Introduction to the complex phases of underdoped cuprates

Since the discovery in 1986 of superconductivity in cuprates this class of materials has represented a paradigmatic example of strongly correlated systems. The intense research activity has led up to the understanding of many interesting properties not strictly connected with superconductivity. In particular the complex magnetic phases in the underdoped region of the phase diagram (see Fig.1), in addition to their possible relevance for superconducting mechanisms, seem to have remarkable analogies with soft matter physics.

Figure 1: Schematic phase diagram of cuprates.

Typically the key structural elements are represented by CuO$_2$ layers. They are separated by other elements (La, Bi, O, Y, Ba) which play the role of charge reservoirs. The
parent compound is a Mott insulator with long-range antiferromagnetic (AFM) order, that can be modelized with a two-dimensional Heisenberg model describing Cu spins. The partial substitution of the interlayer elements with atoms of different valence, brings exceeding electrons or holes in CuO_{2} layers. A progressive increasing of this chemical doping can destroy the AFM ordered phase of the stoichiometric compound.

In this thesis we will focus our attention on the hole-doped lanthanum cuprates like La_{2-x}Sr_{x}CuO_{4} (LSCO). In this class of materials a superconducting phase appears with the highest \( T_{c} \) at around \( x = 0.16 \) holes per Cu (optimum doping). Higher doping (overdoping) eventually leads to a conventional Fermi liquid. But the subject of this project will be the complex electronic phases which appear reducing the doping respect to the optimal one (underdoping). Although the low temperature AF long-range order is destroyed above a concentration of added holes per planar copper \( x \approx 0.02 \), signatures of the magnetic order persist in the dynamical spin and charge correlations up to the overdoped regime. In particular the low temperature state of these materials for hole concentration in the range between about \( x = 0.02 \) and \( x = 0.05 \) (until the onset of superconductivity), is called in literature “cluster spin glass phase” [1], i.e. a phase made of patches of locally antiferromagnetically ordered spins with an axis of magnetization that varies from patch to patch. This phase represents the low temperature state of these materials.

It is important to define a type of order in the underdoped region of cuprates in such a way that the superconducting phase can be viewed as a consequence of the strong fluctuations in the quantum critical point between an ordered region and the Fermi liquid phase. This is what can be observed in many other unconventional superconductors, like heavy fermion systems or pnictides, in which the superconducting region forms a ‘bell’ around a quantum critical point. The presence of a region characterized by a pseudogap in the normal phase of the underdoped cuprates, that is a gap in the electronic spectrum observed only in certain directions of the Brillouin zone, can suggest the preformation of the Cooper pairs that lead up to superconductivity only when a coherence of phase is established. Although we do not reject a priori this scenario, we look for broken symmetries that may have interesting analogies with the liquid crystal phases as suggested by experimental results.

In LSCO, neutron scattering experiments have revealed low energy incommensurate magnetic excitations at wave vectors \( \frac{\pi}{a}(1 \pm \delta, 1) \) and \( \frac{\pi}{a}(1, 1 \pm \delta) \) in the underdoping regime, where the incommensurability \( \delta \) (defined as the shift of the magnetic Bragg peaks from the antiferromagnetic wave-vector \( Q_{AF} \) in reciprocal lattice units) depends linearly on \( x \) from \( x = 0.02 \) up to \( x = 1/8 \). By decreasing doping below \( x < 0.5 \), scattering undergoes a rotation toward the diagonal direction [2, 3]. In some situations the scattering become elastic with Bragg peaks showing the appearance of long range order [4]. This can be explained by quasi-one-dimensional structures called stripes, made by holes that condense into charged straight lines aligned parallel to each other in coincidence with domain walls of the AFM order, where the phase of the staggered magnetization changes by \( \pi \) [5, 6, 7]. Stripes with long-range order are electronic analogues of the smectic phase of liquid crystals [8].

There are also situations in which the incommensurate scattering is only inelastic,
long-range order does not exist but still the $C_4$ symmetry of the lattice appears broken to $C_2$. An interesting case is that of YBa$_2$Cu$_3$O$_{7-x}$ (YBCO), in which the absence of long-range charge order is accompanied by evidence for rotational symmetry breaking in neutron scattering [9, 10]. This suggest the analogous of the nematic order of liquid crystals [8]. The underlying charge nematic order is believed to consists of unidirectional charge stripes which drive the formation of an incommensurate spin modulation [6].

Evidence for some form of stripe correlations comes from neutron, x-ray scattering and tunneling experiments [6], and its complete understanding could shed light on the observed strong relationship between superconductivity and the low energy spin fluctuations responsible for incommensurate scattering. Indeed both these phenomena disappear at the same concentration of holes suggesting an intimate relation between them [11].

During my thesis work I will study the phase diagram of cuprates in the underdoped regime. In particular I want to clarify the way in which the system destroys the long range magnetic order to reorganize itself with another type of order still not well defined. We will use a variety of approaches. First we will obtain the energy of different spin textures using a microscopic model and the Gutzwiller approximation.

Vortex-Antivortex pairs as building blocks

Our purpose is to explain the neutron scattering experiments on underdoped region of lanthanum cuprates in terms of a phase which breaks rotational and inversion symmetry. It is formed by oriented stripe segments which do not need to have positional order thus we call it ferromagnetic.

As a starting point of our work, we look at variational computations [12], which suggest that at very small concentration holes tend to localize in the core of a vortex of the AF spin order. Such vortices have an energy which diverges logarithmically with the system size. The system avoids this large energy cost by forming tightly bound vortex-antivortex (VA) pairs. The residual attraction between pairs competes with the Coulomb repulsion due to the charged doping holes in the core of the spin vortices. The idea which I will explore in my thesis is that such charged VA pairs can be used as building blocks of the underdoped phase diagram.

In order to study these textures we have performed variational calculations based on the Gutzwiller approximation (GA) of the extended one-band Hubbard model, whose Hamiltonian reads

$$\mathcal{H} = \sum_{i,j,\sigma} t_{ij} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \right) + U \sum_i n_{i,+} n_{i,-}. \quad (1)$$

The first part is the kinetic energy due to hopping between sites $i$ and $j$. We consider hopping restricted to nearest neighbors and next-nearest neighbors. The interaction term is assumed to be extremely short range. The ratio between on-site repulsion $U$ and nearest-neighbor hopping $t$ is set to $U/t = 8$ as suggested in Ref. [13, 14], while the ratio between next-nearest neighbors hopping $t'$ and $t$ is set to $t'/t = -0.2$.
As a first approximation we use the standard Hartree-Fock decomposition method on this model on a square lattice which keeps both \( z \) and \( x, y \) components of the spins,

\[
U \sum_i n_{i,\uparrow} n_{i,\downarrow} \approx U \sum_i \langle n_{i,\uparrow} \rangle c_{i,\uparrow}^\dagger c_{i,\downarrow} + \langle n_{i,\downarrow} \rangle c_{i,\downarrow}^\dagger c_{i,\uparrow} - \langle S_z^+ \rangle c_{i,\uparrow}^\dagger c_{i,\downarrow} - \langle S_z^- \rangle c_{i,\uparrow} c_{i,\downarrow}^\dagger \\
-\langle n_{i,\uparrow} \rangle \langle n_{i,\downarrow} \rangle + \langle S_z^- \rangle \langle S_z^+ \rangle.
\] (2)

The Hamiltonian written in this way can be easily diagonalized, obtaining self-consistent solutions by iteration. More accurate solutions can be achieved by using the GA [15, 16, 17], which allows to deal with the strong on-site repulsion.

Through this type of computations we have seen that the interaction between the pairs is dominated by an anisotropic short-range core-core contribution which originates from the charge distribution of the localized holes. This results in a head-to-tail aggregation of VA pairs which tend to form chains in such a way that only the vortex and the antivortex on the extremes contribute to the long range distortion. Fig 2(a) shows the spin and the charge structure for 8 holes corresponding to 4 VA pairs. Examination of the spin current (b) allows to visualize the VA pair nucleated at the extremes and the fact that the texture breaks inversion symmetry. This allow us to treat a segment of VA pairs like an oriented dipole. We see that the segments tend to form an antiphase domain wall of the AF order although the transition from finite segments to infinite stripes is non trivial and will be object of my future work.

![Figure 2](image)

**Figure 2:** a) Stripe segment for 8 holes (corresponding to 4 VA pairs) obtained by minimizing the GA energy on a 16 \( \times \) 16 lattice in the one band Hubbard model with \( t'/t = -0.2 \). The arrows are the staggered magnetization while the circles are proportional to the excess hole charge. b) Spin currents currents defined from the conservation of the \( z \) component of the magnetization [12].

Since the textures are planar and we are interested on the large scale behavior we can treat this configuration as a classical XY-model with nearest neighbor interaction \( J \). If we consider the staggered magnetization \( S_{i}^{stg} = S_{i} e^{-i(\pi,\pi)\cdot r_{i}} \), the relevant model is ferromagnetic. The segments are modeled as a chain of vacancies which alternately correspond to the center of a vortex and antivortex. The spin structure is then determined
from the minimization of the classical energy but we can show that it can be well described by the linear superposition of the spin deformation due to each single vortex of the chain.

The Hamiltonian of the classical two-dimensional XY-model is given by

\[ \mathcal{H} = -J S_0^2 \sum_{i} \sum_{\delta=x,y} \cos(\phi_i - \phi_{i+\delta}), \]

(3)

where \( x, y \) indicate the nearest neighbor site in the two directions. If the spin phase changes slowly passing from a site to its nearest neighbors we can consider \( (\phi_i - \phi_{i+\delta}) \) as a small quantity and we can approximate the Hamiltonian using \( \cos(x) \approx 1 - \frac{1}{2} x^2 + O(x^4) \) (in an antiferromagnetic background the cosine must be developed around \( \pi \) ) obtaining the continuum limit

\[ \mathcal{H}_{cl} = \frac{1}{2} \int d^2x \rho_s |\nabla \phi(x)|^2, \]

(4)

where the stiffness is defined by \( \rho_s = JS_0^2 \). If we introduce the quantity \( I_{i,i+\delta} = 2\rho_s \sin(\phi_{i+\delta} - \phi_i) \), one can show that it must satisfy the Kirchoff’s law of the nodes in an electric network, in order to minimize the energy of the system. So it may be interpreted as the spin current between the site \( i \) and \( i+\delta \). In the continuum limit it becomes \( \mathbf{J}(x) = 2\rho_s a \nabla \phi \).

Vortices represent topologically stable excitations of the ordered phase. If the spin phase \( \theta \) is a spatially continuum variable a vortex can be defined by

\[ \phi(\mathbf{r}) = k \theta, \]

(5)

where \( k \) is the winding number stating the strength of the vortex. We will use \( k = 1 \) for vortices and \( k = -1 \) for antivortices. \( \theta \) is the angular coordinate of the position \( \mathbf{r} \), such that \( \mathbf{r} = (r, \theta) \Rightarrow \theta = \arctan(y/x) \). So the influence of a collection of segments, like that showed in Fig. 2(a), on spins at point \( \mathbf{r} \), is given by

\[ S^x(\mathbf{r}) = S_0 \exp(iQ\mathbf{r}) \cos \Phi(\mathbf{r}); \]

\[ S^y(\mathbf{r}) = S_0 \exp(iQ\mathbf{r}) \sin \Phi(\mathbf{r}), \]

(6)

where \( Q = (\pi, \pi) \) is the AF wave-vector and

\[ \Phi(\mathbf{r}) = \sum_{i=1}^{N_{seg}} \left[ \arctan \left( \frac{y - y_{i,1}}{x - x_{i,1}} \right) - \arctan \left( \frac{y - y_{i,2}}{x - x_{i,2}} \right) \right], \]

(7)

is the angular spin distortion due to the \( N_{seg} \) segments with a vortex at \( \mathbf{r}_1 = (x_{i,1}, y_{i,1}) \) (tail) and an antivortex at \( \mathbf{r}_2 = (x_{i,2}, y_{i,2}) \) (head), with \( l = |\mathbf{r}_1 - \mathbf{r}_2| \). So we can approximate the ‘phase field’ produced by segments of more than one VA pair, with the one produced by segments of the same length but made by a single vortex and antivortex at the extremes. Fig.3(a) reports the spin phase distribution for a particular distribution of stripe dipoles with segment length \( N = 8 \) at \( x = 0.03 \), each oriented along \([-1,1]\) direction [18]. One observes a monotonous increase on the phase of the staggered magnetization along \([1,1]\) direction, although the distribution of stripe segments is completely
Figure 3: Spin phase distribution for (a) macroscopically and (b) randomly polarized
distribution of segments in a 160 × 160 sites system. Segments have a length of
8 sites on the diagonal (4 VA pairs) and are represented by arrows indicating
the length ad orientation [18].

random. In Fig.3(b), also for the same distribution of segments, the associated orientation
of the segments is completely random. In this case the system disaggregates into
large areas with similar phase. It can be shown that the phase distribution generated by
oriented segments induces incommensurate peaks of the spin structure factor in excellent
agreement with experiments [18]. We can call this configuration ferroelectric, since it
displays only an orientational order of the segments (they are aligned in a ferroelectric
way) and not a positional order. This leads to a C4 rotational and inversion symmetry
breaking. The parameter that characterize this symmetry breaking is represented by the
average spin current, that is proportional to ⟨∇Φ(r)⟩. It can be analytically calculated
in our lattice of dimension L2, obtaining

⟨∇Φ(r)⟩ = π ẑ × Nseg
          L2 (r1 − r2) = π ẑ × lNseg ẑ,

where ħ is the versor specifying the orientation of the segments. We can define the
macroscopic polarization vector as

P = lNseg
    L2 ħ

in such a way that ⟨∇Φ(r)⟩ = π ẑ × P. Clearly P plays the role of the ferroelectric order
parameter. It can be expressed in term of the concentration x of the charge carriers and
of the filling factor ν, that is the number of charges per segment length, i.e. P = x/l

In Ref.10, the authors propose an order parameter proportional to the incommens-
urability of the neutron scattering peaks, to characterize the phase of the underdoped
cuprates. We can show that it can be found a relation between this incommensurability
and the polarization P that we propose as order parameter. Indeed the constant spin
current implies an incommensurate spin response perpendicular to the segments, whose
modulus is q ⊥ = πP.
Perspectives

My future objective is to perform a Monte Carlo analysis to study the temperature and doping evolution of the complex phases of cuprates described in the previous section. To simplify the numerical implementation it is useful to remember that an XY vortex can be mapped to a 2D Coulomb charge [19] or alternatively to current wires perpendicular to the 2D plane. The sign of the charges or the direction of the current is determined by the winding number \( k \) of the vortices. In this way we can leave the interacting topological charges free to evolve in the thermal bath, without taking into account the spin configuration. Only at the end of the simulations we can reconstruct the total spin distribution. The long range interaction between these topological charged is given by a central potential described by the Bessel function \( K_0(r/\lambda) \), where \( \lambda \) is a screening length. To this we have to add the real 3D Coulomb repulsion between the holes, and the short range force arising from the quantum superposition of the atomic orbitals (we can extract it from Gutzwiller calculation).

With these simulations we want to characterize possible thermodynamic transitions and to find other type of order in the phase diagram of cuprates, for example the possible presence of a nematic phase (rotational symmetry broken but inversion symmetry preserved), between the ferronematic region and the disorder. Furthermore we will extend this approach to study the progressive evolution of the stripe-segment ferronematic phase to the phase with very long or infinite stripes.

Another problem we want to analyze is the study of the effect of dislocations on the long range antiferromagnetic order. A dislocation is a topological defect of the crystal structure. It arises naturally for example due to the misorientation between two crystal domains in a polycrystalline structure. Some types of dislocations (edge dislocations) can be visualized as being caused by the termination of a plane of atoms in the middle of a crystal, distorting nearby planes of atoms. Fig.4 shows the deformation due to two dislocations in an AF ordered 2D lattice. In such a case we expect a deformation of

![Crystal structure distortion due to two edge dislocations](image)

**Figure 4:** Crystal structure distortion due to two edge dislocations on an AF ordered square lattice. This structure has been calculated considering an elastic interaction between each nearest neighbor sites.
the spin structure similar to that generated by a vortex and an antivortex. We will use mean field techniques like those showed in the previous section, i.e. Hartee-Fock and/or Gutzwiller calculation, to obtain the low energy states of this type of systems, and to study its properties as the distance between dislocations is changed. We expect that the domain wall could become metallic in some cases, giving rise to a quantum wire.

References