Term Paper – Physics 498ESM – Spring 2004

"STM Studies of Cuprate Superconductors"

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The paper summarizes recent STM experiments that have found spatial modulations on the tunneling conductance on $Bi_2Sr_2CaCu_2O_{8+\delta}$. In the superconducting phase those modulations have been related to quasi-particle interference due to scattering from defects. Similar modulations found on the pseudogap phase don't seem to fit to the quasi-particle explanation. In the end discuss how those experiments fit on the big picture and try to give some personal inputs on the subject.

1. Background

For almost twenty years, the superconductors with high transition temperatures (high-T_c) have been keeping many physicists busy. The challenge to explain the microscopic mechanism of the High-T_c superconductivity have generated numerous proposals and discussions†.

Scanning Tunneling Microscopy (STM) is a powerful tool to investigate the electronic states of conducting materials at atomic scale. In this paper I will give an overview of results obtained by applying this technique on high-T_c superconductors. The measurements reveal that the electronic states have an spatial modulation. This results could be used as a way to verify the diverse proposals for ordering in cuprates.

1.1 What do you measure with STM?

Before I start I just want to give the reader a better idea of what STM consists.

The STM uses an conducting tip in order to scan the density of states of an conducting sample. Once the tip gets close enough (about 10A) to the sample, it is able to tunnel current to it. So by keeping the current constant as it scans, one obtains a topographic image of the sample. The (bias) voltage you apply to the sample, will define until which electronic state you are tunneling (also, the polarity will define if you are tunneling to electrons or holes states).

The most interesting feature is that if you are able to measure the differential tunneling conductance, the derivative of the tunneling current on the bias voltage (V_b), at a certain point, you will be obtaining the local density of states(LDOS)[1]:

$$\mathrm{LDOS}(E,r) \propto dI(V_b, r)/dV_b \qquad \text{with } E = eV_b \qquad (1)$$

And by LDOS one should understand the following:

$$\mathrm{LDOS}(E,r) \propto \Sigma_k \, |\Psi_k(r)|^2 \, \delta(E - \varepsilon(k)) \qquad (2)$$

with Ψ_k are the eigenstates for (quasi)particles with dispersion relation $\varepsilon(k)$.

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† Curiosity: if you goggle Ref. [3], the high-Tc discovery, on the web of science, you will find it received more than 6810 citations! Not bad!

One kind of experiments that is often used to contrast STM data is the angle-resolved photoemission spectroscopy (ARPES). Refer to [2] for a good review. As an scattering method, ARPES will make the spectroscopy map on the momentum phase space, providing you the dispersion relation $\varepsilon(k)$.

Bottom line is: STM allow you to obtain a map in real space of the LDOS. Most of the data I will be showing here consists of those LDOS maps.

1.2 What is interesting in High-T_c superconductors?

The materials I will be interested are the so called cuprates. Those are ceramic compounds in which some elements, e.g. Yttrium and Barium, are sandwiched between Copper-Oxygen planes. Initially being insulators, superconductivity will arise once we dope the Cu-O plane with holes. This is done by substitution of some of the sandwiched element. For example, in the pioneer experiment [3], the material La_2CuO_4 have some of the La atoms, which have 3 available electrons, replaced by Sr, which has only 2 electrons available, making $La_{2-\delta}Sr_{\delta}CuO_4$.

The superconductivity on those materials is different from the one with low-T_c. The mechanism to understand the formation of the Cooper pairs can no longer be understood in terms of BCS. One of the striking features is that BCS pairs have zero angular momentum (s-wave symmetry) while most of the High-T_c ones have non-zero angular momentum (d-wave symmetry).

The general behavior of the cuprates as we change temperature and doping is illustrated in the phase diagram below (figure1).

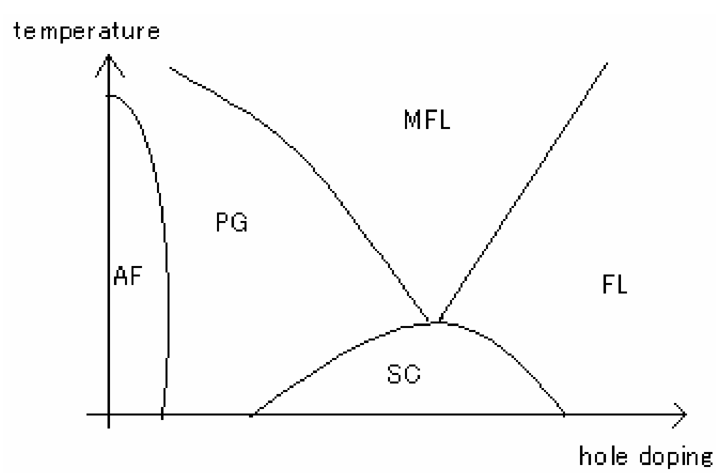


Figure 1: "Typical" cuprate phase diagram. Electronic behavior as function of the Temperature and hole doping.

In this paper I will be showing data obtained in both the superconducting phase(SC) and the pseudogap region (PG). The other areas are the ones that are understood the best. On zero doping, the cuprates are insulators and with temperatures low enough, they present an antiferromagnetic (AF) transition. At high doping we are in a metal phase, well understood well by introducing the quasiparticle concept, forming the so-called Fermi liquid (FL). The central area (MFL, marginal Fermi liquid), above the superconduting regime and between the Fermi liquid and pseudogap region is characterized by a similar behavior to the Fermi liquids but with some transport properties quite different. I will not enter in details about these here, let's instead focus our attention to our two area of interest.

The superconduting phase is characterized by the Coopper pair formation, related presence of a energy gap (with d-wave symmetry in cuprates), which leads to zero resistivity. So even if the ingredients are known, the challenge is to find the mechanism for the formation of this gap.

The pseudogap regime is not superconducting but also have direct indications of a presence an energy gap. Energy gap can be easily seen when we take a look at the density of states. Let's take a look at the STM data taken by Renner et al.[4] shown in (figure 2):

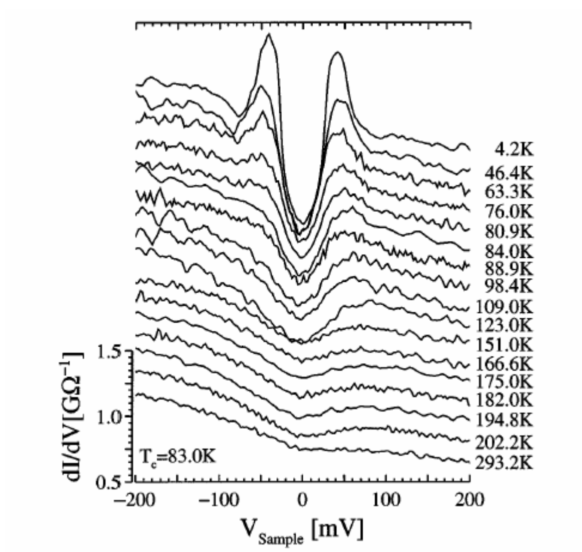


Figure 2: Conductance as function of the bias voltage at various temperatures. This data was taken in slightly underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) which has T_c = 83K. The peaks on the gap boundaries are related to the superconductivity coherence. Notice that once we move to the pseudogap regime we don't have those peaks. The scale correspond to the data at 293K and the offset is for clarity. Fig. taken from [4].

This data shows the presence of a gap in temperatures way higher than T_c and having still a tiny presence even in room temperature. In STM experiments we are not able to visualize the symmetry of the gap, because, as it is shown in equation (2), as we map in real space the LDOS we don't have the angle dependence in momentum k. Data from other experiments, e.g. ARPES, have shown that the pseudogap has the same symmetry as the superconducting gap (d-wave). For a good experimental review paper on the pseudogap, I recommend the reader to check [5].

Now if the superconducting gap is related to the pair formation, one may ask "what kind of order is related to the pseudogap"? This no one knows. Many think they do though... Various models have arisen trying to explain all experimental data but little agreement have been achieved. A fast look in the literature and one finds models with pair formation without long-range order, charge or spin order, circulating currents, quantum critical points, etc. I could write ten papers going through those models. So let's restrict ourselves to analyzing later how some of those models stands to experiments described next.

2. Data

Almost all STM data was taken in single crystals of $Bi_2Sr_2CaCu_2O_{8+\delta}$. The reason is that to perform and experiment, a very clean and flat surface is needed. This is achieved by cleaving the sample in situ, in ultra high vacuum. This cleaving process is very effective in $Bi_2Sr_2CaCu_2O_{8+\delta}$ but very arduous in other cuprates. The sample is not cleaved in the Cu-O plane (where superconductivity happens) but in the Bi-O plane. It is believed though that the tip is able to probe the electronic states in the Cu-O plane.

In an experiment performed in J. C. Davis' lab [6], they mapped the tunneling conductance for various values of sample bias. One of those can be seen in (figure 3). Their data is taken at 4K, scanning nearly optimum doped samples (with T_c ranging from 78K to 85K) The topography map shows the ability to scan with atomic resolution and gives a better idea of the location and resolution in which the data was taken. As the atoms are displaced from their ideal square lattice, they form this supermodulation along the crystal b-axis shown on the inset. The second image is an example of the tunneling conductance map.

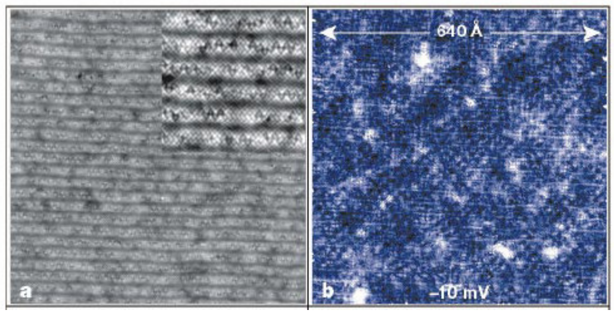


Figure 3: Atomic resolution images taken with a 640A field of view(FOV). (a) Topographic image of the Bi-O plane. The inset is a x2 magnification to show better the quality of the image. (b) Tunneling conductance map, $g(r,V_b)$, taken with bias voltage V_b = -10mV. Images found in [7].

Now in order visualize modulations on real space we can take a Fourier transform of the maps and visualize the reciprocal lattice. Constant modulations in real space will be represented by points in momentum space. Examples The result can be seen below:

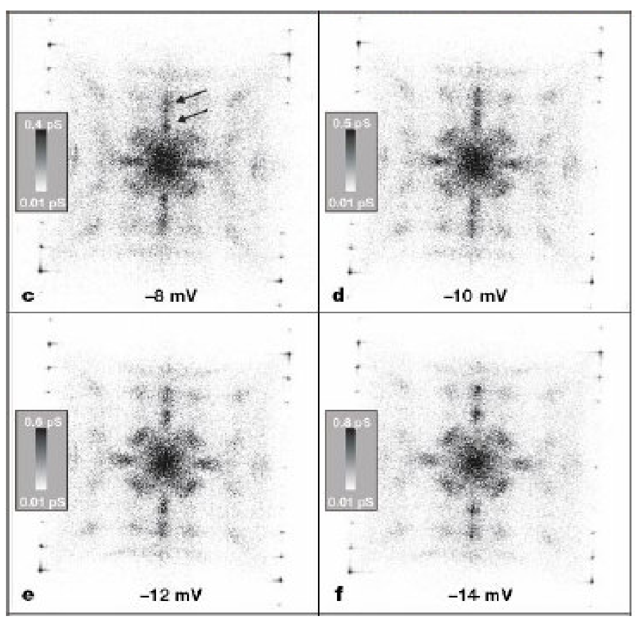


Figure 4: Examples of the conductivity in the reciprocal space, $g(q,V_b)$. The bias voltages are indicated in each image. The arrows point to non-dispersive b-axis supermodulations. The other point like features are the dispersive modulations of interest

The data taken is a collection of maps at various values of bias, V_b. By observing the position of the peaks in the reciprocal space, one can find out if the modulation disperses, if it changes its period for different energy levels. The peak position has a clear dispersion as it can be seen on (figure 5a). I will enter in more details on the implications on the next section.

(a) (b)

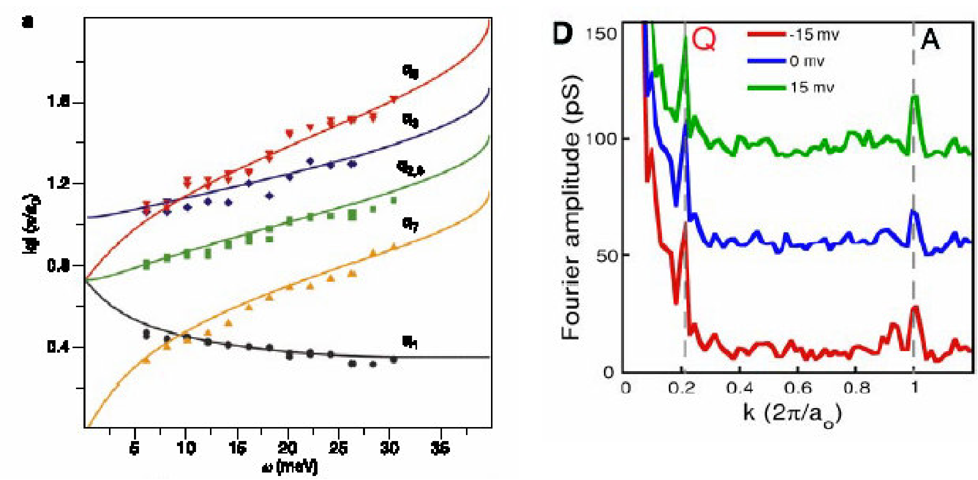


Figure 5: (a) The measured dispersion of the modulations at low temperature. The peak position is plotted as function of the bias. The different colors correspond to different peaks. The solid line is theoretical prediction. [7](b) A cross section of the Fourier map, illustrating the peaks as functions of |q|, with different colors corresponding to different bias.[8]

In another experiment [8], performed in Yazdani's Lab, they were able to get measurements of those modulation but at higher temperatures. Their data in low temperatures (in side the superconducting phase, T=40K) agrees with the one found in [6,7] but the striking feature is that above T_c, into the pseudogap regime (T=100K), they found modulations and they don't seem to disperse as the ones in low temperatures (figure 5b). The periodicity has a fixed value of $4.7 \pm 0.2\ a_0$ (where a_0 is the Cu-Cu distance)

3. Analysis

Let's start with a search for a possible explanation for origin the modulations in the superconducting phase.

The most obvious explanation could be some kind of structural effect. The b-axis supermodulation is an example of structural effect. In this case the peaks should not disperse. (It can be verified in both group's data that the b-axis modulation does not disperse.) So this explanation would be only suitable for the pseudogap modulation. In order to verify that, Yazdani's group measured the peak intensity. It is expected that for structural effects the peak intensity increases the same way as the LDOS does. But by plotting how the LDOS changes as function of the bias voltage, they notice that the atomic peaks and the b-axis modulation ones follow the DOS trend but the new modulation does not. Quite the opposite: while the DOS is smaller at low voltages (gap region!) the modulations have their maximum intensity in this region.

A good model for the superconducting modulations is based on quantum interference of quasiparticle states caused by scattering defects [6,7]. The quasiparticle dispersion relation ε(k) has been mapped by ARPES. For energies below the maximum of the energy gap, the contours of constant energy have a peculiar banana like shape (Figure6a). The quasiparticle density of states for a given energy is proportional to $\int|\nabla_k \varepsilon(k)|^{-1}dk$ at this energy. The end of the bananas are the terms that give the maximum contribution for the $|\nabla_k \varepsilon(k)|^{-1}$. So elastic scattering between those ends should generate the most intense modulations in the LDOS.

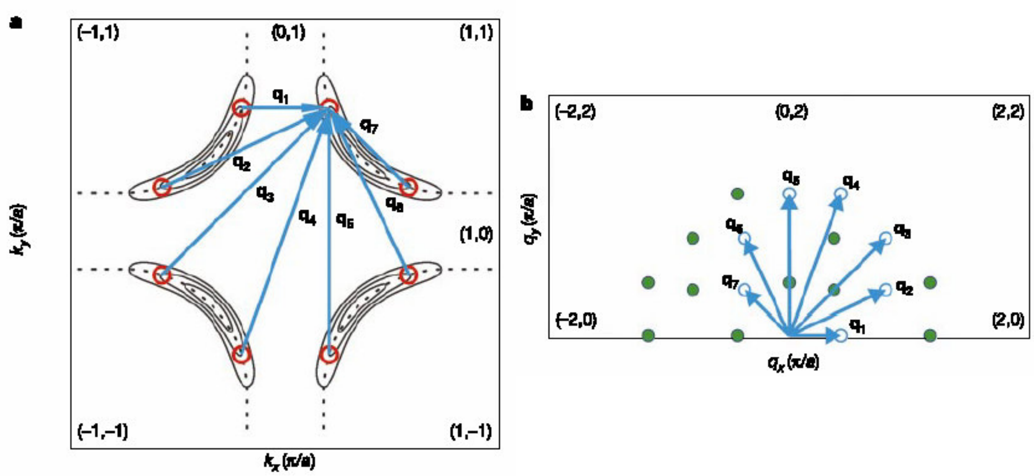


Figure 6 [7]: (a) The banana-like contour are the constant energy contours. Scattering between the red zones should dominate the modulations at the LDOS map. (b) the all possible scattering q-vectors are put with common origin. The ones in blue are the ones shown in the (a). there is a total of possible 16 distinguishable symmetric pairs of q-vectors.

In [7], it is possible to identify 12 of those 16 modulations. On (figure 5a) the solid lines represent expected dispersion relation for the modulations using this quasiparticle model. They fit the data in a remarkable way.

On the other hand the experiment on the pseudogap cannot use the same model. The strongest argument is based on the fact the period of the modulations is constant. This period was verified the same in different samples, with different concentrations of defects and impurities, showing that the value is very robust. (Another difficulty for this I think, is in defining the concept of quasiparticle on the pseudogap, where it is ill defined.

A popular suggestion for ordered state in the pseudogap phase is the one dimensional charge ordering, stripes. The value of the period of the modulations found in [8] is unfortunate because it makes it hard to think of how one would get the $4.7a_0$ value. Proposals for a $4.0a_0$ modulation have been made but this is far away from the error bar of the experiment. Another factor is that those modulations have a checkerboard (two dimensional) nature and not one dimensional.

The stripes interpretation cannot be underestimated. On an extensive review [9], Kivelson *et al.* suggests how fluctuating stripes could give the same checker-board pattern found in STM. The counter-argue the quasiparticle mechanism as the only mechanism generating modulations. The arguments fall is beyond my knowledge and I am no way able evaluate them.

4. Conclusions

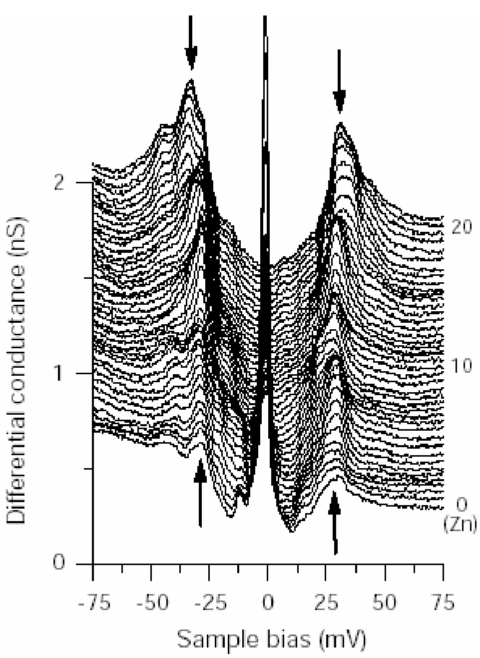
The patterns found on STM support that the cuprate phase diagram has a complex competition between different orders. These experiments are just one more among various phenomena found on cuprates that have controversial explanation.

On the experimental side, I believe there is a need to go beyond the limitations of the STM. Even though it give us rich information the single particles states, usually theories urge for measurements of correlation functions. Such information could select better which kind of orders are present.

On the theorist point of view, I believe there is a necessity of giving more predictions of effects that could be observed on single particle spectra or related to transport, thermodynamics, etc., properties. Sometimes I have the feeling that adjusting theories to fit experimental data is not as convincing. Many models come up with some order that fits well with some experiments and let other effects without explanations. For example, after reading some papers about stripes I could not understand how it is even related to the pseudogap energy magnitude or how can it produce the d-wave gap symmetry. Proposals with spin-charge separation, adjust better to those properties but also receives its critics.

5. Epilogue

There are other couple of neat experiments performed by Davis' group that caught my attention[10,11]. In those we can see individual impurities effects on the cuprate superconductivity. They measured how the differential conductance changes as you walk towards the site of the impurity. This way, we can see the evolution of the superconducting gap. They use two different kinds of samples, one having Ni as impurity and other having Zn. The impurity will substitute the Cu in Cu-O plane, forming for example $Bi_2Sr_2Ca(Cu_{1-x}Ni_x)_2O_{8+\delta}$.



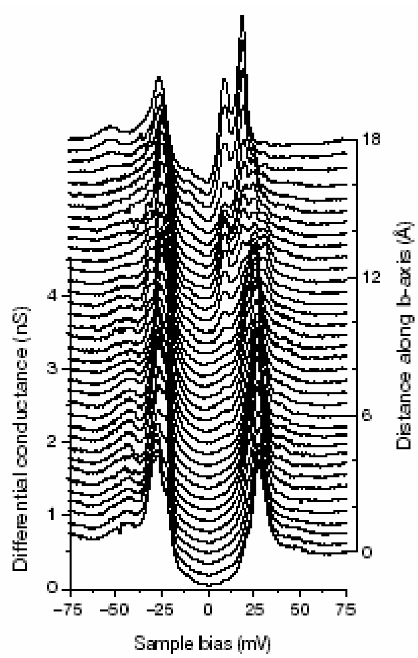


Figure 7: (a) Evolution of the differential tunneling conductance as we walk away from the Zn site. The arrows point out the suppression of the coherence peaks. (b) Similar plot but with the Ni impurity. The right scale is bit misleading: the top most graphic correspond to the Ni site while the bottom most to somewhere far. All data taken at 4K.

The measurements of the LDOS in the impurity site (Figure7) shows that the Zn destroys the gap locally while the Ni does not. The Ni is believed to be a magnetic impurity while the Zn not. In conventional superconductors, magnetic impurities are destructive to the superconductivity. Here, however, we notice quite the opposite. The fact that Ni impurities have smaller effects on the superconductivity then Zn support models with magnetic mechanisms.

6. References

[1] For a book with details on the STM theory and techniques: J. A. Stroscio and W. J. Kaiser "*Scanning Tunneling Microscopy*", Academic Press (1993)

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