Experimental evidence of pseudogap and its emergence

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May 11, 2018

Abstract

Energy gap is necessary in superconductor phase transition, as physicists widely agree with. Unconventional superconductors, especially cuprates, among other novel properties, has been believed to exist a so-called pseudogap state, where only wave vectors oriented in copper oxide bond are allowed, within a temperature range, while higher than Tc. Experiments on underdoped superconductors such as BSCCO reveal its close relationship with preformed Cooper pairs. The recently observed pair density wave is possible to correspond with its spatial distribution. However, the origin of pseudogap is still under debate. Here we mainly present a review of the experiment evidence. We will also briefly introduce several theoretical progress on its emergence.

1 Introduction

1.1 Superconductivity

In 1911, superconductivity was first discovered in mercury. Here comes the era of condensed matter physics. Superconductor is characterized by several interesting experimental effects, for example zero resistance and Meissner effect. Below certain temperature, (usually we call it T_c), the resistance falls to zero Ohms. In fact, T_c is a function of magnetic field. Generally speaking, the stronger the magnetic field is, the lower T_c becomes. We have known from Electro and magnetism that there will be no electric field inside a metal when existing a static electric field outside. However, it usually will not happen for magnetic field. While Meissner effect tells us, this could happen for superconductor if the magnetic field not too strong.
In 1972, a Nobel Prize was awarded for BCS theory. BCS points out several key facts about superconductors. One is Cooper pair. In BCS, electrons with wave vector $\boldsymbol{k}$ and -$\boldsymbol{k}$ will pair up together. BCS Hamiltonian is basically involved with s-wave pair, which is usual the case for conventional superconductors. Another one is the energy gap. BCS predicts a finite energy gap delta between the ground state energy and Fermi energy. Later we will see how these two facts play a significant role in so-called unconventional superconductor, (or Type-2 superconductor).

1.2 Cuprates

In 1987, another Nobel Prize was awarded for superconductor, thrilling the world. The transition temperature of unconventional superconductor is above the liquid nitrogen boiling temperature, having potential for great application. Up to now, many of the unconventional superconductors are cuprates i.e. complexes with oxides and copper. Lets first take a look at the crystal structure of cuprate, for example $La_{2-x}Sr_2CuO_4$(LSCO).[1]

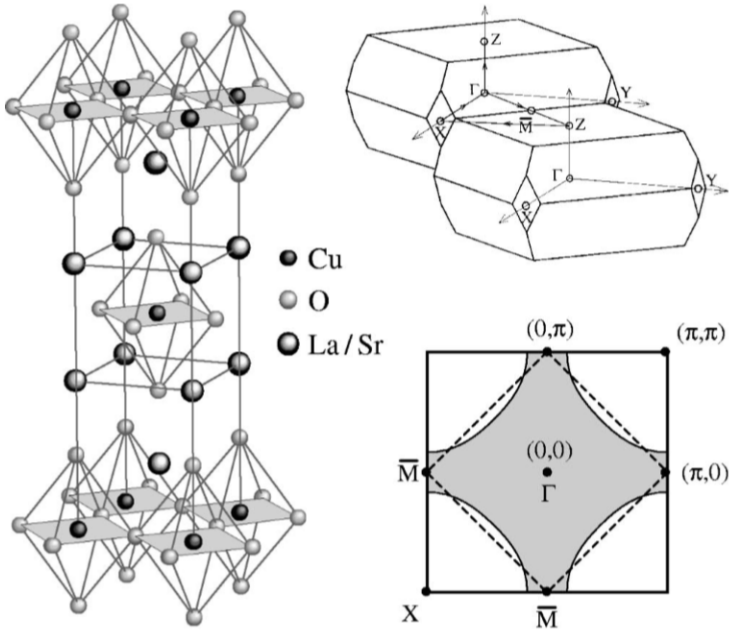

Fig 1. Crystal structure of LSCO and its Fermi surface[1]

From Fig 1, we can clearly see that LSCO is in a layer-by-layer structure. It has a tetragonal unit cell. Here c is much longer than a. From band theory, we can expect anisotropic properties in cuprates, for example anisotropic resistance. The copper atom and its nearest oxygen atoms form an octahedron. These octahedrons form a BCC structure. While Lanthanum and Strontium atoms insert between the octahedron layers. This complex structure originates from its parent compound La_2CuO_4. Actually, after Sr doping, there exists distortion in this tetragonal structure. More interestingly, when the temperature is lowered, the octahedron will slightly rotate and thus many exotic phases comes out, for example superconductor and pseudogap[1]. The top inset is the shape of Brillouin zone. Compared with its crystal structure, it is clear that the $\gamma-\bar{M}$ is in the direction of copper-copper bond. The $\gamma-$X line is in the direction of copper-oxygen bond. The bottom inset is the calculated fermi surface, including the next-nearest-neighbor hopping. Here, the fermi surface is a hole-like fermi surface.

The origin of its superconductivity is still under debate. Actually, it goes beyond BCS. For example, the parent compound La_2CuO_4 is a Mott insulator. For BCS, we usually expect a metallic material, having small resistance at room temperature and suddenly resistance dropping to zero at some temperature. Maybe, this is one of reason why it takes 70 years to find unconventional superconductor after superconductivity firstly discovered.

1.3 Mott insulators

For better understanding of cuprates and its amazing phase diagram, let us talk about Mott insulator first. Band theory is one of most fundamental theory in condensed matte physics. It achieves a great success by predicting many properties in solids. For example, if certain material has a partially occupied band, it is predicted to be a conductor and vice verse. It does work for a lot of materials. However, not for Mott insulator. Because of strong electron-electron interaction, La2CuO4, for example, turns out to be an insulator, even if its band is not fully occupied. Here comes a question. Is there a way to overcome this electronelectron interaction and turn these Mott insulators into conductors? The answer is 'Yes'. Thanks to those genius scientists, they find the strong electron electron interaction can be broken by doping and introducing distortion into the crystal[2]. Lets take a look at the phase diagram of two doping types.

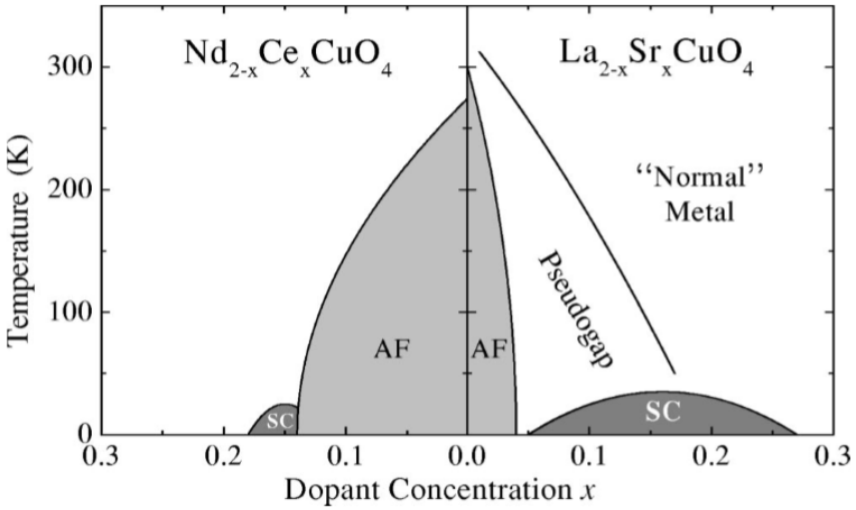

Fig 2. Phase diagram of $Nd_{2-x}Ce_xCuO_4$ and $La_{2-x}Sr_xCuO_4$[1]

There are two types of doping, electron doping and hole doping. In Fig 2, $Nd_{2-x}Ce_xCuO_4$ is electron doped and $La_{2-x}Sr_xCuO_4$ is hole doped. When not doped, both of materials are antiferromagnetic insulators. After a small dopant concentration, $La_{2-x}Sr_xCuO_4$ is a so-called pseudogap phase. Then, within a wide dopant concentration range, $La_{2-x}Sr_xCuO_4$ becomes a superconductor. While $Nd_{2-x}Ce_xCuO_4$ behaves differently during the phase transition. First, it does not have pseudogap state. Second, the dopant concentration range for antiferromagnetic phase is wide and that of superconductor is not. In this essay we will mainly focus on pseudogap state. It is worthy to note that there is no clear boundary of pseudogap phase. Later we will see it clearly.

2 Pseudogap

Pseudogap is referred as a phenomenon that a gap is opened near the Fermi surface when this gap is transparent for wave vectors in certain directions, as shown in Fig 3[3]From Fig 2, phase diagram, we can find pseudogap usually exists in the underdoped superconductors. Below is the shape of fermi surface in $Bi_2Sr_2CaCu_2O_8$(Bi2212).

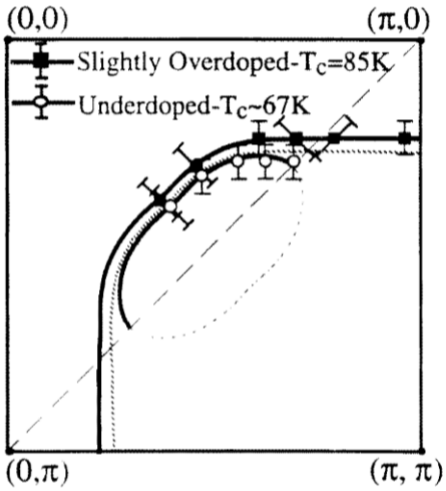

Fig 3. Fermi surface of overdoped and underdoped $Bi_2Sr_2CaCu_2O_8$[3]

In Fig 3, for overdoped superconductor there is clearly a closed Fermi surface, more exactly a closed hole like Fermi surface. For underdoped superconductor, there only exists a so-call Fermi arc. And this Fermi arc stopped at (0,π) and (π,0) line. From BCS, we know below T_c, an energy gap Δ exists between ground state energy and Fermi energy. More importantly, this energy gap is an isotropic energy gap, meaning that a gap exists for all directions of wave vector. This energy gap we usually call it superconductor gap. Here we need to clarify several properties of such superconductor gap. First, it is independent of temperature. More exactly, the number of Δ/k_BT_c remains a constant. This means the higher transition temperature is, the deeper the superconductor gap becomes. And the optimally-doped cuprates have the deepest superconductor gap. Second, such gap opens only below T_c and does not exists above T_c. In another word, in BCS system, there is a clear Fermi surface above T_c. In overdoped system, it is quite similar. However, in underdoped system, it opens a partially transparent gap near the Fermi surface.

2.1 Existence of pseudogap based on ARPES Research

Up to now, ARPES is still one of the basics experimental tools for pseudogap research. To understand the anisotropicity of the pseudogap quantitatively, lets read a ARPES image of Bi2212

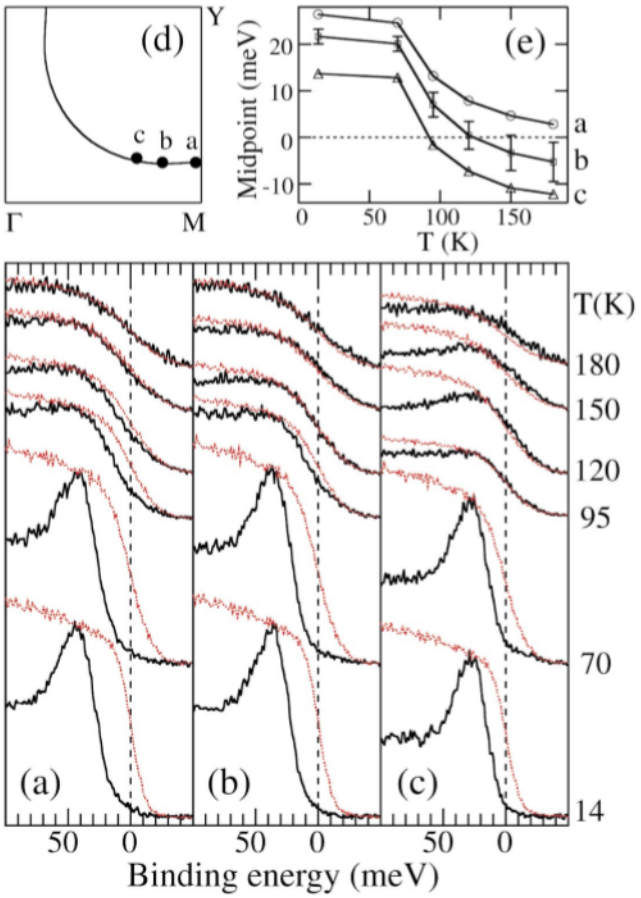

Fig 4. ARPES image of underdoped Bi2212 (T_c=84)[1]

Fig 4 shows the energy absorption at different position, marked in the inset (d). The inset (e) shows the leading-edge midpoint shift according to the temperature. The black line is the data for Bi2212 and the red line is that for Polycrystalline Pt. Comparing (a) and (c), we can find the midpoint of leading-edge pulling back at position (a) at 120K and 95K. This pulling back implies a gap opens at position (a). From inset (b), we can conclude that the size of pseudogap in the reciprocal space, not the value of the gap, grows as the temperature decreases. Since there is no pulling back in the leading-edge at 120K and it exists at 95K. When analyzing the temperature dependence of the gap, pseudogap behaves similarly with superconductor gap, both independent of temperature[1][4].Taking these two aspects, size growing when lowering the temperature and depth remaining, some scientists argue that as the temperature lowered, the pseudogap develops into the superconductor gap,[1] as shown in Fig 5[3].

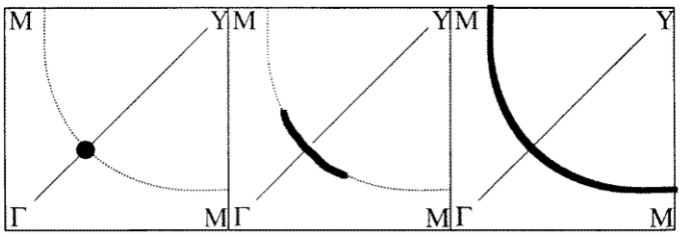

Fig 5. The size of the gap shrinks as the temperature rising (from left to right)[3]

2.2 Debate on pseudogap

2.2.1 The relationship between pseudogap and superconductor gap

ARPES shed light onto the existence of pseudogap while STM brought a great debate on its nature. At first, lets see some data from early tunneling conductance research.

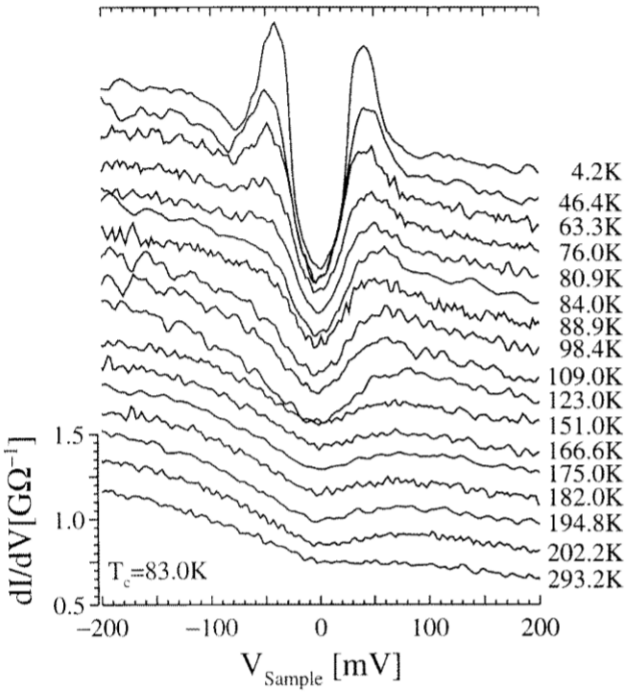

Fig 6. Tunneling conductance for underdoped Bi2212[3]

In Fig 6, below T_c, there is a deep dip centered at the Fermi energy and two peaks indicating superconductor gap. The dip extends out close to room temperature while the peak vanishes above T_c. Besides, the slope of peaks decreases as the temperature go down. Such suppression of the excitation is believed to have relationship with pseudogap. Same story happens to the suppression of the dip. [3]As we mentioned before, the separation of the peaks does not

change with the temperature, implying the superconducting gap independent of temperature. However, early research did not show the spatial inhomogeneity or measure the pseudogap energy directly. So far it seems to correspond with the model we mention above, i.e. the pseudogap evolving into superconductor gap. However, some of the scientists argue that the gap measured here is not the superconductor gap, instead, being pseudogap. And they refer the energy of the superconductor gap to the energy for breaking the Cooper pairs[5].

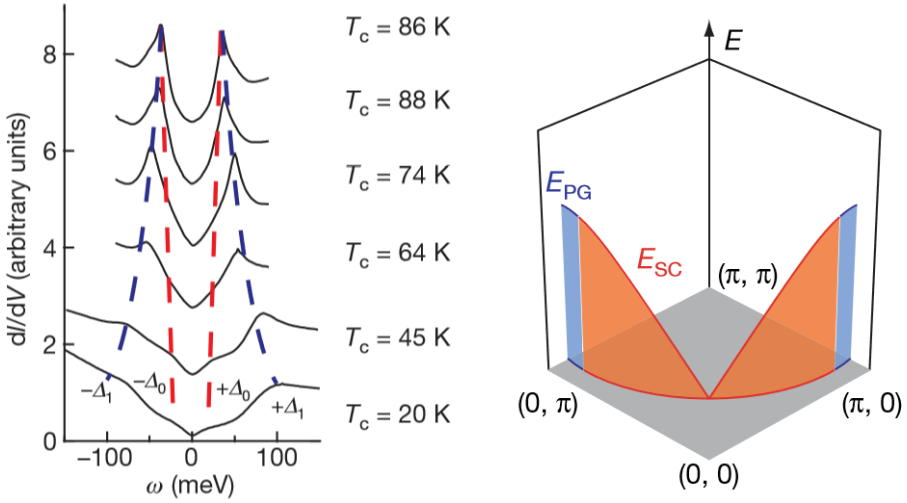

Fig 7. Spatially averaged tunneling spectrum of Bi2212[5] and electronic structure in 3D plot[4]

According to Fig.7, Bi2212 samples, with different dopant concentration, apparently have different energy gap. They claimed, the peak, marked by blue dash, signals the pseudogap here they call it delta1[4]. The red dash is the superconductor gap. Actually, here they defined the superconductor energy by the extinction energy of Bogoliubov quasiparticles. Or we can interpret it as the energy for breaking the Cooper pair. The right inset shows the relationshiphip between these two energy scales. The orange part stands for the d-wave superconductor gap. The blue part stands for the pseudogap. Here, both of the two energy gaps are temperature independent, however, the superconductor gaps will close above T_c and pseudogap stays.

2.2.2 Symmetry breaking and order parameter candidates

Up to now, the symmetry in a pseudogap phase is under most severe debate. Actually, they have consensus, for example, translational and rotational symmetry breaking. However, as for the rotational symmetry, there also exist disagreements. Some assume pseudogap maintain C4 symmetry[6], some insist on C4 symmetry reducing to C2[5]. Besides, other symmetries, like mirror symmetry breaking and time-reversal symmetry breaking, are both supported by partial scientists[7].

Along with the mysterious symmetry is its unknown order parameter. Some scientists believe in the close relationship between the pair density wave and pseudogap[8]. While, some

other scientists argue they are separate phenomena since they have different critic doping concentration[9].

2.2.3 Two theory of pseudogap

Marginal fermi liquid phenomenology Marginal Fermi-liquid phenomenology is one of a popular theory in cuprates. A trial to apply this theory to pseudogap is based on a so-called circulating current (CC) phase. In marginal Fermi-liquid phenomenology hypothesis, excitations which contribute to both the charge and spin polarizability of the form, shown as below, exist over a wide range of momentum $\boldsymbol{q}$[10].

$$\mathrm{Im}\tilde{P}(\mathbf{q},\omega)\sim\begin{cases}-N(0)(\omega/T) \text{ for } |\omega|<T,\\ -N(0)\mathrm{sgn}\omega \text{ for } |\omega|>T,\end{cases} \qquad (1)$$

One particle Green's function turns out to be incoherent near Fermi surface. Apply this method into solving the general Hamiltonian, where interactions on Cu and on O and the nearest neighbor interaction between Cu and O are included. Then, a phase, with time-reversal symmetry breaking and rotational symmetry breaking, occurs automatically[11]. However, as we mentioned above, the rotational symmetry breaking is still under debate. According to some STM research, C_4 symmetry might also be broken[7]. Also, the next nearest neighbor interaction is necessary to obtain the hole-like Fermi surface.[1]

t-J model t-J model is a strong coupling model. A spin-spin interaction term is included, since pseudogap has a close relationship with Mott insulator. Also, next nearest neighbor term is included by allowing t_{ij} varying on different positions.

$$H=P\left[-\sum_{\langle ij\rangle,\sigma}t_{ij}c^{\dagger}_{i\sigma}c_{i\sigma}+J\sum_{\langle ij\rangle}\left(\boldsymbol{S}_i\cdot\boldsymbol{S}_j-\tfrac{1}{4}n_in_j\right)\right]P. \qquad (2)$$

By adding more elaboration terms, t-J model is still active in pseudogap theory.

3 Strange Metal

When talking about the pseudogap, it is natural to mention strange metal. Let us read a phase diagram of cuprates.

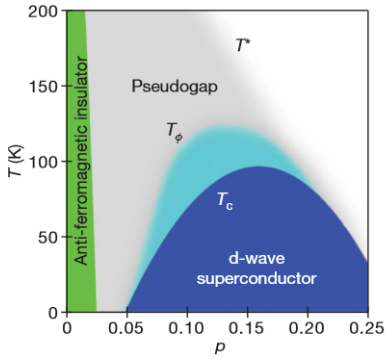

Fig 11. Phase diagram of Bi2212[5]

Pseudogap phase occupies a domain, having a long temperature range. From pseudogap phase, if we raise the temperature, we can obtain a so-called strange metal phase, which is the white part in Fig 11. Notably, there is no clear boundary between pseudogap and strange metal, even though there is a charactoristic temperature T^*.

3.1 Fermi liquid theory

For normal metal, there is a famous Wiedemann-Franz (WF) Law. It shows a universal relation between heat conductivity and electrical conductivity[12].

$$\frac{\kappa}{\sigma T} = L_0$$

κ is heat conductivity. σ is electric conductivity. L_0 is a universal constant.
Actually, such result is a natural conclusion of Fermi liquid theory. Let us first introduce the conventional picture. For a metal, it is clear that the charge carrier is electron, which is a Fermion. When carrying heat, electrons, again, play an important role. Besides, the lattice vibration, or we usually say phonons, transport heat, too. However, at low temperature, some degrees of freedom will be frozen, for example, phonon. As a result, at low temperature, electron is both charge carrier and main heat carrier. From a conventional view, WF law implies that the charge carrier and heat carrier in a metal are Fermions and more exactly, the same Fermion.
Fermi liquid theory gives us a similar picture, except that the charge carrier and heat carrier are not electrons. In fact, they are Fermion-like quasi-particles. While, such quasi-particles do have a close relationship with electrons. They are excited modes of electrons. We know that in Fermi gas model, the Fermions are treated as non-interactive free particles, still obeying Fermi-Dirac distribution. However, it is not true in a real metal. There exists electron-electron interaction, let alone electron-phonon interaction. Fermi liquid theory points out only electrons near Fermi surface are involved in those transportation processes, and the excited modes just behave like a free electron except for modified effective mass and energy spectrum.
Up to now, Fermi liquid theory achieve a great success. Most of the metallic materials obey the WF law, behaving like a Fermi liquid. Actually, even superconductors obey such law, apparently not at their superconductor states. At superconductor state, the charge carrier

is mainly Cooper pair, not quasi-particle. Since the Cooper pairs do not carry entropy, they cannot transport heat. The heat carrier is still Fermion-like quasi-particle. While, some of the cuprates do not obey WF law above T_c[12]. Instead, they behave strangely. This is why scientists call it strange metal.

3.2 Breakdown of Fermi liquid theory

Cuprates like $(Pr, Ce)_2CuO_4$ (PCCO)[12] $Bi_{2.1}Sr_{1.9}CaCu_2O_{8+x}$(BSCCO)[13] seem to have separate carriers for heat and charge transportation, more exactly, 'spin-charge separation'[14]. In BSCCO, a moment-energy-independent continuum of fluctuation has been reported recently[13]. Lets take PCCO as an example to have a brief introduction to strangle metal.

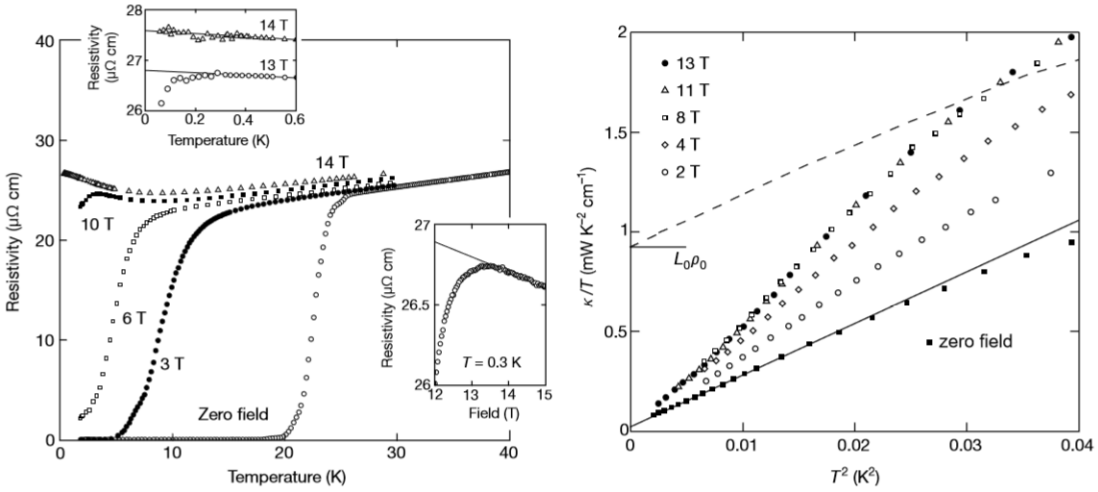

Fig 12. Electric resistance and thermal conductivity of PCCO[12]

The zero field transition temperature of this PCCO sample is around 20K. When $B = 14T$, the superconducting state is totally broken. Above T_c, the resistance evolves in a power law as $a + bT^{\alpha}$, $\alpha = 1.7$[12]. In the upper inset of the left figure in Fig 12, resistance rises slightly as the temperature goes down at B=14T. The authors attribute it to the weak location and they demonstrate it by applying a transverse magnetic field as shown in the bottom inset. Thus the charge carrier behaves like a quasi-particle.

However, in the right figure, such carrier seems not to contribute to the heat conductivity as it is expected. $L_0\rho_0$ is the value calculated based on the resistance measured in the left figure. We know the thermal conductivity of the free Fermions is supposed to be linear in temperature. While that of free bosons is supposed to be proportional to T^3. Another strange phenomenon is related with the saturate magnetic field. To fully destroy the superconducting state, about 14T magnetic field is necessary. However, the magnetic field saturates around 8T in the right figure. The mismatch between the two characteritic magnetic field implies more physics deep inside the pseudogap.

4 Conclusion

There remains great deal of research to do on pseudogap, both theoretical and experimental. The symmetry, the order parameter, even its origin are all ambiguous. Perhaps, we just did not classify it clearly. Or maybe there are several different types of pseudogap, governed by different mechanism. Whatever the mystery is, research on pseudogap will definitely lead us to a better understanding in superconductors as well as the whole condensed matter physics.

References

[1] A. Damascelli, Z. Hussain, and Z.-X. Shen, "Angle-resolved photoemission studies of the cuprate superconductors," *Reviews of modern physics*, vol. 75, no. 2, p. 473, 2003.

[2] N. Mott, "Conduction in non-crystalline materials: Iii. localized states in a pseudogap and near extremities of conduction and valence bands," *Philosophical Magazine*, vol. 19, no. 160, pp. 835–852, 1969.

[3] T. Timusk and B. Statt, "The pseudogap in high-temperature superconductors: an experimental survey," *Reports on Progress in Physics*, vol. 62, no. 1, p. 61, 1999.

[4] Y. Kohsaka, C. Taylor, P. Wahl, A. Schmidt, J. Lee, K. Fujita, J. Alldredge, K. McElroy, J. Lee, H. Eisaki, *et al.*, "How cooper pairs vanish approaching the mott insulator in bi 2 sr 2 cacu 2 o 8+ δ," *Nature*, vol. 454, no. 7208, p. 1072, 2008.

[5] M. Lawler, K. Fujita, J. Lee, A. Schmidt, Y. Kohsaka, C. K. Kim, H. Eisaki, S. Uchida, J. Davis, J. Sethna, *et al.*, "Intra-unit-cell electronic nematicity of the high-t c copper-oxide pseudogap states," *Nature*, vol. 466, no. 7304, p. 347, 2010.

[6] M. Karmakar, "Thermal transitions, pseudogap behavior, and bcs-bec crossover in fermi-fermi mixtures," *Physical Review A*, vol. 97, no. 3, p. 033617, 2018.

[7] L. Zhao, C. Belvin, R. Liang, D. Bonn, W. Hardy, N. Armitage, and D. Hsieh, "A global inversion-symmetry-broken phase inside the pseudogap region of yba 2 cu 3 o y," *Nature Physics*, vol. 13, no. 3, p. 250, 2017.

[8] M. Hamidian, S. Edkins, S. H. Joo, A. Kostin, H. Eisaki, S. Uchida, M. Lawler, E.-A. Kim, A. Mackenzie, K. Fujita, *et al.*, "Detection of a cooper-pair density wave in bi 2 sr 2 cacu 2 o 8+ x," *Nature*, vol. 532, no. 7599, p. 343, 2016.

[9] S. Badoux, W. Tabis, F. Laliberté, G. Grissonnanche, B. Vignolle, D. Vignolles, J. Béard, D. Bonn, W. Hardy, R. Liang, *et al.*, "Change of carrier density at the pseudogap critical point of a cuprate superconductor," *Nature*, vol. 531, no. 7593, p. 210, 2016.

[10] C. Varma, P. B. Littlewood, S. Schmitt-Rink, E. Abrahams, and A. Ruckenstein, "Phenomenology of the normal state of cu-o high-temperature superconductors," *Physical Review Letters*, vol. 63, no. 18, p. 1996, 1989.

[11] C. Varma, "Pseudogap phase and the quantum-critical point in copper-oxide metals," *Physical Review Letters*, vol. 83, no. 17, p. 3538, 1999.

[12] R. Hill, C. Proust, L. Taillefer, P. Fournier, and R. Greene, "Breakdown of fermi-liquid theory in a copper-oxide superconductor," *Nature*, vol. 414, no. 6865, p. 711, 2001.

[13] M. Mitrano, A. Husain, S. Vig, A. Kogar, M. Rak, S. Rubeck, J. Schneeloch, R. Zhong, G. Gu, C. Varma, *et al.*, "Singular density fluctuations in the strange metal phase of a copper-oxide superconductor," *arXiv preprint arXiv:1708.01929*, 2017.

[14] S. A. Kivelson, D. S. Rokhsar, and J. P. Sethna, "Topology of the resonating valence-bond state: Solitons and high-t c superconductivity," *Physical Review B*, vol. 35, no. 16, p. 8865, 1987.