W. Y. The electronic specific heat of cuprate superconductors. Physica C 235-240, 134 (1994).

[34] Dzhumanov S. and Karimboev E. X. Competing pseudogap and impurity effects on the normal-state specific heat properties of cuprate superconductors. Physica A 406, 176 (2014).

[35] Naumov V. N., Frolova G. I., Amitin E. B., Fedorov V. E. and Samoilov P. P. Electron heat capacity and moments of phonon density of states of $HoBa_2Cu_3O_{7-\delta}$. Physica C 262, 143 (1996).