Specific heat behavior of high temperature superconductors in the pseudogap regime

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Experimental data obtained from thermodynamic measurements in underdoped high temperature superconductors show unusual anomalies in the temperature dependence of the electronic specific heat both in the normal state and at the critical point associated to the superconducting phase transition. The observed deviations from the standard behavior are probably linked with the opening of a pseudogap in the energy spectrum of the single-particle excitations associated with the normal state. Based on a phenomenological description of the pseudogap phase we perform analytical and numerical calculations for the temperature dependence of the specific heat for both the superconducting and normal state. The reduced specific heat jump at the transition point can be explained by a modified electronic single particle contribution to the specific heat in the presence of the normal state pseudogap. The hump observed in the normal state specific heat can be explained by the electronic pair contribution associated with strong fluctuations of the order parameter in the critical region. The obtained theoretical results are discussed in connection with experimental data for cuprates.

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I. INTRODUCTION

One of the most controversial properties of high temperature superconductor materials (HTSC) is the presence of a gap in their normal state single particle excitation spectrum. Usually addressed as the pseudogap, this relatively new feature just added a new controversy on the long list of unusual properties of the normal phase of HTSC. The pseudogap phase is seen in the underdoped region of the HTSC phase diagram for temperatures above the superconducting critical temperature $T_c$ and below a characteristic temperature $T^*$. The presence of the pseudogap phase was experimentally proved by direct measurements of the single particle excitation spectra in angle resolved photoemission spectroscopy (ARPES) and tunneling experiments, but also in nuclear magnetic resonance (NMR), specific heat, resistivity, infrared conductivity, and Raman spectroscopy experiments. However, in spite of a large amount of experimental data, there is still no general consensus on the nature of the pseudogap phase, especially regarding the doping dependence of the onset temperature $T^*$ around the optimal doping point. As a function of doping, in one possible scenario, $T^*$ merges with $T_c$ in the overdoped region, whereas in a different scenario, $T^*$ falls from large values in the underdoped region to a zero value at a critical point, universally identify for all HTSC at $\rho_c = 0.19$. From the theoretical point of view, these two scenarios involve different approaches. In the first one, the superconducting and pseudogap phases are strongly connected, the pseudogap being associated with the formation of precursor Cooper pairs ($T_c < T < T^*$), pairs which become coherent and condense at $T_c$, leading to the superconducting phase. A different theoretical approach leading to the same conclusions with respect to the onset temperature $T^*$ consider the role of the pair fluctuations above the critical temperature $T_c$. In the second scenario, the key role is played by the presence of an antiferromagnetic region in the phase diagram at low doping values, the pseudogap being a consequence of the direct interaction between the electrons and fluctuations of the antiferromagnetic order parameter. Unfortunately, despite this large theoretical effort, an agreed description of the normal state in HTSC (including the pseudogap phase) is still lacking.

In a recent work, Moca and Janko performed a detailed theoretical analysis of the electronic specific heat in HTSC. Starting from a phenomenological description of the pseudogap, it is argued that a correct description of the specific heat behavior in the normal state can be obtained only with the inclusion of the electron pair contribution. Such a scenario is sustained by the presence of strongly enhanced fluctuations of the order parameter in the critical region above the transition temperature in quasi-two dimensional systems such as HTSC. In this way the observed maximum in the coefficient of the electronic heat capacity, $\gamma(T) = C/T$, can be fully explained. However, the anomalies related to the specific heat behavior are observed also in the specific heat coefficient jump, $\Delta \gamma(T_c)$, at the transition point. In the overdoped region, where the presence of a pseudogap is still questionable, the specific heat jump remains almost constant. As the doping decreases, around the optimal doping point, where the pseudogap is supposed to open, the specific heat jump starts to decrease. Once the doping value is in the underdoped region, $\Delta \gamma(T_c)$ falls...
sharply, the larger the pseudogap is, the smaller the specific heat jump becomes. The goal of this paper is to calculate the temperature dependence of the electronic specific heat, both for the superconducting and normal phase of HTSC, and to analyze its jump at the critical point based on a modified BCS theory which includes the pseudogap effects. A similar approach of the electronic specific heat behavior was considered by Loram et al.\textsuperscript{14} in order to explain the anomalous properties induced by the pseudogap in YBa\textsubscript{2}Cu\textsubscript{3}O\textsubscript{6+x}.

The paper is organized as follows: In Section II we discuss a phenomenological theoretical approach based on the validity of Gorkov’s equations and we obtain the modified gap equation starting from a normal state characterized by the presence of a pseudogap, $E_g$. In Section III we discuss the specific heat behavior based on the proposed model. Analytical results are obtained for the specific heat jump at the critical point using Pauli’s theorem. Numerical results for the specific heat coefficient, $\gamma(T)$, are presented based on an analytical expression of the free energy as function of temperature, below and above the critical temperature $T_c$. A comparison between analytical and numerical results for the specific heat jump at the transition point is also presented. Section IV gives our conclusions.

II. THEORETICAL MODEL

In the following we will consider a simple model based on the Gorkov’s equations formalism in which the normal state Green’s functions will include the presence of the pseudogap. A similar analysis was used by different authors\textsuperscript{16,17,18} in order to study the effect of the pseudogap phase on different properties of the superconducting state. Our theoretical approach is based on the assumption that in the pseudogap phase the self-energy corrections to the free electronic Green’s function are given by:

\[
\Sigma(k, i\omega_n) = -E_g^2(k)G_0(-k, -i\omega_n), \tag{1}
\]

where $G_0(-k, -i\omega_n)$ represents the free electron Green’s function, $E_g(k)$ the pseudogap, and $\omega_n = (2n + 1)\pi T$ is the usual fermionic Matsubara frequency. This phenomenological form of the self-energy was already used to explain the form of the spectral function, $A(k_F, \omega)$, observed in ARPES experiments.\textsuperscript{19} A similar behavior of the electronic self-energy was reported late in the seventies by Schmid\textsuperscript{20} as a direct consequence of electron-pair fluctuation interactions in the critical region around the transition temperature. However, it is not our goal to understand the origin of this phenomenological self-energy, but to use it in order to extract different properties of the superconducting state in cuprates. The normal state Green’s function can be obtained with the aid of Dyson’s equation as:

\[
G(k, i\omega_n) = \frac{u_k^2}{i\omega_n - E_k} + \frac{v_k^2}{i\omega_n + E_k}, \tag{2}
\]

where $E_k^2 = \xi_k^2 + E_g^2(k)$, $u_k^2 = (1 + \xi_k/E_k)/2$, and $v_k^2 = (1 - \xi_k/E_k)/2$ ($\xi_k$ denotes the electron energy measured from the Fermi level).

In terms of Green’s function formalism the standard BCS theory is recovered by the use of the Gorkov equations:

\[
\begin{align*}
G_0^{-1}(k, i\omega_n)G(k, i\omega_n) + \Delta(k)F^\dagger(k, i\omega_n) &= 1 \\
\Delta^*(k)G(k, i\omega_n) - G_0^{-1}(-k, -i\omega_n)F^\dagger(k, i\omega_n) &= 0 \tag{3}
\end{align*}
\]

$G(k, i\omega_n)$ and $F(k, i\omega_n)$ represent the normal and anomalous Green’s functions in the superconducting state. The superconducting order parameter, $\Delta(k)$, is defined in the usual way in terms of the anomalous Green’s function, $F(k, i\omega_n)$, as:

\[
\Delta(k) = -T\sum_n \int \frac{dp}{(2\pi)^2} V(k, p)F^\dagger(p, i\omega_n). \tag{4}
\]

The interaction term, $V(k, p)$, supposed to be attractive, is responsible for the formation of the Cooper pairs. The anomalous superconducting state Green’s function can be easily obtained from Gorkov’s equations and using Eq. (4) the standard BCS gap equation is recovered.

Our theoretical model assumes the validity of Gorkov’s equations for the case of HTSC, where the free electron Green’s function, $G_0(k, i\omega_n)$, is replaced by the more general Green’s function given by Eq. (2). In this way the effects of the pseudogap on the superconducting gap equation are considered. A simple calculation leads to the following general gap equation:

\[
\Delta(k) = -T\sum_n \int \frac{dp}{(2\pi)^2} \frac{\Delta(p) \left[ (i\omega_n)^2 - \xi_p^2 \right]}{\left| \Delta(p) \right|^2 \left[ (i\omega_n)^2 - \xi_p^2 \right]^2 - \left[ (i\omega_n)^2 - \xi_p^2 - E_g^2(p) \right]^2}. \tag{5}
\]

The sum over the Matsubara frequencies can be performed analytically and the gap equation becomes:

\[
\frac{1}{V_d} = \int \frac{dp}{(2\pi)^2} 2\sqrt{\Delta^4(T) + 4\Delta^2(T)E_g^2} \times \frac{A^2(T)}{\sqrt{\xi_p^2 + A^2(T)\psi^2(p)}} \tanh \frac{\sqrt{\xi_p^2 + A^2(T)\psi^2(p)}}{2T} - \frac{B^2(T)}{\sqrt{\xi_p^2 + B^2(T)\psi^2(p)}} \tanh \frac{\sqrt{\xi_p^2 + B^2(T)\psi^2(p)}}{2T}, \tag{6}
\]

where

\[
\begin{align*}
A^2(T) &= E_g^2 + \frac{1}{2} \left[ \Delta^2(T) + \sqrt{\Delta^4(T) + 4\Delta^2(T)E_g^2} \right] , \\
B^2(T) &= E_g^2 + \frac{1}{2} \left[ \Delta^2(T) - \sqrt{\Delta^4(T) + 4\Delta^2(T)E_g^2} \right]. \tag{7}
\end{align*}
\]
Secondly, we considered a parameter, which is known to be more appropriate for the gap at $T = 0$ of the ratio $\Delta(0)/\Delta_0(0)$, as function of the ratio $E_g/\Delta(0)$ obtained from both the numerical (full line) and analytical (dashed line) calculations.

Unfortunately, the exact analytical solution for the gap equation (6) at any temperature in the superconducting state ($0 < T < T_c$) is difficult to obtain. Instead, we performed a numerical calculation for the gap temperature dependence considering different values of the normal state pseudogap. As a general observation we note that the superconducting state is suppressed by the presence of the normal state pseudogap. The value of the superconducting gap at $T = 0$ K, $\Delta(0)$, transition temperature, $T_c$, and superconducting gap, $\Delta(T)$, decrease as the pseudogap increases. As an example of the numerical solution, in Fig. 1(a) we present the temperature dependence of the superconducting order parameter, $\Delta(T)$, as function of temperature for different values of the pseudogap, $E_g$. However, some simplifications in Eq. (6) can be made in order to approximate some of the superconducting state properties, such as the value of the critical temperature, $T_c$, and the superconducting gap at $T = 0$, $\Delta(0)$. First of all the integration over the momenta is replaced by an energy integration using the corresponding density of states (DOS) in the normal state (DOS) in the normal state:

$$N(\xi) = \begin{cases} \frac{1}{2} N_0 \xi, & |\xi| < E_g \\ \frac{1}{2} N_0, & |\xi| > E_g \end{cases},$$

where $N_0$ denotes the DOS of a two dimensional (2D) free electron gas. This form of the density of states resembles the one seen experimentally in HTSC and is different from the constant density of states used in Ref. 14. We assume also the following energy scale, $E_g < \Delta(0) < W/2$, with $W$ being the bandwidth. This choice of the energy scale is valid in the doping region around the optimal doping point. Based on this assumption one finds:

$$T_c = T_{c0} \left[ 1 - \frac{1}{4} E_g - \frac{21\xi(3)}{16\pi^2} \left( \frac{E_g}{T_{c0}} \right)^2 \right],$$

$$\Delta(0) = \Delta_0(0) \left[ 1 - \frac{E_g}{\Delta_0(0)} - \frac{3}{2} \left( \frac{E_g}{\Delta_0(0)} \right)^2 \right],$$

with $T_{c0}$ and $\Delta_0(0)$ being the critical temperature and zero temperature order parameter obtained in standard $d$-wave BCS calculations. As we can see, the effect of the pseudogap is to decrease both the critical temperature and the superconducting gap at $T = 0$ (See Ref. 18), in agreement with the numerical results. Fig. 1(b) compares the analytical result of Eq. 9 for the pseudogap dependence of the $T = 0$ K order parameter with the exact numerical result obtained by solving the gap equation 6. The slopes of the curves are slightly different, but such a behavior is expected as for the analytical results a number of simplifications were made.
III. SPECIFIC HEAT

One of the most systematic experimental studies of the thermodynamic properties of the HTSC are the specific heat measurements. Anomalies in the specific heat behavior are reported especially in the normal state, the coefficient of the electronic specific heat capacity, $\gamma(T)$, in underdoped samples being no longer constant as function of temperature as we expect from the standard Fermi liquid theory. The broad maximum observed in $\gamma(T)$ at a specific temperature $T_m \sim T^*$ is associated with the onset of the pseudogap. Moreover, the specific heat jump at the transition point is a function of doping, a lower value than the standard one predicted by the BCS theory being observed in the underdoped region.

In this section we calculate the temperature dependence of the specific heat below and above the critical temperature, extract the specific heat jump at the critical point and compare our analytical and numerical results with the available experimental data.

A. Pauli’s theorem

According to the Pauli’s theorem the difference between the superconducting and normal state thermodynamic potential at the transition point can be calculated based on the following formula:

$$\frac{O_s - O_n}{v} = \int_0^\Delta d\Delta' \left( \Delta' \right)^2 \frac{d(1/V_d)}{d\Delta'},$$

(10)

where $O_s$ and $O_n$ are the thermodynamic potentials in the superconducting and normal state respectively, and $v$ is the sample volume. In the critical region the direct dependence between the inverse of the interacting potential, $1/V_d$, and the superconducting gap, $\Delta(T)$, can be extracted from Eq. (10) considering that close to the transition point the value of the order parameter is small. Accordingly, one finds that

$$\frac{1}{V_d} = -T \sum_n \int \frac{d\mathbf{p}}{(2\pi)^2} \frac{\psi^2(\mathbf{p}) \left[ (i\omega_n)^2 - \xi_p^2 \right]}{\left[ (i\omega_n)^2 - \xi_p^2 - E_p^2 \psi^2(\mathbf{p}) \right]^2},$$

$$-\Delta^2(T) T \sum_n \int \frac{d\mathbf{p}}{(2\pi)^2} \frac{\psi^4(\mathbf{p}) \left[ (i\omega_n)^2 - \xi_p^2 \right]}{\left[ (i\omega_n)^2 - \xi_p^2 - E_p^2 \psi^2(\mathbf{p}) \right]^2},$$

(11)

a result which together with Eq. (10) leads to

$$\frac{O_s - O_n}{v} = -\frac{\Delta^4(T)}{2} T \sum_n \int \frac{d\mathbf{p}}{(2\pi)^2} \frac{\psi^4(\mathbf{p}) \left[ (i\omega_n)^2 - \xi_p^2 \right]}{\left[ (i\omega_n)^2 - \xi_p^2 - E_p^2 \psi^2(\mathbf{p}) \right]^2},$$

(12)

The electronic contribution to the specific heat can be calculated based on the thermodynamic potential as $C = -T \partial^2 Q / \partial T^2$. One can see that the knowledge of the specific heat jump at the critical point requires the knowledge of the temperature dependence of the superconducting gap in the critical region, below the phase transition point. A laborious, but straightforward calculation based on Eq. (11) gives

$$\Delta^2(T) = \frac{32\pi^2 T_c^2}{21\zeta(3)} \left( 1 - \frac{T}{T_c} \right) \times \left[ 1 - 3.14 \frac{E_g}{\Delta_0(0)} + 7.6 \left( \frac{E_g}{\Delta_0(0)} \right)^2 \right],$$

(13)

a result which inserted in Eq. (12) gives for the specific heat jump at the transition point the following value

$$\frac{C_s - C_n}{v} = \frac{8\pi^2 T_c N_0}{21\zeta(3)} \left[ 1 - 0.53 \frac{E_g}{\Delta_0(0)} - 1.46 \left( \frac{E_g}{\Delta_0(0)} \right)^2 \right]^2.$$

(14)

It is clear from Eq. (14) that the presence of the pseudogap in the single particle excitation spectrum in the normal state is responsible for the observed suppression of the specific heat jump at the critical point. Such an effect seems to be universal, as it is observed in the underdoped region of most of the HTSC materials such as Bi2212, Bi2201, and YBa2Cu3O7-δ.

B. Numerical results

The electronic single particle contribution to the specific heat has a simple linear $T$-dependence above $T_c$ and an exponential temperature dependence below the critical temperature. A detailed numerical analysis of the temperature dependence of the specific heat coefficient in underdoped HTSC was done in Ref.13. The main conclusion of this study was that the electronic single particle contribution to the specific heat is not enough to correctly describe the experimental data in the normal state, the inclusion of the electronic pair contribution being required in order to understand these data. The electronic pair contribution, associated to strong fluctuations of the order parameter in the critical region above the phase transition point, induces a bump in the normal state specific heat at a temperature of the order of $T^*$, and has to be considered to understand the general behavior of the specific heat in the normal state of HTSC.13 However, no numerical results were presented for the specific heat jump at the transition point.

In the following we will present numerical result for the temperature dependence of the specific heat coefficient,
γ(T), in both the superconducting and normal state. Our analysis will include both electronic single particle and electronic pair contributions. From the numerical point of view, a more reliable way to extract the specific heat temperature dependence is to compute C as the first derivative of the electronic free energy, \( C = dE/dT \). In general the electronic free energy, \( E \), can be calculated based on the following relation:

\[
E = T \sum_{\mathbf{k},n} (i\omega_n + \xi_\mathbf{k}) \mathcal{G}(\mathbf{k},i\omega_n) .
\]

Below the transition temperature the normal Green’s function \( \mathcal{G}(\mathbf{k},i\omega_n) \) can be obtained from Gorkov equations, while for temperatures above the critical temperature the normal state Green’s function, \( G(\mathbf{k},i\omega_n) \), given by Eq (2) should be used instead. Two steps are performed in order to extract the temperature dependence of the specific heat coefficient. First, we will sum over the Matsubara frequencies and, secondly, we will numerically integrate over the momentum space, \( \mathbf{k} \). The general result can be written as:

\[
E = \sum_k S_k ,
\]

where \( S_k \) has different values in the superconducting and normal states. For the superconducting state, at temperature smaller than the critical temperature, \( T_c \), after the summation over the Matsubara frequencies is performed, \( S_k \) can be calculated from the following relation

\[
S_k = \frac{1}{\psi^2(k) \sqrt{\Delta(T)^4 + 4\Delta^2(T)E_g^2}} \\
\times \left[ \frac{2\xi_k \psi^2(k) (A^2(T) - E_g^2) \sqrt{\xi_k^2 + A(T)^2 \psi^2(k)}}{\sqrt{\xi_k^2 + A(T)^2 \psi^2(k)} + \frac{2\xi_k^2 + A(T)^2 \psi^2(k)}{2T}} \right. \\
- \frac{2\xi_k \psi^2(k) (B^2(T) - E_g^2) \sqrt{\xi_k^2 + B(T)^2 \psi^2(k)}}{\sqrt{\xi_k^2 + B(T)^2 \psi^2(k)} + \frac{2\xi_k^2 + B(T)^2 \psi^2(k)}{2T}} \\
+ \left. \frac{2\xi_k \psi^2(k) (B^2(T) - E_g^2) \sqrt{\xi_k^2 + A(T)^2 \psi^2(k)}}{\sqrt{\xi_k^2 + A(T)^2 \psi^2(k)} + \frac{2\xi_k^2 + A(T)^2 \psi^2(k)}{2T}} \right] ,
\]

whereas in the normal state, at temperatures larger than the critical temperature, \( T_c \), one has:

\[
S_k = \frac{1}{\sqrt{\xi_k^2 + E_g^2 \psi^2(k)}} \left[ 2\xi_k \sqrt{\xi_k^2 + E_g^2 \psi^2(k)} \right. \\
- \left. (2\xi_k^2 + E_g^2 \psi^2(k)) \tanh \frac{\sqrt{\xi_k^2 + E_g^2 \psi^2(k)}}{2T} \right] .
\]

The results obtained for the temperature dependence of the total energy, \( E \), obtained by integrating Eqs. (17) and (18), match perfectly at the critical point but the slopes of the curves are different, indicating a discontinuity of the specific heat at the transition point. The specific heat coefficient can be calculated in a straightforward manner by taking the derivative as a function of temperature. The results are presented in Fig. 2(a). Two important features are observed: first, as the analytical results predicted, the specific heat coefficient jump at the critical point, \( \Delta\gamma(T_c)/\Delta\gamma_0(T_c) \), (\( \Delta\gamma_0(T_c) \) represents the value of the specific heat coefficient jump at the transition point in the absence of the pseudogap) as function of the ratio \( E_g/\Delta_0(0) \) obtained from both the numerical (full line) and analytical (dashed line) calculations.

![FIG. 2: (a) Temperature dependence of the electronic single particle contribution to the specific heat coefficient, \( \gamma(T) \), for different values of the ratio \( E_g/\Delta_0(0) \). (b) The normalized specific heat coefficient jump at the critical point, \( \Delta\gamma(T_c)/\Delta\gamma_0(T_c) \), (\( \Delta\gamma_0(T_c) \) represents the value of the specific heat coefficient jump at the transition point in the absence of the pseudogap) as function of the ratio \( E_g/\Delta_0(0) \) obtained from both the numerical (full line) and analytical (dashed line) calculations.](image-url)
heat coefficient jump at the transition point as function of the ratio $E_g/\Delta_0(0)$, as extracted from numerical and analytical calculations. As expected, there are slight differences between the slopes of the numerical and analytical curves, a feature which is due to successive approximations used in the analytical calculation.

As we already mentioned different contributions to the specific heat coefficient, $\gamma(T)$, have to be considered for a better understanding of the HTSC specific heat data at high temperatures corresponding to the normal state. One possible mechanism was considered by Moca and Janko, and is related to the strong nature of the order parameter fluctuations in the critical region, leading to an important electronic pair contribution to the specific heat coefficient in the normal state. This contribution has been evaluated previously and we quote here the result for completeness, $C_{\text{pair}}^{\text{an}} \sim (T^*/T)^5 \exp(-2T^*/T)$, where $T^* = 2\pi E_g^2/g$ and $g$ describes the quasiparticle interaction. Fig. 3 presents the temperature dependance of the specific heat coefficient in the presence of a normal state pseudogap ($E_g/\Delta_0(0)$).

Electronic single particle and electronic pair contributions are summed to obtained the total electronic specific heat coefficient. The electronic single particle contribution is important for the specific heat coefficient jump at the transition point, whereas the electronic pair contribution can explain the broad maximum observed in the specific heat coefficient at high temperatures in the normal state. Note that no specific heat coefficient jump at the transition point is associated to the electronic pair contribution. A similar qualitative behavior of the total electronic specific heat coefficient was reported for HTSC.

IV. CONCLUSIONS

The nature of the pseudogap is still an open question and its explanation is beyond the scope of this paper. Using a simple phenomenological model we have investigated the temperature dependence of the specific heat coefficient both below and above the critical point for HTSC characterized by the presence of a pseudogap in the excitation spectrum of the normal phase. The single particle contribution is the most important contribution to the electronic specific heat, but this is not sufficient to explain the hump that develops at high temperatures in the normal state.

An important result that emerges from our calculations is the behavior of the specific heat jump at the critical point. Experimentally, in the underdoped region, where the pseudogap energy is large, the jump is very small in contrast with the overdoped region where the pseudogap is practically absent and a BCS-like behavior emerges with a large jump at the critical point. We have calculated the electronic single particle contribution to the specific heat jump at the critical point in the presence of the pseudogap and a similar dependence to the one experimentally observed was obtained. Increasing the pseudogap the specific heat jump at $T_c$ starts to decrease. This feature can be understand in terms involving the suppression of the superconducting state in the presence of the pseudogap, as both the superconducting gap and critical temperature are smaller due to a loss of states at the Fermi level. The specific heat anomaly presented in HTSC at high temperatures ($T > T_c$) can be successfully understood in terms of two particle (electronic pair) contributions to the specific heat. Note that the pair contribution to the specific heat does not affect the specific heat jump at the transition point.

Our analysis is based both on analytical and numerical calculations. The restrictions imposed by the approximations used in the analytical calculation lead to differences between the analytical and numerical results. Basically, the analytical results are reasonable around the optimal doping point and in the overdoped region, where the value of the observed pseudogap is small. With respect
to the phase diagram one should mention that the model we used is valid only in the second scenario discussed in the introduction, as the pseudogap presence leads to a reduction of the normal-superconducting phase transition temperature, meaning that the pseudogap should completely disappear around the optimal doping point. However, it is generally accepted that in the overdoped region the standard Fermi liquid and BCS theories are still valid, any inclusions of a pseudogap in the description of the system properties being inappropriate.

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