

The superconductivity project: Magnetic and charge dynamics of underdoped high temperature superconductors

1. Aims of the project.

The quest for understanding the mechanism of high-temperature superconductivity in the copper oxide materials has been at the forefront of condensed matter physics for two decades. Since there is currently widespread consensus that strong electron correlations are at the heart of this phenomenon, magnetic and charge excitations - which can be regarded as “fingerprints” of these correlations - are of central importance for this field. Two experimental probes yield incisive and complementary information about magnetic excitations in the copper oxides: neutron scattering probes the wave vector and energy dependent magnetic susceptibility over the entire Brillouin zone in an energy range from about 1 to 200 meV, and nuclear magnetic resonance (NMR) probes the local magnetic susceptibility at particular lattice sites. Two other experimental techniques provide complementary information about the charge excitations. The angular resolved photoemission probes the wave vector and energy resolved excitations in the energy range from a fraction of eV to a few eV. Measurements of the dc and ac conductivities probe the low energy charge response integrated over the Brillouin zone.

There has been very substantial progress in experiments during the past several years. The incommensurate dynamic [1, 2, 3, 4, 5, 6] and static [7, 8, 9, 10, 11] spin responses have been studied by neutron scattering in the $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ and $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ families of copper oxides. It has been well established that the response is a generic property of the copper oxides [12]. The sensitivity and accuracy of photoemission measurements has increased dramatically. In particular, small Fermi arcs have been observed in underdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ across the superconductor-insulator transition down to the doping level $x=0.03$ [13]. Another very important development is the observation of dc and ac transport anisotropies in the spin glass phase of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [14, 15], showing anisotropies as large as 50 to 70%. These measurements became possible due to the development of de-twinning techniques for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ crystals. The phase diagram of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, first suggested in Ref. [16] and shown in Fig.1Left, is widely known: the three-dimensional antiferromagnetic Néel order identified below 325 K in the parent compound disappears at doping $x \approx 0.02$ and gives way to the so-called spin-glass phase which extends up to $x \approx 0.055$. In both the Néel and the spin-glass phase, the system essentially behaves as an Anderson insulator and at low temperature exhibits only hopping conductivity. Superconductivity then sets in for doping $x > 0.055$ [17]. For a long time there was widespread consensus that this was the generic diagram for the hole doped copper oxides. However, recent studies of $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ have revealed that it is not so [18, 19, 20, 21]. In this compound antiferromagnetic order exists down to the superconducting phase, and moreover, it is likely that antiferromagnetism and superconductivity overlap, see Fig.1Right. Another very important distinction between $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ and $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ is that before onset of superconductivity (oxygen content smaller than $y=0.35$, see Fig.1Right) $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ behaves as a normal conductor (with some indications of weak localization) [20, 21, 19]. Note that while x in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ in Fig.1Left is approximately equal to the hole doping, the y in $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$, Fig.1Right, is just oxygen content. The hole doping is smaller than the oxygen content and it is approximately 6-7% at $y \approx 0.37$, see Ref. [22].

Thus, the experimental situation has advanced dramatically during the past several years. The observation of static incommensurate structures in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ caused a renewal of theoretical interest in the idea of spin spirals in copper oxides [23, 24, 25, 26, 27, 28, 29, 30, 31].

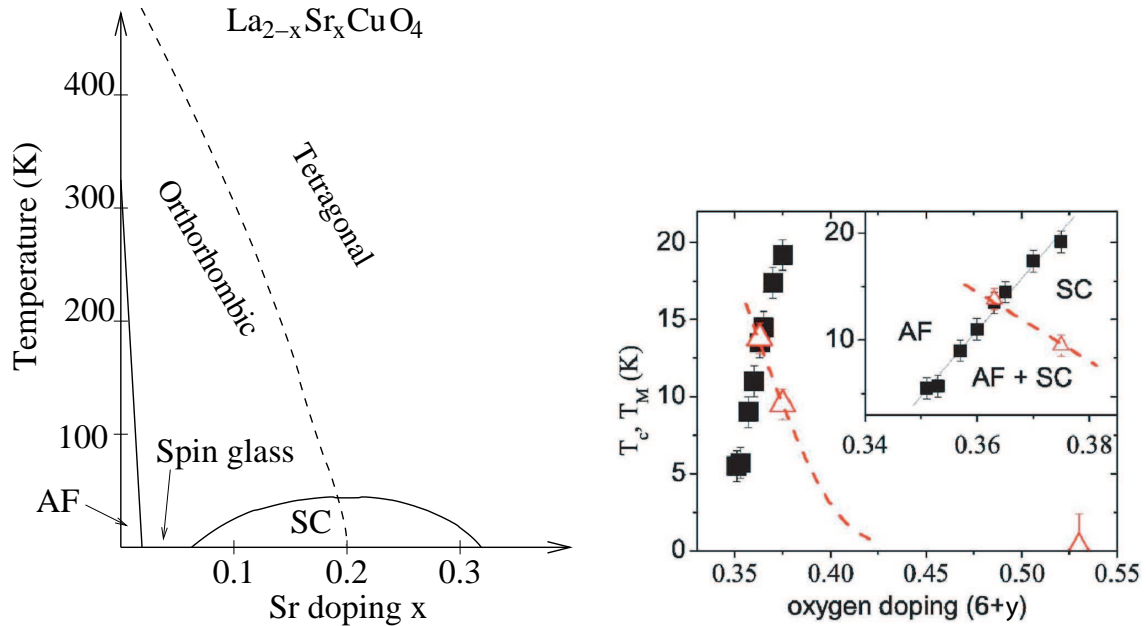


Figure 1: Left [16]: Phase diagram of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$; the superconducting (SC) and the anti-ferromagnetic (AF) phases are separated by the spin glass phase. Right [18]: Phase diagram of $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$; the superconducting and the antiferromagnetic phases overlap near $y \approx 0.37$.

This renewed activity has finally lead to a breakthrough in our understanding of the spin glass phase of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ [32]. It is widely believed that the $t - J$ model describes the essential low-energy physics of the copper oxides [33, 34, 35]. In a recent series of works we found a fully controlled solution of the model at small doping. The great simplification that has allowed us to find the solution is the localization of holes due to Coulomb pinning by Sr ions. Based on this approach we have explained a number of effects that previously had not been understood:

- 1) Ref. [27] explains why the incommensurate neutron scattering structure rotates by 45° exactly at the insulator-superconductor transition point. The effect was observed in Ref. [10].
- 2) Ref. [28] explains the anisotropy in the in-plane dc and ac conductivities, observed in Refs. [14, 15].
- 3) Ref. [31] explains the coexistence of incommensurate and commensurate neutron scattering peaks in the Néel phase, observed in Ref. [11].
- 4) Ref. [31] explains the pinning of the incommensurate structure to the orthorhombic b-axis, observed in Refs. [8, 9, 10].
- 5) Ref. [31] explains the dramatic dependence of the uniform magnetic susceptibility on doping [31], observed in Ref. [36].
- 6) Ref. [37] explains the negative in-plane magnetoresistance, observed in Refs. [38, 39].
- 7) Finally, in Ref. [32] we have built the full theory of the spin glass phase of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. In Fig.2 we present the neutron scattering experimental data [10] together with the theoretical curve from [32]. The agreement is remarkable, especially bearing in mind that the theory has no fitting parameters.

Now we plan to attack even more complex problems related to the magnetic and the charge structure of the copper oxides. In point **9** of the program presented below we will also address superconductivity; however, at the moment the primary goal is the study of the magnetic and the charge correlations. We will extend and develop the outlined approach that proved to be highly successful in explaining the low temperature properties of the Néel and spin glass phases

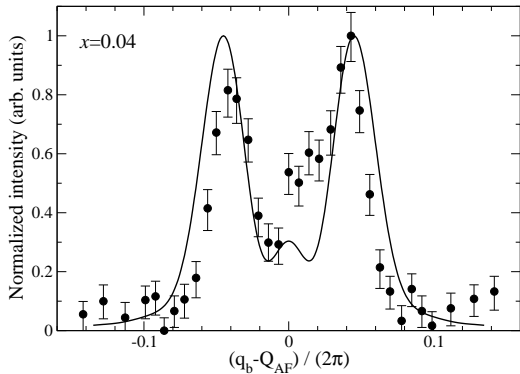


Figure 2: Neutron scattering probability versus momentum transfer in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ for $x = 0.04$. Experimental points are taken from Ref. [10]. The theoretical curve is from Ref. [32]. The theory does not contain any fitting parameters.

of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. The central point of the approach is an expansion in powers of doping x (implemented via chiral perturbation theory). Therefore, the approach is applicable to underdoped copper oxides. More specifically we plan to address the following problems:

- 1) Evolution of the Dzyaloshinski-Moriya interaction with doping, and pinning of the spiral polarization in the spin glass phase of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$.
- 2) Temperature dependence of the spin-wave gaps and of the interplane antiferromagnetic interaction in the parent compound La_2CuO_4 .
- 3) Theory of the full NMR experiment for La_2CuO_4 in magnetic field directed along the orthorhombic b-axis.
- 4) Theory of the NMR experiment for Zn doped La_2CuO_4 .
- 5) Calculation of the Hall coefficient in lightly doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ at high temperature.
- 6) Calculation of the in-plane resistivity in lightly doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ at high temperature.
- 7) Theory of angular resolved photoemission in the spin glass state of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$.
- 8) Theory of Li doped La_2CuO_4 .
- 9) Solution of the uniformly doped two-dimensional t-J model at doping $x \rightarrow 0$.
- 10) Theory of inelastic neutron scattering in the uniformly doped state.
- 11) Underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ and the influence of interplane interactions on magnetic stability.
- 12) Ca doped $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$, and the possible localization of holes.

2. Importance of the project

This project is aimed at studies of the physics behind high temperature superconductivity - a phenomenon that is still not understood, despite the numerous research efforts undertaken since its discovery two decades ago. The quality of experimental data has improved dramatically over the past several years, and as a result many new effects have been discovered and investigated in depth. The experimental developments have provided a number of novel insights. Broad international efforts, both experimental and theoretical, aimed at the resolution of this challenging problem, are becoming more and more coordinated. These studies are in parallel with the development of applications based on high-temperature superconductivity. The next generation of experiments is expected to be even more accurate and systematic, mostly related to improvements of material quality, energy and momentum resolution, application of polarized

beams, etc. This is a challenge for the theory, and perhaps more importantly, it provides an opportunity for the theory to get deeper insights and address specific questions.

Our group has been working on underdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ over the past few years. We chose $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ because systematic experimental data at low doping were available for this compound. This work has led to a breakthrough, we now fully understand the structure of the Néel and spin glass states of the compound [32]. Our theoretical approach is based on chiral perturbation theory which allows us to build a systematic and fully controlled expansion at low doping. The chiral perturbation theory was originally developed in particle physics where it has been widely used, but it is little known in condensed matter physics. Recently the group of Prof. Wiese (Bern, Switzerland), following our footsteps, has realized the power of the method and started to apply it to the copper oxides [40]. Another clue to success in the understanding of the spin glass state of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ was the analysis of the neutron scattering data of Prof. Yamada's group (Tohoku University, Japan) [7, 8, 9, 10, 11]. This data gave a very important guiding line for the theory. It was hardly possible to understand the spin glass state before having these measurements.

We plan to further develop our success and attack more complex problems. A list of the problems was presented in the previous section and details will be discussed in the next section. The main idea is to combine very specific questions aimed at particular experiments (like theory of the full NMR experiment for La_2CuO_4 in magnetic field directed along orthorhombic b-axis), with generic theoretical problems, such as solution of the uniformly doped t-J model at very small doping (a spin liquid with separated scales). We strongly believe that specific questions can shed light on generic problems and that advancements in solution of generic problems can guide experiments. As a main theoretical tool we will continue to use the chiral perturbation theory in which we have expertise and a great advantage compared to other groups. However, we will combine this with other analytical and numerical methods.

We work in a close collaboration with experimental groups of Prof. B. Keimer (Max-Planck-Institute for Solid State Research, Stuttgart, Germany) and Prof. J. Haase (Leipzig University, Germany). Many points of the present project are directly related to current or planned experiments in these groups. We also collaborate with many theoretical groups, Prof. A. Milstein (Novosibirsk), Prof. G. Sawatzky (Vancouver), Prof. W. Metzner (Stuttgart), Prof. O. Andersen (Stuttgart), Prof. R. Singh (Davis). We strongly believe that these collaborations are vital for the success. We also believe that the project will contribute to the physics program at the ANSTO OPAL reactor.

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