

Fractional fermi fluid as a model to understand the pseudogap regime in high temperature cuprate superconductors

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Abstract

At low temperatures, $T < T_c$, atoms form Cooper pairs in the superconducting state. Because it takes energy to break these pairs, there is no way to remove a single particle without adding energy to the system. This leads to a gap in the single-particle energy spectrum. When temperature is increased such that $T > T_c$, remnants of this gap, where certain energy ranges have few states associated with them, remain. These have been termed pseudogaps. This pseudogap behavior has been found to exist in underdoped cuprates and is temperature and doping dependent. This paper aims to review the pseudogap regime of cuprate superconductors and to discuss the experimental observations of this pseudogap. Then it will introduce the fractional fermi liquid model as an explanation for this pseudogap.

1 Introduction

Since their discovery by Bednorz and Muller in 1986, high temperature superconducting cuprates have been one of the most studied correlated electron materials. However, the origin of this superconductivity still remains a mystery. It was discovered that cuprate superconductors exhibit a wide range of phases as a function of hole doping. In particular, this paper will focus on the pseudogap regime of under-doped superconducting cuprates. In this regime, a pseudogap emerges in the electron energy spectrum at temperatures much larger than the superconducting transition temperature T_C . Additionally, various forms of competing order seem to emerge. This paper is structured in the following way: first, an analysis of the the crystal structure of the of cuprates, then a brief discussion of the cuprate superconducting state, followed by a summary of the behavior observed in the pseudogap regime of under-doped cuprates. Finally, an introduction to the Fractionalized Fermi Liquid (FL*) model will be given, which provides an explanation for the emergence of the pseudogap regime.

2 Crystal structure of cuprates

The crystal structure of high temperature superconducting cuprates is characterized by two-dimensional superconducting CuO_2 sheets separated by non-superconducting layers as seen in Figure 1. The copper ions in these planes are either in their +2 or +3 oxidized states, so that each ion has either one or two holes located in its 3d orbital. These CuO_2 layers are the key to the superconductivity of cuprates.

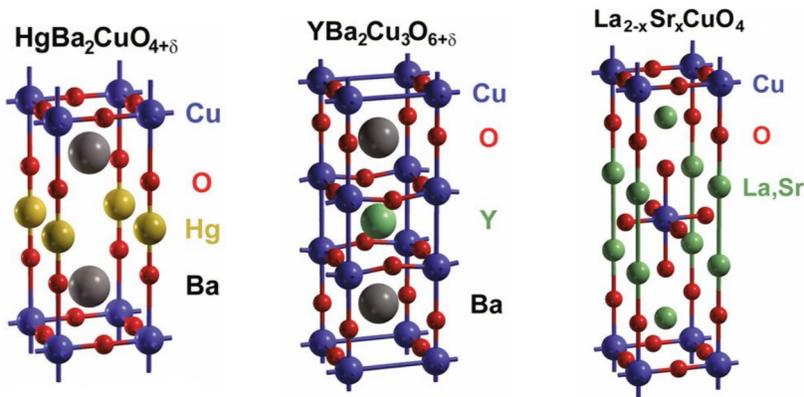


Figure 1: The layered crystal structure of high temperature superconducting cuprates [1]. CuO_2 planes separated by insulating spacer layers.

In Figure 1, we see that each copper ion is enclosed by six oxygen atoms. This octahedron enclosure of oxygen atoms in conjunction with the 3d orbitals of the copper ions, shown in Figure 2, immediately gives rise to a splitting of energy levels. Because the $d_{x^2-y^2}$ and d_{z^2} orbitals point toward the oxygen atoms while

the d_{xy} , d_{yz} , and d_{xz} orbitals point away from them, the $d_{x^2-y^2}$ and d_{z^2} orbitals experience a larger relative Coulomb repulsion raising them to a higher energy level. Additionally, another energy splitting occurs because the $d_{x^2-y^2}$ orbital is closer to the in-plane oxygen atoms than the d_{z^2} orbital. This means that the $d_{x^2-y^2}$ orbital is at a higher energy level than the d_{z^2} orbital. This results in the $d_{x^2-y^2}$ orbital being the one that is half-occupied.

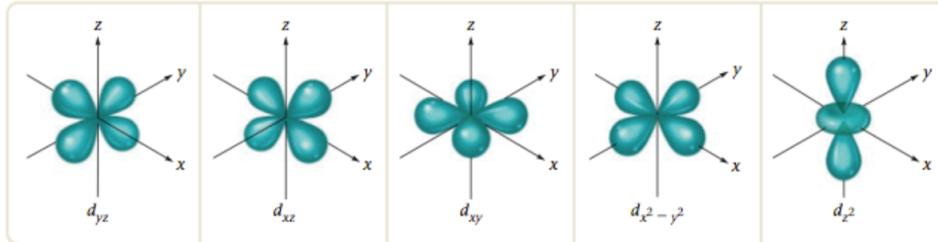


Figure 2: The layered crystal structure of high temperature superconducting cuprates [?]. CuO_2 planes separated by insulating spacer layers.

The oxygen ions, on the other hand, have full a $2p$ orbital. Using the same argument as for the copper ions, because the in-plane p_x and p_y orbitals are closer to the copper ions than the p_z orbital, the p_x and p_y orbitals are at a higher energy level than the p_z orbital. This indicates that we need to focus on the $2p_x$ and $2p_y$ orbitals of the oxygen ions. In summary, to understand high temperature superconducting cuprates, we need to consider the overlapping $3d_{x^2-y^2}$ orbital of the copper ions and the $2p_x$ and $2p_y$ orbitals of the oxygen ions.

3 Parent antiferromagnetic state

Because the copper $3d_{x^2-y^2}$ orbitals are half-filled in the undoped parent system, it would be reasonable to assume that this system would be a conductor. However, because the energy required for the double occupancy of electrons at a single site is much larger than the energy required for electrons to hop between nearest neighbor sites, the electrons remain localized and the parent compound is actually an insulator.

Although the electrons are localized and do not actually occupy the same site, they can virtually hop between sites with the superexchange interaction. The Pauli exclusion principle states that electrons with the same spin cannot occupy the same site, so this virtual hopping of anti-parallel spins of copper ions onto the same oxygen site gives rise to antiferromagnetism.

4 Hole doping

The magnetic nature of cuprate superconductors has been shown to be dependent on temperature and doping level. Doping is accomplished by either adding or removing electrons to or from the spacer layers between the CuO_2 planes. When holes are added, electrons are pulled away from the CuO_2 planes leaving behind holes to maintain charge neutrality. Figure 3 shows the phase diagram for hole-doped cuprates. Because this paper will focus on hole-doped cuprates, the question then becomes in which orbital will the doped holes choose to reside when they are introduced to the CuO_2 layer. Because the oxygen orbitals are already full, one could assume that the holes would occupy the copper orbitals. However, spectroscopy measurements have shown that the holes actually prefer the oxygen orbitals [1]. This is because hole occupancy of the oxygen orbitals is more energetically favorable than double occupancy of the copper orbitals.

A closer look at Figure 3 shows that the antiferromagnetic state is destroyed at a doping of $p_{min} \approx 0.05$, the critical doping at which superconductivity sets in. The transition temperature T_C then grows to a maximum at an optimal doping of $p_{opt} \approx 0.16$. It then decreases for higher doping, eventually vanishing at $p_{max} \approx 0.27$ [2]. Materials with a doping of $p_{min} < p < p_{opt}$ are classified as under-doped, while materials that have a doping of $p_{opt} < p < p_{max}$ are called overdoped. Regions of this phase diagram that are now well-understood include the antiferromagnetic phase, the fermi liquid, and the superconducting state. The strange metal and the pseudogap are not-well understood. However, this paper will primarily focus on the pseudogap regime.

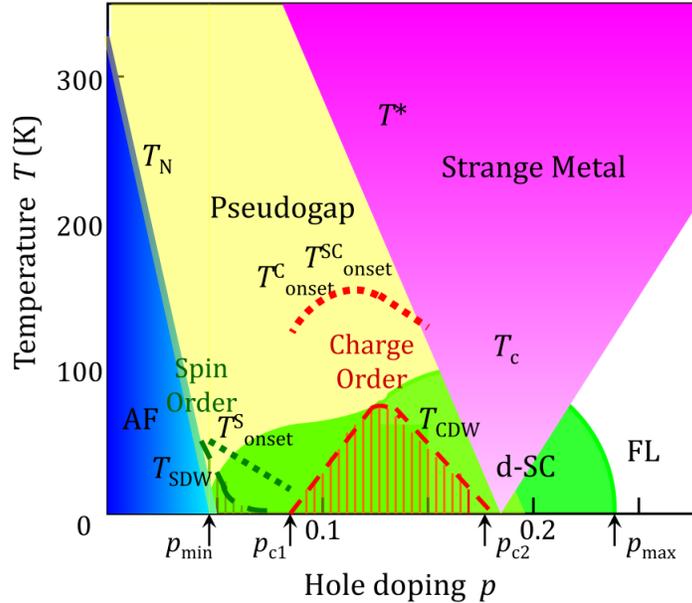


Figure 3: Phase diagram for cuprates [2]. The x-axis is the doping level of the system, which controls the electron concentration per copper site on the CuO_2 planes. The y-axis is temperature.

5 High temperature superconducting cuprates

Since the 1986 discovery of high temperature superconducting cuprates, a qualitative understanding of the nature of their superconductivity has been achieved. First, it is interesting to note that cuprates were originally materials not considered to be able to exhibit superconductivity. This was due to the fact that cuprates are such poor conductors at room temperature and that they become insulating antiferromagnets if their chemical composition is even slightly altered []. Also magnetism arises from strong repulsive interactions between electrons while conventional superconductivity comes from induced attractive interactions. Clearly, the highly correlated electronic nature of superconducting cuprates complicates things.

One of the most notable aspects of superconducting cuprates is their high transition temperature T_C , which exceeds the transition temperature of other materials by almost an order of magnitude and surpassed what was widely believed at the time of their discovery to be the highest possible temperature that superconductivity could survive. This high transition temperature is strange because according to BCS theory, despite strong Coulomb repulsions, relatively weak attractions between electrons induced by the coupling to phonons can bind the electrons to form Cooper pairs that condense in a manner similar to the way bosons condense to form superfluids. These Cooper pairs have an energy smaller than the phonon energy $\hbar\omega_D$. This should imply that T_C would be small because $k_B T_C \ll \hbar\omega_D \ll E_F$, and it was believed for a while that T_C could never exceed $30K$ [2]. But as seen in Figure 4, cuprates have a T_C that is significantly larger than this supposed upper bound.

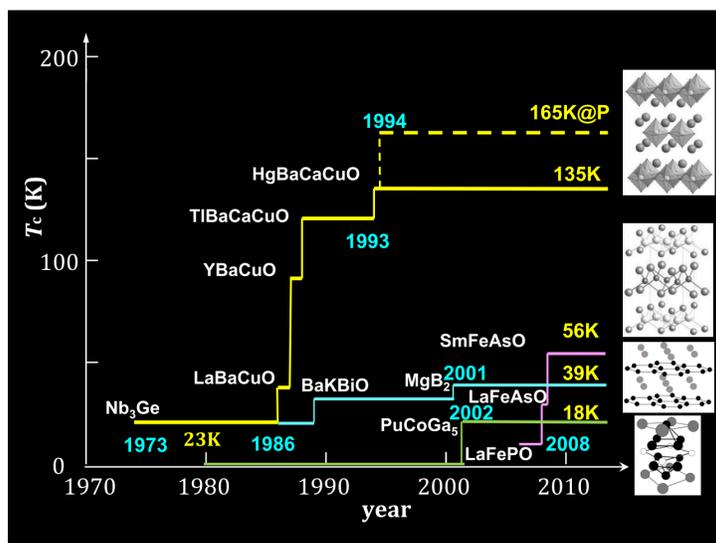


Figure 4: Timeline of the discovery of superconducting materials and their transition temperatures. [2]

Classic BCS theory is able to describe some of the behavior of superconducting cuprates. For example, BCS theory states that the superconducting ground is a condensate comprised of Cooper pairs. This is

also the ground state for superconducting cuprates [?]. Also in line with classic BCS theory, photoemission experiments indicate the presence of quasi-particles and reveal the Bogoliubov-type dispersion [?]. However, the behavior of superconducting cuprates quickly begins to diverge from classical superconductivity theory. An example of this deviation is the d-wave symmetry exhibited by the cuprate superconductors as opposed to the predicted s-wave symmetry of conventional superconductors [3]. This deviation indicates that superconductivity in cuprates may have a different origin than classical superconductors.

Cuprate superconductors are also unique because they seem to be robust to any forms of disorder. Because of their doped nature, they can be considered to be quite impure and BCS theory dictates that any form of potential disorder, like the impurities in cuprates, should suppress the superconducting state [4]. Even though under-doped cuprate superconductors have a disordered lattice, the d-wave hole-doped superconductor still persists. To understand the superconducting state, there needs to be an understanding of the states out of which the superconducting state emerges, namely the strange metal and the pseudogap regime. Behaviors seen in the pseudogap regime follow.

6 The pseudogap regime

The question now becomes: how is the pseudogap phase related to the superconducting phase. In hopes of answering this question, much recent research has focused on the pseudogap regime of under-doped cuprates. The pseudogap was first discovered when nuclear magnetic resonance measurements found a drop in the spin susceptibility $\chi_s(T)$ [5]. A reduced density of states was later confirmed with specific-heat data [6]. Its name is derived from this observation of a reduced density of states and the fact that there is a partial gap that appears at the Fermi surface at temperatures much larger than T_C . This gapped region retains its conducting properties, but with increased doping, the gap diminishes and the materials become more metallic. There is substantial evidence of competing orders different from superconductivity that are at play in this regime.

6.1 Fermi surface reconstruction

Early efforts to map the Fermi surface of the pseudogap regime consisted of quantum oscillation measurements performed on $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ at optimal doping. Instead of seeing a large Fermi surface that enclosed the total number of electrons n_e , these measurements revealed the existence of a small Fermi pocket that existed instead [5].

These quantum oscillation measurements were soon replaced by angle-resolved photoemission spectroscopy (ARPES), which would provide a direct map of the Fermi surface of the pseudogap regime in momentum space. These ARPES measurements revealed the existence of a large Fermi surface in cuprates but also showed that as doping was reduced to the parent insulating phase, the Fermi surface does not remain intact but breaks up into Fermi arcs [5]. It was found that these gaps are located at the antinodal regions of the Brillouin zone, as shown in Figure 5. A gapped Fermi surface is expected for the superconducting state, but what was interesting about the measurements of these Fermi arcs was the appearance of the gap at temperatures much higher than the transition temperature T_C . It was thought that these holes were might be due to some kind of density-wave reconstruction given the antinodal locations of the pockets [5].

Later, it was found that the appearance of the Fermi arcs was temperature-dependent and that existed only in the pseudogap regime. They collapsed to nodes below T_C , and the full Fermi surface was recovered above T^* , the temperature at which the pseudogap disappears [5]. This lead to the thought that the pseudogap regime was actually the precursor to the superconducting phase. This explanation states that Cooper pairs start to form in the pseudogap regime, but phase fluctuations keep them from condensing into the superconducting order until the temperature is lowered. This idea is supported by measurements of diamagnetism which is observed up to about $T = 150\text{K}$ [5].

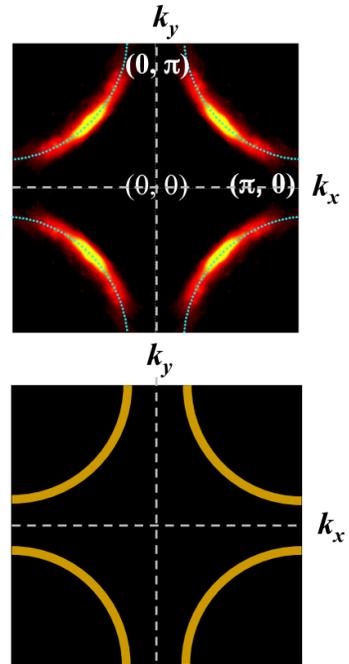


Figure 5: Fermi arcs of the pseudogap regime [2].

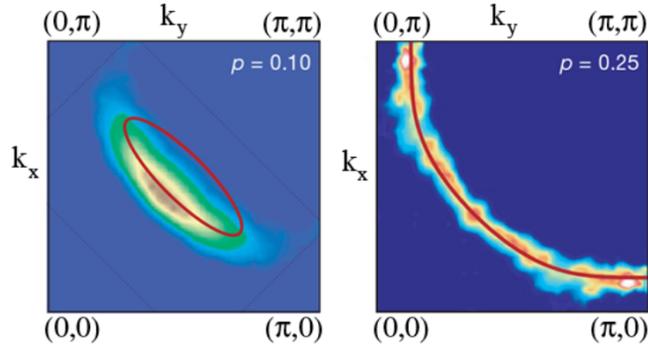


Figure 6: ARPES measurements of the Fermi arc seen in the pseudogap regime for low hole doping (left) and the full Fermi surface seen for large hole doping [5].

The best support for this theory of pre-formed pairs comes from scanning tunneling microscopy (STM) measurements that show a smooth evolution of the pseudogap into the superconducting state energy gap. These measurements also show that in the superconducting state, the low energy excitations near the nodes behave like one would expect for a BCS d-wave state, but at higher energies, charge stripes were found to exist [7], a form of charge order.

6.2 Charge order

To better understand this pseudogap that forms, experiments were that were directly related to electron charge, such as measurements of electrical conductivity, were performed. Two outcomes are possible: there could be an in-plane charge response in the CuO_2 layers or a response for charge transport between planes. It was found that the charge current is confined to be just in the CuO_2 plane [6].

In the 1990s, neutron scattering experiments showed a stripe-like charge order in that formed in the underdoped LSCO family. These stripes are characterized by a segregation of the antiferromagnetic order and charge. These stripes of charge are unique because they stay metallic and even superconduct at low temperatures. This system can now be viewed as a partially crystallized superconductor formed from electron pairs [7]. It was also found that these charge stripes form pair density waves, of which the phase reverses from stripe to stripe [7]. X-ray experiments measured that this short-range charge order gradually appears between $T = 100\text{K}$ and $T = 200\text{K}$. High energy x-ray scattering and NMR experiments confirmed that the charge order is static [8]. Uni-directional stripes of doped holes separated by undoped antiferromagnetic regions.

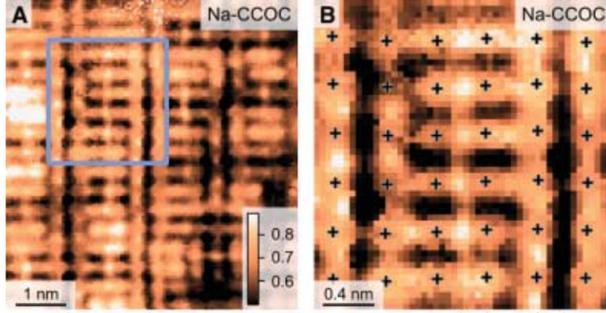


Figure 7: Charge order seen in under-doped cuprates [9].

6.3 Quantum liquid crystal

There is also evidence that a quantum liquid crystal structure exists in the pseudogap regime, which indicates a breaking of rotational symmetry. A temperature-dependent resistivity was measured at for different levels of doping for $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ [8]. Figure 8 shows that from panels (a)-(c) transport anisotropy decreases with decreased doping, but between panels (c) and (d), the transport anisotropy suddenly increases again. Neutron scattering experiments performed on $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ showed an instability to form uni-axial domains at low temperatures $T = 150\text{K}$ [8], providing further evidence of a nematic phase.

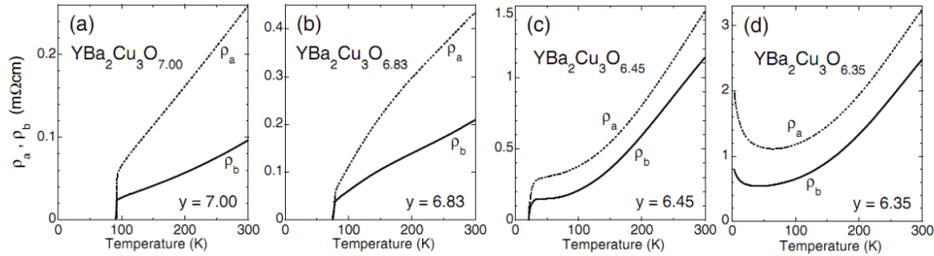


Figure 8: Resistivity measurements of $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$

[8]

7 Fractionalized Fermi liquid model

As we have now seen, the normal state for above the superconducting state is not the standard Fermi liquid but rather what is known as the pseudogap regime, which has well-defined low-energy excitations but small Fermi surfaces. The Fractionalized Fermi liquid (FL^{*}) model was introduced to explain the physical origin of the pseudogap regime. This model applies at a temperature just below T^* , where evidence for the pseudogap

regime is just measured suppression in the spin susceptibility and the appearance of the Fermi arc in the electron spectral function.

First, consider the structure of a doped spin liquid. Start with a doped antiferromagnetic with p holes per unit cell. Note that although the antiferromagnetic has p holes, the band insulator has $p + 1$ holes. To see this, start with the band insulator, which has full occupancy. To get the antiferromagnet, remove an electron from each site, alternating up and down spins. p electrons are further removed, leaving the p -doped antiferromagnet. As p increases, the antiferromagnetic order is destroyed so that the system becomes a spin liquid with p holes. The spins of the antiferromagnet become pairs into singlets. The remaining holes carry a spin and charge $+e$ and are called holons. Neutral spin- $\frac{1}{2}$ excitations called spinons also exist in the system as shown in Figure 9.

Now, add an attractive potential between the holons and the spinons. The holons and spinons then pair up to form bound states with charge $+e$ and spin- $\frac{1}{2}$. If we consider the strong coupling limit in which this pairing only happens between nearest neighbor sites, then we get the FL^* model shown in Figure 9. These fermionic dimers that form between the holons and spinons resonate with the original spin singlet pairs. Because there is a dilute gas of these fermionic dimers, they form a metallic state with a Fermi surface and the picture is similar to the Fermi liquid picture.

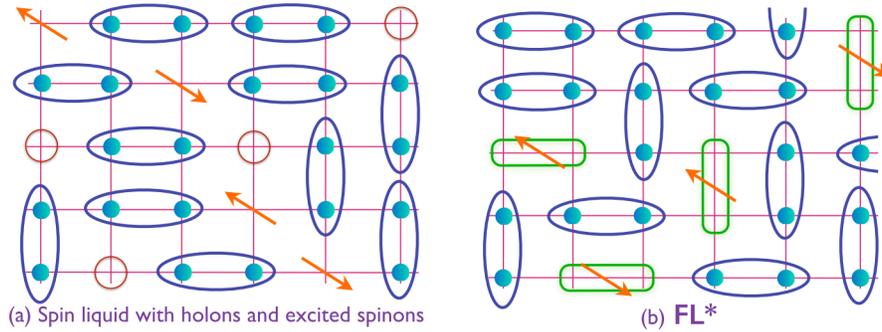


Figure 9: ARPES data for two levels of hole doping of YBCO [5]. The left image is data for a doping of $p = 0.1$ and shows the Fermi arc that forms. The right image is data for a doping of $p = 0.25$ and shows that a large Fermi surface forms instead.

However, there are differences between the FL^* model and the Fermi liquid model. In the FL^* model, a density of p spin- $\frac{1}{2}$ particles with charge $+e$ are enclosed by the Fermi surface while a density of $1 + p$ particles is enclosed in a Fermi liquid. This is a clear violation of the Luttinger's theorem, which states that the particle number enclosed by the Fermi surface would be equal to the total number of electrons n_e or a hole density of $1 + p$, followed by Fermi liquids. Also in contrast with the Fermi liquid model, the FL^* model introduces a second type of quasi-particle, which are the dimers that form between the holons and

the spinons.

8 Conclusion

Studying the physics of cuprates was originally inspired by trying to understand why superconductivity can happen at such a high temperature. However, there is still plenty of research that needs to be done to explain the competing order in the pseudogap regime.

References

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