Nonlinear Lattice Dyamics in High–T_c Superconductors

Ph.D. thesis of Francesco Piazza

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Abstract

After 15 years since it was discovered, the microscopic mechanism of High–T_c superconductivity remains elusive. In particular, the role of lattice vibrations in the electronic coupling is still very dibated. Many of the proposed models invoke unusual vibrational properties, such as nonlinearity in the interatomic potentials. In this thesis we present a combined experimental and theoretical study of lattice anharmonicities in cuprates.

We first introduce and describe our Extended X–Ray Absorption Spectroscopy (EXAFS) experiment. We then develop a novel data analysis technique, which enables us to measure directly the nonlinearity in the interatomic potentials of the copper-oxide planes, which constitute the basic structural unit of all cuprates. Finally, based on our experimental results, we introduce a simple dynamical model of the copper–oxide layers. We study this model both analytically and numerically, showing the emergence of anharmonic localised excitations known from nonlinear physics as discrete breathers. The general layout of the thesis is the following.

The first chapter is devoted to a review of the basic structural and physical properties of cuprates. In particular, we review and discuss the existing experimental data regarding the Cu–O interatomic potential in the $\mathrm{CuO_2}$ planes. In the second chapter we introduce the basics of EXAFS spectroscopy. From a simple derivation of the main features of the theory underlying it, to a simple but complete discussion of the details of our experiment. The last three chapters are entirely dedicated to the original contribution to this thesis. First, we introduce and develop a pair distribution function based on quantum perturbation theory. It is designed to incorporate directly the parameters describing the interatomic potential of the Cu–O pair through a Taylor expansion. We thorougly illustrate the properties of the distribution function and carefully examine its sensitivity to the potential parameter. For this purpose, we set up an easy and robust procedure based on the statistical F–test. In chapter four we present the data analysis of our experiment. We begin presenting the general fits of the whole spectra. Then we move on to a closer examination of the contribution from the Cu–O pair. and present a complete analysis of the Cu–O interatomic potential based on the pair distribution function developed in the previous chapter. The last chapter is entirely devoted to a detailed study of the lattice dynamics of the $\mathrm{CuO_2}$ planes. As a start, we present a careful analytical and numerical analysis of the linear spectrum (phonon bands) based on a simple model with two force constants. This analysis provides the necessary background for the interpretation of the subsequent numerical experiments. Based on the experimental results discussed in the first part, we simulate a simple nonlinear model and show how it is possible to observe the spontaneous emergence of discrete breathers in a copper–oxide plane. We discuss the properties of such solutions and attempt a definition and a quantitative estimate of their lifetime, based on a simple non–linear stability analysis.