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Thermodynamic properties of the superconductivity in quasi-two-dimensional Dirac electronic systems

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Abstract. The thermodynamic properties of superconducting Dirac electronic systems is analyzed in the vicinity of quantum critical point. The system is characterized by a quantum critical point at zero doping, such that the critical temperature vanishes below some finite value of interaction strength. It is found that the specific heat jump of the system largely deviates from the conventional BCS theory value in the vicinity of quantum critical point. We investigated the region of applicability of the mean-field theory using the Ginzburg-Landau functional.

1 Introduction

A lot of attention has been devoted recently to quasi-two-dimensional condensed matter systems containing electrons that may be described by a relativistic Dirac – type Lagrangian, namely Dirac electrons. These are evidently non-relativistic systems, though the kinematics of such electrons is described by a Dirac instead of a Schrödinger term in the Hamiltonian [1–3]. This arises from the fact that in some materials there are special points in the Brillouin zone where two bands touch in a single point around which the electron dispersion relation may be linearized. The Fermi surface reduces to a point, the Fermi point, where the density of states vanishes. The elementary excitations around a Dirac point are Dirac electrons [4].

There are many important quasi-two-dimensional Dirac electrons systems. These includes high- T_c cuprates [5–8], graphene [9–20], and transition metal dichalcogenides [21–23].

The discovery of the high- T_c superconductors made a large impact on condensed matter physics, and in such systems, the superconductivity is considered to occur in a quasi-two-dimensional system of copper oxide (CuO_2) plane [24]. The Dirac points appear in the intersection of the nodes of the d -wave superconducting gap and 2D Fermi surface. The low-energy quasiparticle dynamics is determined exclusively by these points since they are occupied even at very low temperatures [1,6–8]. Because of these nodes, the low-energy quasiparticle spectrum is gap-

less and the dispersion relation can be linearized. Thus, Dirac electrons are expected to play an important role in the cuprates.

Dirac electrons also appear in semi-metals such as graphene sheets or stacks, namely graphite, where the vanishing density of states at the Fermi points has important consequences in the electronic properties [9–12,15–20]. Moreover, graphene can display unusual properties as a part of normal-superconducting hybrid structures, for instance, the Andreev reflection phenomenon.

Thorough investigation of graphite has revealed also the evidence of intrinsic superconductivity in doped samples [25]. Theoretically, various mechanisms of superconductivity in graphene have been considered. Both phonon- and plasmon- mediated mechanisms [26] as well as resonating valence bond and density wave lattice models [27,28] have been proposed. Recently, first principle calculations have predicted that doped graphene as a high-temperature electron-phonon superconductor [29]. It has been shown within the time tested BCS model that superconducting properties in undoped graphene [4,19,20,23,30,31] posses a quantum critical point (QCP), which connect the normal and superconducting phases. It is controlled by the magnitude of the effective superconducting interaction strength. However, the Cooper theorem of pairing is no longer valid as one expect in the absence of Fermi surface due to doping.

The quasi-two-dimensional transition-metal dichalcogenides (TMD) 2H-TaSe₂, 2H-TaS₂ and 2H-NbS₂ are layered compounds where s-wave superconductivity coexists with a charge-density wave (CDW) [32,33] at low temperatures and Dirac electrons produces interesting effects in the system. The Dirac points are formed in the

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intersection of the Fermi surface with the nodal lines of the charge-density wave order parameter [21–23]. This is a particular example of nodal liquids, which in general contain Dirac electrons [34].

Uchoa and co-workers have proposed theory for *s*-wave superconductivity in nodal liquids [23]. It was also observed, in contrast to the original BCS theory, which is not critical, there exist a QCP in the critical coupling parameter for undoped system. That is, when the system is doped, the superconducting gap is strongly changed as the coupling constant parameter is modified and the QCP is suppressed. The transport and thermodynamic properties of the nodal liquids deviate from the BCS theory of conventional superconductors.

For these reasons mentioned above, we are encourage to believe that Dirac electrons are expected to play an important role in the understanding of the superconductivity in various materials. Thus, the superconductivity in two-dimensional systems is of great relevance in the condensed matter physics.

Considering a two-dimensional model requires a few comments concerning the applicability of the mean field approach. It is well known that the superfluid transition in a two-dimensional system occurs in the form of the Berezinskii-Kosterlitz-Thouless transition at a temperature lower than the mean field transition temperature [4,35,36]. Thus, the transition temperature will give the temperature scale at which the amplitude of the order parameter becomes non-zero, whereas phase coherence occurs only at the lower transition temperature. Nevertheless, the applicability of the mean field approach improves for some material like graphite, where a nonzero interplanar coupling is always present [19,20,27].

Our aim in this paper is to investigate the thermodynamic properties of the Dirac electrons system in general form. We employ the Ginzburg Landau functional to establish the region of applicability of mean field approximation. This analysis will be perform using the standard *s*-wave BCS model for the Dirac electrons without invoking any nature of pairing mechanism (see Refs. [19,20]).

The rest of the paper is organise as follows, in Section 2, we use the standard BCS theory in two dimension to calculate the superconducting energy gap and the critical temperature as functions of the doping level and the pairing interaction. Also in that section, we analyse the behaviour in various coupling limit. Then, Section 3 is devoted to the derivation of thermodynamic properties of the Dirac electrons system. The applicability of the theory is considered within the context of Ginzburg Landau theory in Section 4. Finally, the Section 5 will be devoted to the discussion of results and conclusions.

2 BCS gap equation and temperature analysis

In this section, we employ the standard *s*-wave BCS gap equation in two-dimension to analyze the behavior of the system at both zero and finite temperature. The BCS gap equation in a spatially two dimensional uniform system is

given as [19,20,37]

$$1 = \frac{1}{2} \int |V_p| \frac{d^2p}{(2\pi\hbar)^2} \frac{1}{E_p} [1 - 2n(E_p)], \quad (1)$$

where the energy of excitations is $E_p = \sqrt{\xi_p^2 + \Delta^2}$ and $n(E_p)$ is the equilibrium Fermi distribution of quasiparticles with energies E_p . The energy measured from the Fermi level, $\xi_p = v_F p \pm \mu$, where v_F is the Fermi velocity and μ is the measure of doping. $|V_p|$ determines the pairing interaction.

Using the standard BCS theory of Dirac spectrum without including any form of pairing mechanism in other to be general, we assume an *s*-wave pairing interaction $V_p = -|V_p|$ that depends on the range of interaction. The coupling constant, λ is introduced using the relation:

$$\frac{|V_p|}{\pi\hbar^2 v_F^2} = \begin{cases} \lambda/\xi_m, & |\xi_p| < \xi_m, \\ 0, & |\xi_p| > \xi_m \end{cases} \quad (2)$$

where the ξ_m determines the range of the attractive interaction.

2.1 Zero temperature analysis

The zero temperature BCS gap equation for both electron and hole doping can be obtain as:

$$\begin{aligned} \frac{\xi_m}{\lambda} &= \frac{1}{2} \left[2 \int_{\mu}^{\xi_m} \frac{\xi_p}{\sqrt{\xi_p^2 + \Delta_0^2}} d\xi_p + 2\mu \int_0^{\mu} \frac{d\xi_p}{\sqrt{\xi_p^2 + \Delta_0^2}} \right] \\ &= \sqrt{\xi_m^2 + \Delta_0^2} - \sqrt{\mu^2 + \Delta_0^2} - |\mu| \log \left[\frac{|\mu| + \sqrt{\mu^2 + \Delta_0^2}}{\Delta_0} \right]. \end{aligned} \quad (3)$$

At zero temperature limit and when the system is undoped, $\mu = 0$, the BCS gap equation yields [19,20],

$$\Delta_0 = \xi_m \frac{\lambda^2 - 1}{2\lambda}. \quad (4)$$

This shows that the gap equation has a QCP, indicating that superconductivity can exist only above a minimum range of coupling interaction. Assuming that $\lambda = 1 + \varepsilon$, it can be shown that in the limit of $\lambda \rightarrow 1$ and the $\varepsilon \ll 1$ that $\Delta_0 = \varepsilon \xi_m$. Considering a finite but low doping case when the gap, Δ_0 is very small, equation (3) becomes

$$\Delta_0 = 2|\mu| \exp \left(\frac{-\xi_m (1 - \lambda)}{|\mu| \lambda} - 1 \right). \quad (5)$$

This shows that the gap is largely depend on the doping level, $|\mu|$ rather than the range of interaction and assure that gap exist for any finite doping in the system.

2.2 Finite temperature analysis

Considering both electron and hole doping, the finite temperature gap equation as a function of interaction coupling constant and doping parameter can be written as [19,20,23]:

$$\frac{\xi_m}{\lambda} = 2T \ln \left\{ \frac{\cosh(\sqrt{\xi_m^2 + \Delta^2}/2T)}{\cosh(\sqrt{\mu^2 + \Delta^2}/2T)} \right\} + |\mu| \int_0^{|\mu|} \frac{d\xi_p}{\sqrt{\xi_p^2 + \Delta^2}} \tanh \left(\frac{\sqrt{\xi_p^2 + \Delta^2}}{2T} \right). \quad (6)$$

For zero doping limit, $\mu = 0$, equation (6) becomes

$$\frac{\xi_m}{\lambda} = 2T \ln \left\{ \frac{\cosh(\sqrt{\xi_m^2 + \Delta^2}/2T)}{\cosh(\Delta/2T)} \right\}. \quad (7)$$

Using $\lambda \approx (1 + \varepsilon)$ in the low temperature limit, $\xi_m \gg T_c$, ($T = T_c$, $\Delta \rightarrow 0$) we have,

$$\xi_m = \xi_m + \varepsilon \xi_m - (1 + \varepsilon) 2T_c \ln 2. \quad (8)$$

Employing the relation, $\Delta = \varepsilon \xi_m$, we observe that in the vicinity of QCP, $\lambda \rightarrow 1$, we have $2\Delta_0/T_c = 2.77$. Far from the QCP, in the limit $\lambda \gg 1$, the critical temperature, $T_c = \xi_m \lambda/4$ and the zero gap dependence on the transition temperature is obtained as $2\Delta_0/T_c = 4$. These results agree with references [19,20,30,31]. We have seen that from the finite temperature analysis at zero doping, $\mu = 0$; the BCS universal ratio for normal metal $\kappa_0 \sim 2\Delta_0/T_c = 3.52$ is not satisfied at vicinity of QCP and strong coupling limit.

At finite doping, the critical temperature in the weak-coupling regime is obtain as:

$$T_c = \frac{2|\mu|e^\gamma}{\pi} \exp \left(\frac{-\xi_m(1-\lambda)}{|\mu|\lambda} - 1 \right) \quad (9)$$

where $e^\gamma = 1.781$. Substituting the zero temperature gap equation of equation (5) into equation (9), we get $2\Delta_0/T_c = 3.52$. Also, in the strong coupling limit ($\mu/\Delta \ll 1$), equation (6) can be written as:

$$\frac{\xi_m}{\lambda} = 2T_c \ln \frac{\cosh\left(\frac{\xi_m}{2T_c}\right)}{\cosh\left(\frac{\mu}{2T_c}\right)} + \frac{\mu^2}{2T_c}. \quad (10)$$

After some expansions; in the limit of $\lambda \rightarrow 1$, that is $\lambda \sim 1 + \varepsilon$; equation (10) can be simplify into

$$T_c = \frac{\Delta_0 + \sqrt{\Delta_0^2 + \mu^2 \ln 4}}{2 \ln 4}. \quad (11)$$

This is the expression for the superconducting transition temperature of the system when doped at strong coupling limit [23]. It can be observe that when the system is not doped, $\mu = 0$, we recover the relation $2\Delta_0/T_c = 2.77$.

Let now consider the behavior of the gap equation near T_c in the limit of $\Delta/2T \ll 1$. Considering the case of zero doping, $\mu = 0$, equation (6) is:

$$\frac{\xi_m}{\lambda} = 2T \ln \left\{ \frac{\cosh\left(\frac{\xi_m}{2T}\right)}{\cosh\left(\frac{\Delta}{2T}\right)} \right\}. \quad (12)$$

After expanding equation (12) and taking the limit $\lambda \rightarrow 1$, $\lambda \sim 1 + \varepsilon$ we have

$$\Delta = 2\sqrt{T_c \Delta_0} \tau^{1/2} \quad (13)$$

where $\tau = 1 - T/T_c$ and $T_c = \Delta_0/2 \ln 2$. Figure 1 shows the dependance of the superconducting gap to temperature when the system is not doped.

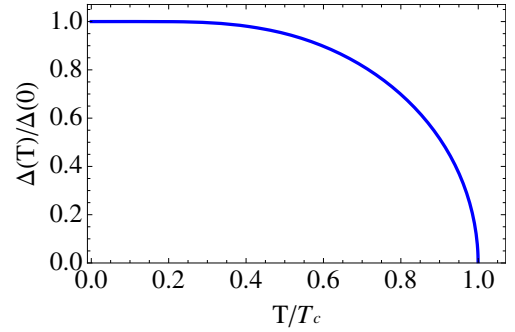


Fig. 1. (Color online) Superconducting gap dependence on temperature.

When the system is doped, $\mu \neq 0$, equation (6) becomes;

$$\frac{\xi_m}{\lambda} = 2T \ln \left\{ \frac{\cosh\left(\frac{\xi_m}{2T}\right)}{\cosh\left(\frac{\sqrt{\mu^2 + \Delta^2}}{2T}\right)} \right\} + \frac{\mu^2}{2T}. \quad (14)$$

We performed Taylor's series expansion in the limit, $\Delta/2T \ll 1$, and some algebraic simplifications near phase transition to obtain

$$\Delta = 2\sqrt{T_c \Delta_0 + \frac{\mu^2}{4}} \tau^{1/2}. \quad (15)$$

Equation (15) yields the behaviour of the gap close to phase transition when the system is doped and the gap vanish when the temperature equals the critical temperature ($T = T_c$). The dependence of the superconducting gap on doping for various temperature near T_c is shown in Figure 2. It is observed that the superconducting gap increases with doping at a finite temperature. Also, the low gap size corresponds to the temperature close to the transition temperature, T_c .

3 Thermodynamic properties

We proceed with calculating the difference between the thermodynamic potentials for the system in the superconducting and normal phases using the standard procedure [38]. The difference in thermodynamic potential is

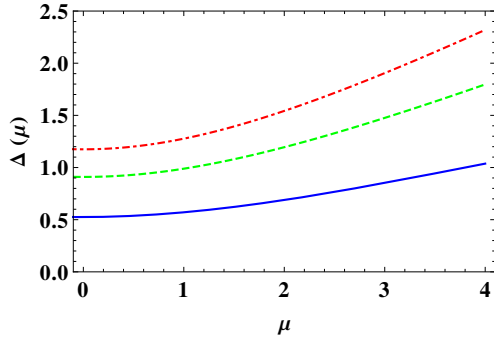


Fig. 2. (Color online) The superconducting gap of the Dirac electronic system as a function of the μ for different T . The temperature, $T = 0.75 T_c$ (red, dotdashed line), $0.85 T_c$ (green, dashed line) and $0.95 T_c$ (blue, solid line) for the parameter $T_c = 1$.

defined as follows;

$$\Omega_s - \Omega_n = V \int_0^\Delta d\Delta \Delta^2 \frac{d(1/\tilde{\lambda})}{d\Delta} \quad (16)$$

where $\tilde{\lambda} = \frac{\pi \hbar^2 v_F^2}{\xi_m} \lambda$ from equation (2). Expanding equation (12), the gap equation at low temperature limit for zero doped system ($\mu = 0$) can be re-written as:

$$\frac{\xi_m}{\lambda} = 2T \left(\frac{\xi_m}{2T} - \frac{\Delta}{2T} \right) + 2T \ln \frac{1 + e^{-\xi_m/T}}{2} - 2T \ln \frac{1 + e^{-\Delta/T}}{2}. \quad (17)$$

Expanding equation (17) in the low temperature limit, $\xi_m \gg \Delta$, we obtain the relation:

$$\Delta = \Delta_0 - 2T \exp(-\Delta/T). \quad (18)$$

To obtain the thermodynamic potential, we start by differentiating equation (17) with respect to Δ and incorporating $\tilde{\lambda}$ to obtain (we have assume $\hbar = 1$);

$$\frac{d}{d\Delta} \left(\frac{1}{\tilde{\lambda}} \right) = -\frac{1}{\pi v_F^2} \tanh \left(\frac{\Delta}{2T} \right). \quad (19)$$

At low temperature limit, where $\Delta/T \gg 1$, we approximate $\tanh(\Delta/2T)$ by $1 - 2 \exp(-\Delta/T)$. Applying the result in equation (16) and substituting equation (18) into the resultant equation, we get

$$\Omega_s - \Omega_n = \frac{1}{\pi v_F^2} \left[-\frac{\Delta_0^3}{3} - 4T^2 \Delta_0 e^{-\frac{\Delta_0}{T}} - 4T^3 e^{-\frac{\Delta_0}{T}} + 4T^3 \right]. \quad (20)$$

In the present low temperature limit, the normal phase thermodynamic potential is given by $\Omega_n = -4T^3/\pi v_F^2$. Then, the entropy of the system, $S_{n,v} = -\partial\Omega_n/\partial T = 12T^2/\pi v_F^2$ and the specific heat capacity can be written $C_{n,v} = 24T^2/\pi v_F^2$.

These results should be contrasted with the conventional behaviour of thermodynamic potential for normal metal describe by Landau Fermi liquid theory. In that case, $\Omega_n \sim -T^2$ and therefore both entropy and specific heat are linear in temperature. In the case of Dirac fermions, the density of state is not a constant but depends linear in energy. The energy is counted from nodal point. This feature of the density of state therefore lead to quadratic behaviour of both entropy and specific heat of Dirac fermions at zero doping. We point out that for finite doping, the Fermi surface is a circle (for zero doping, it is just a point). The density of state at the Fermi level is a constant for the doped case. Therefore, the specific heat and entropy will be described by conventional Landau Fermi liquid formulas for normal metal.

Thermodynamic potential for the superconducting material becomes

$$\Omega_s = \frac{1}{\pi v_F^2} \left\{ -\frac{\Delta_0^3}{3} - 4T^2 \Delta_0 e^{-\Delta_0/T} - 4T^3 e^{-\Delta_0/T} \right\}. \quad (21)$$

Thus, the electronic specific heat of the superconducting state of the system is:

$$C_{s,v} = T \frac{\partial S}{\partial T} = \frac{4\Delta_0^3}{\pi v_F^2 T} \exp(-\Delta_0/T). \quad (22)$$

To consider the jump in specific heat capacity of Dirac electrons systems, we start with the gap equation for undoped case in the limit $\mu/T_c \ll 1$ near phase transition (Eq. (12)) and take care of the proper density of state. The thermodynamic potential difference becomes;

$$\begin{aligned} \Omega_s - \Omega_n &= -\frac{2T_c \Delta_0^2}{\pi v_F^2} \tau^2 (1 + \tau) \\ &= -\frac{2T_c \Delta_0^2}{\pi v_F^2} \left(1 - \frac{T}{T_c} \right)^2. \end{aligned} \quad (23)$$

After algebraic simplification, the jump in specific heat capacity at T_c is

$$\Delta C|_{T_c} = \frac{4\Delta_0^2}{\pi v_F^2}. \quad (24)$$

This is one of the result we are after. It can also be observed that the jump in specific heat does not depend linearly on T_c as the standard BCS theory of conventional superconductors. Using the relation $\Omega_n = -4T^3/\pi v_F^2$ and $\Delta_0 = 2T_c \ln 2$, we have

$$\left[\frac{C_s - C_n}{C_n} \right]_{T_c} = 0.32. \quad (25)$$

We observed that the universal constant in the vicinity of QCP is 0.32. This strong decrease from the BCS universal constant value of 1.43 for conventional superconductor is attributed to the vanishing density of states at the Fermi point. We note that Uchoa et al. [23] obtained the value of 0.35 using different approach.

4 Ginzburg Landau functional

In this section, we use the superconducting gap dependence near phase transition and the jump in specific heat capacity to recover the coefficients of the Ginzburg Landau functional when the system is not doped. The fluctuation correction to the specific heat capacity is used to establish the limit of the applicability of the Ginzburg Landau theory. In the zero magnetic field, the Hamiltonian of the system close to superconducting transition related to the presence of the fluctuation Cooper pairs in it can be written as:

$$F[\Psi(r)] = \int dV \left\{ a|\Psi(r)|^2 + \frac{b}{2}|\Psi(r)|^4 + c|\nabla\Psi(r)|^2 \right\} \quad (26)$$

where Ψ is the order parameter, a , and b are the coefficients that depends on temperature. The order parameter coincides with the value of the superconducting gap in spectrum of one-particle excitations and can be denoted as $\Delta(r)$.

From the Landau theory of phase transitions, the superconducting gap, Δ is related to the coefficients and temperature as follow:

$$|\Delta|^2 = -\frac{a}{b} \quad (27)$$

where $a = \alpha|\tau|$ and $|\tau| = \frac{T-T_c}{T_c}$. Also, the jump of the specific heat capacity at the phase transition point can be written as [39,40], $\Delta C = C_s - C_n = \alpha^2/2bT_c$.

Employing equation (13), the superconducting gap equation near phase transition at zero doping, into equation (27) we get $b = \alpha/4\Delta_0 T_c$. Using the relation, $\Delta C = 4\Delta_0^2/\pi v_F^2$ we have, $\alpha = 4T_c \ln 2/\pi v_F^2$. Then, the coefficients a , b , and c becomes

$$a = \frac{4T_c \ln 2}{\pi v_F^2} \left(1 - \frac{T}{T_c} \right); \quad b = \frac{1}{2\pi v_F^2 T_c}, \quad \text{and } c = \frac{1}{\xi_m}. \quad (28)$$

Now, let consider the contribution of fluctuation to the heat capacity in the normal phase of the Dirac electrons system. Restricting ourselves to the region of temperatures beyond the immediate vicinity of transition, where this correction is still small, the fourth-order term in $\Psi(r)$ can be omit with respect to the quadratic one [39].

However, for the Dirac electrons system which is basically 2D systems, the fluctuation correction to the specific heat capacity turns out to be [40]

$$\delta C_{fl} = \frac{1}{4\pi} \frac{\alpha T_c}{c\tau}. \quad (29)$$

This correction allows us to answer quantitatively about the limits of applicability of the GL theory. In the vicinity of the transition point, this theory can be applied up to the temperature when the fluctuation corrections become comparable to the value of the corresponding physical values themselves. The relationship between the fluctuation correction and the change in specific heat is of the form, $\delta C_{fl} \ll \Delta C$;

$$\frac{bT_c}{2\pi c\alpha} \ll \tau \quad (30)$$

where $\bar{G}i = bT_c/2\pi c\alpha$. $\bar{G}i$ is the so-called Ginzburg-Levanyuk number, which is defined as the value of the reduced temperature at which the fluctuation correction reaches the value of the difference in specific heat capacity, ΔC . The mean field approximation is applicable in the region $\bar{G}i \ll \tau$ [40].

Considering undoped Dirac electronic system in strong coupling limit ($\mu/T_c \ll 1$), we substitute the parameters b , c , and α into equation (30) to obtain

$$\bar{G}i(\mu = 0) = \frac{1}{16\pi \ln 2} \frac{\xi_m}{T_c}. \quad (31)$$

Using the relations at zero temperature analysis, we get

$$\bar{G}i(\mu = 0) = \frac{\lambda}{4\pi(\lambda^2 - 1)}. \quad (32)$$

Equation (32) can be used to obtain the range of applicability of the theory in the strong coupling limit. The theory fails in the vicinity of QCP ($\lambda \rightarrow 1$).

When the system is doped, it takes the Fermi surface to becomes that of a normal two dimensional system and the Ginzburg number, $\bar{G}i$ can be written as

$$\bar{G}i(\mu \neq 0) = \frac{T_c}{\mu}. \quad (33)$$

Substituting the value of T_c in the weak coupling limit (Eq. (9)) into equation (33), we have

$$\bar{G}i(\mu \neq 0) = \frac{2e^\gamma}{\pi} \exp\left(\frac{-\xi_m(1-\lambda)}{|\mu|\lambda} - 1\right). \quad (34)$$

Using equations (32) and (34), the regions where the theory is applicable in a 2D Dirac electronic system is established.

5 Conclusions

We have theoretically studied the thermodynamic properties of superconducting Dirac electrons systems and re-examined the superconducting gap at both zero and finite temperatures without invoking any form of pairing mechanism and assuming a standard s -wave.

The thermodynamic properties of the Dirac electrons systems is different from the conventional superconductors. For instance, the specific heat jump of the system is obtained as 0.32 ($\Delta C_v/C_n = 0.32$) in the vicinity of QCP. This is a strong deviation from the BCS universal constant value of 1.43 for conventional superconductor because of the vanishing density of states at the Fermi point. We used the Ginzburg Landau functional parameters which depends on the system of material to analyze the range of applicability of the mean field theory. It is observed that close to the QCP, the theory of superconductivity is not applicable. But different phases BCS and non-BCS exist, which depends on coupling constant, λ , the range of attractive interaction, ξ_m and the level of doping, μ .

Finally, we have presented both qualitative and quantitative description of thermodynamic properties of 2D Dirac electrons system in the vicinity of QCP and established the domain of applicability of the mean-field theory. We presented Ginzburg Landau treatment of fluctuations. The work on time-dependent Ginzburg Landau is in progress.

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