Name of your laboratory
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December 2, 2019
Internship Report

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1 Introduction

Among layered materials, high-Tc superconductors, and especially cuprates, raised a lot of interest. Despite the numerous studies carried out on cuprates, the physics behind these compounds is not yet fully understood. The breakdown of BCS theory calls for more refined theories for explaining the unconventional superconductivity emerging [11]. Indeed, undoped cuprates turn out to be anti-ferromagnetic insulators [2], so no quasi-particle feature appears in their electronic structures preventing from the formation of coherent pairs, but the anti-ferromagnetic fluctuations do play an important role in the emergence of superconductivity with doping. Superconductivity is observed in hole-doped cuprates, suggesting that the question of superconductivity in cuprates is actually rather about how quasi-particles appear with doping. Once the quasi-particles appear, they are very much expected to form coherent pairs. This reasoning, along with the discovery of a rich phase diagram in respect of doping and temperature pushed the investigation of the underlying normal state of cuprates.

The phase diagram for $Nd_{2-x}Ce_xCuO_4$ and $La_{2-x}Sr_xCuO_4$ [2] is given in Fig. 1. These two compounds are cuprates, whose phase diagram in general is close to those of other cuprates. In the undoped region, the cuprate is in an anti-ferromagnetic Mott insulator phase. With increasing hole doping (right part of the diagram) at zero temperature, the cuprate becomes superconducting, and at high doping it becomes a metal.

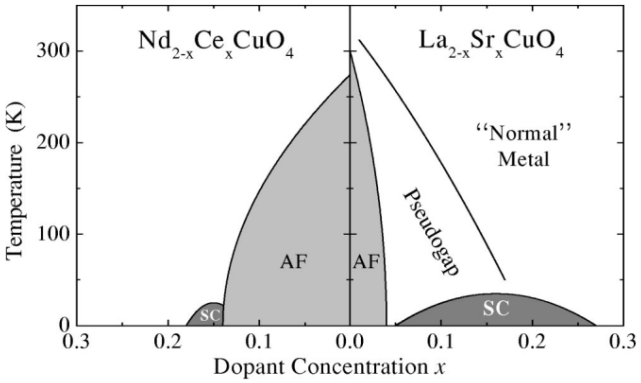

Figure 1: Phase diagram in respect of temperature and doping for $Nd_{2-x}Ce_xCuO_4$ and $La_{2-x}Sr_xCuO_4$. Taken from [2]. Underdoped is said for a doping between zero and optimal doping, and overdoped is used for doping higher than optimal doping (see text).

However, at higher temperatures for hole doping between x = 0.05 and x = 0.15 the cuprate enters in the so-called pseudo-gap (PG) phase. The PG phase is characterized by the opening of an anisotropic gap (also called pseudo-gap) in the Brillouin zone at the Fermi energy [1]. The pseudo-gap is robust as it remains even for temperatures far above the critical temperature for superconductivity (T_C), and it has similarities with the superconducting gap [10]. At temperatures close to the critical temperature for superconductivity, and for a doping close to the optimal doping (doping at which T_C of

superconductivity is the highest), the behavior of the critical line for the PG phase is still under debate.

The similarities between the PG and the superconducting gap point out the fact that they could share the same origin, hence the study of the pseudo-gap seems crucial for the understanding of the cuprates' superconductivity. Our work takes place in this context : we aim at theoretically investigating the pseudo-gap phase in a specific cuprate $Ca_2CuO_2Cl_2$ (CCOC). The choice of this compound was motivated by the fact that it has convenient surface properties for experiments[10] (which makes easier the comparison with theoretical results), and also because we will work along with researchers in Grenoble that can synthesize and analyze such compounds. The usual experiment for probing the pseudo-gap phase is Angle Resolved Photoemission Spectroscopy (ARPES) [2], but we will mainly focus here on the optical properties (optical conductivity for instance) of CCOC which can be used to highlight the emergence of a pseudo-gap.

CCOC belongs to the class of layered materials, it consists of layers of CuO_2 separated by Ca and Cl atoms in a tetragonal structure, see Fig. 2. Cu, O and Cl atoms form octahedras. The CuO_2 layers are well separated hence they have a strong 2D character which is one of the essential aspects of high-T_C superconductors. Undoped CCOC is a half-filled anti-ferromagnetic Mott insulator [10]. When holes are introduced, i.e when CCOC becomes hole-doped, e.g by Na substitution, an anisotropic gap opens : instead of a continuous Fermi surface, the latter is composed of disconnected arcs around $(\pm\pi/2, \pm\pi/2)$ [9]. Since the energy dispersion around the arcs is very similar to d-wave energy dispersion, the correlated half-filled d-orbitals of Cu atoms are expected to be (partly, at least) responsible for the pseudo-gap. Moreover, the p_x and p_y orbitals of Oxygen are expected to be hybridized with the Cu d-orbitals because of the geometry of the CuO_2 layers. Indeed, LDA calculations that I performed for CCOC show that the $d_{x^2-y^2}$ of Cu and the p_x and p_y are hybridized and both contribute to the band crossing the Fermi energy. Such an hybridization is very similar to the Zhang-Rice singlet [12] which has been proposed for creating an effective one-band hamiltonian for cuprates. One can notice here that the Density Functional Theory (DFT) calculation predicts undoped CCOC band structure to be metallic, which is expected from DFT when dealing with a Mott insulator, so it is clear that a theory going beyond the single-electron picture is needed.

This strong d-wave character of the pseudo-gap motivates the use of theoretical tools suited for such correlated orbitals. We chose to work within the framework of Dynamical Mean Field Theory [3] (DMFT) which is known for being powerful when dealing with correlated materials. The anti-ferromagnetic Mott insulator phase at low doping also motivates the use of DMFT. Indeed, the Mott insulator phase is due to two-body interactions which can be captured within DMFT, but not within the one-particle picture of Density Functional Theory (DFT). Moreover, it has been shown that the investigation of the pseudo-gap phase using DMFT requires to take into account non-local correlations [5, 7]. Indeed, as the pseudo-gap is an anisotropic feature, and since it is needed to account for the anti-ferromagnetic fluctuations, k-dependent observables are needed so the local self-energy approximation of single-site DMFT would prevent us to capture the PG. Hence we will use an extension of DMFT : Cluster DMFT (C-DMFT) [6, 8] in which the lattice problem is mapped onto a cluster of atoms embedded in a self-consistent bath of free electrons. This cluster of multiple atoms allows the anti-ferromagnetic fluctuations to be included. Such a construction allows us to take into account explicitly the correlations inside the cluster, i.e correlations on the size of the cluster will be treated exactly. This is more powerful than standard single-site DMFT that only considers on-site correlations. In this study, we will consider oriented 2-site clusters, which are supposed to be the minimal cluster size to investigate the pseudo-gap phase [5, 7]. The similarity of the hybridization of d- and p-orbitals in CCOC with the effective single-band Zhang-Rice singlet suggest that we can treat the problem within C-DMFT considering only one effective band on each atom of the cluster. This effective band will be extracted from LDA calculations. The strong 2D character of the CuO_2 layers allows us to consider a 2D Hubbard Hamiltonian with nearest, next-nearest and next-next-nearest neighbor hopping within the 2 dimensional plane, and on-site interactions between electrons. The layers are so well separated that we can neglect the in-

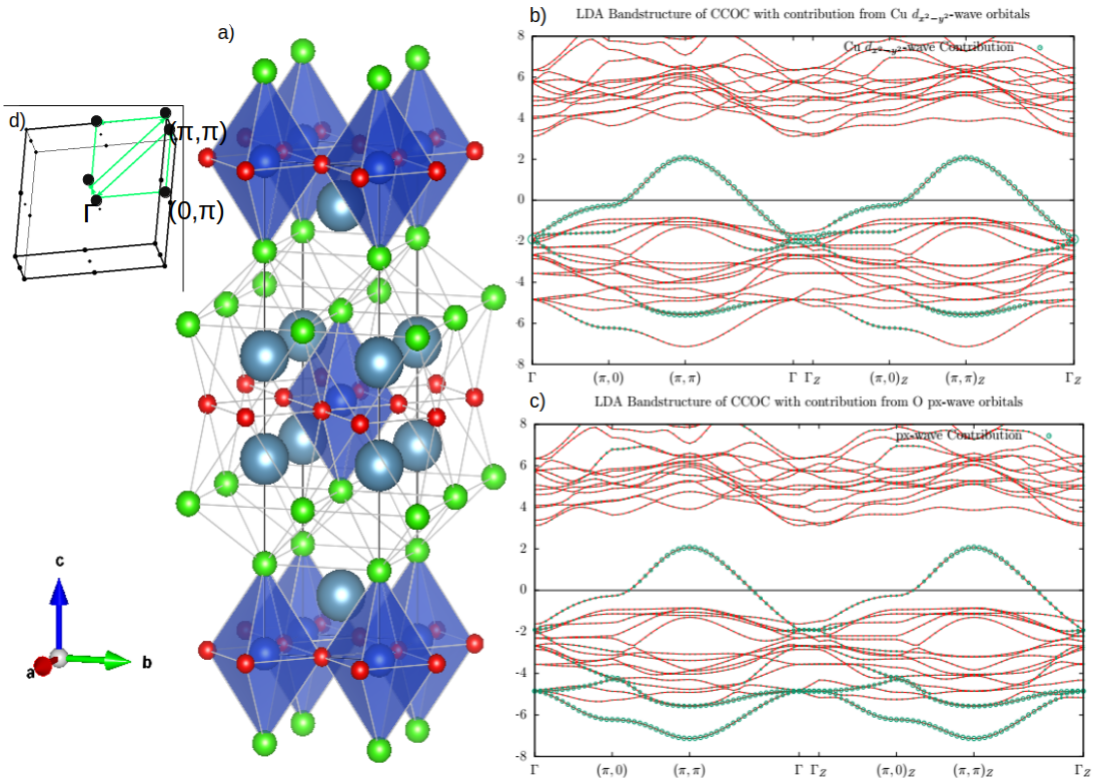

Figure 2: **a)** CCOC crystal structure. Green balls : Cl, red balls : O, dark blue balls : Cu, light blue balls : Ca. **b) and c)** Bandstructure of undoped CCOC with contribution from $d_{x^2-y^2}$ and p_x orbitals respectively. **d)** : k-path used in the Brillouin Zone for the LDA calculation.

teractions between each other.

I will first review the idea and concepts behind C-DMFT and then its practical implementation with oriented 2-sites clusters. I will then compare first preliminary results with 'benchmark' results [4] obtained with Quantum Monte Carlo techniques. This comparison is necessary to confirm that the program I wrote matches with results that are well established and reliable. Then I will present calculations of the electronic structure of CCOC using DFT+C-DMFT and the computed optical properties of such compounds.

2 Theory and Implementation of Cluster-Dynamical Mean Field Theory

2.1 Single-site Dynamical Mean Field Theory

2.2 Towards Dimer Dynamical Mean Field Theory

2.3 Analytic continuation

2.4 Optical Conductivity

3 Results and discussion

3.1 Single-site versus dimer Dynamical Mean Field Theory

3.2 $Ca_2CuO_2Cl_2$

4 Conclusion

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