Orbital-selective Mottness and pairing in Iron-based superconductors

Phd student: Marcello Carta
Advisors: Massimo Capone, Marco Grilli

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Superconductivity: zero resistance to current flow and perfect diamagnetism (a.k.a. Meissner effect)

- 1911: Kamerlingh Onnes discovers that, below 4K, in metallic Mercury electric current persists indefinitely.
- 1933: Meissner & Ochsenfeld discover that Sn and Pb, if cooled under $T_c$, expel the magnetic field from the bulk.
- 1957: Bardeen, Cooper, Schrieffer formulate BCS theory (Nobel Prize 1972), which describes conventional superconductors ($T_c < 23K$).
- 1986: Muller & Bednorz discover superconductivity in $LaSrCuO$, a cuprate, with $T_c \simeq 35K$. Subsequently, many other Copper-based superconductors are discovered, with critical temperature up to 135K (Nitrogen boiling point: 77.35 K). $\rightarrow$ High $T_c$ superconductors.
- 2008: Kamihara, Watanabe, Hirano & Hosono discover superconductivity in compounds containing Iron and a pnictogen (As, F) or a chalcogen (Se, Te) ligand; subsequently, other pnictides are synthesized, with $T_c$ up to 55K.
Presence of a superconducting dome, with maximum at a certain optimal doping of holes or electrons.

Presence of magnetic ordering at low level of doping, antiferromagnetic for cuprates, spin-density wave for pnictides.

In pnictides, for certain values of the doping, there is possible competition/coexistence between superconductivity and magnetic ordering.

Occurrence of a 'pseudogap' region in cuprates.

Undoped cuprates are Mott insulators, undoped pnictides are (bad) metals.
Mott insulators: insulators due to strong electronic correlation.

The fact that the cuprates are Mott insulators (for low level of doping), indicates that electronic correlation plays a major role in the description of these materials. The simplest model which contains electronic correlation is the Hubbard model:

\[ H = - \sum_{(i,j),\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \]

The \( U \) term is a simple modelization of Coulomb repulsion between electrons on the same lattice site.

There is competition between the two terms:

- for \( U \ll t_{ij} \) the first term prevails, thus giving energy bands (in tight binding approximation), and we may have a metal.
- for \( U \gg t_{ij} \), due to very strong on site repulsion, electrons are not encouraged to jump between sites, and we have a (Mott) insulator (if at half filling).

→ somewhere in between these two regimes we have a phase transition between a metal and an insulator, known as Mott-Hubbard transition.

As one might guess from the opposite character of the two terms of the Hubbard hamiltonian, the Mott-Hubbard transition is a non-perturbative phenomenon.
However,

- while in cuprates only the $d_{x^2−y^2}$-generated band is relevant, in pnictides, due to the ligand and to the different electron count, all the five d-generated bands cross the Fermi energy, and thus play a role.

- only the cuprates are Mott insulators at low doping; this may mean that, despite the similarity of the phase diagrams, electron-electron interaction in pnictides is somewhat weaker than in cuprates.

- in cuprates, the superconducting gap $\Delta_k$ is known to have a $d_{x^2−y^2}$-wave symmetry (in $k$ space); regarding pnictides, $p$ and $f$ symmetries have been excluded, but otherwise the symmetry of the gap is possibly non-universal and still debated.

- in either class of materials, it is not known what is the nature of the coupling between electrons causing the formation of pairs, thus causing superconductivity (remember that in conventional superconductors the attraction between electrons is given by the exchange of a phonon).
To reconcile the possible presence of the strong electronic correlation with the absence of a Mott insulating state in the phase diagram, it has been recently proposed a scenario in which the degree of correlation varies with the band index, so that electrons can interact strongly or weakly depending on the band they belong to.

Given the typical lattice structure of a typical Iron-based superconductor, one can derive the following Hamiltonian:
\[
H = \sum_{ij,mm',\sigma} t_{ij}^{mm'} d_{im\sigma}^{\dagger} d_{jm'\sigma} + H_{int} \quad m, m' = 1, \ldots, 5
\]

\[
H_{int} = U \sum_{i,m} n_{im\uparrow} n_{im\downarrow} + \left( U' - \frac{J}{2} \right) \sum_{i,m>m'} n_{im} n_{im'}
\]

\[
- J \sum_{i,m>m'} \left[ 2 S_{im} \cdot S_{im'} + \left( d_{im\uparrow}^{\dagger} d_{im\downarrow}^{\dagger} d_{im'\uparrow} d_{im'\downarrow} + h.c. \right) \right]
\]

where
\[
S_{im} = \frac{1}{2} \sum_{\sigma\sigma'} d_{im\sigma}^{\dagger} \tau_{\sigma\sigma'} d_{im\sigma'}
\]

Our work is to study this model, in order to gain information about Iron-based superconductors; above all we aim to get knowledge about the symmetry of the superconducting order parameter and about the nature of the electron-electron pairing mechanism.

We use several non-perturbative man-body techniques, namely:

- **Dynamical Mean Field Theory (DMFT)**
- **Slave-Particles methods**
DMFT: Quantum analog of classical mean field theory.

We want to build a single site effective theory, approximating the interaction with the rest of the lattice with an effective quantum bath.
The key quantities in DMFT are the local Green’s function at a given lattice site

\[ G_{ii}^{\sigma}(\tau) = -\langle T_{i\sigma}(\tau)c_{i\sigma}^{\dagger}(0) \rangle \]

and the local self-energy \( \Sigma_{ii}(k, \omega) \), given schematically by the following series

Following the usual procedure, we can sum the geometric series obtaining

\[ G(k, \omega) = \frac{1}{\omega - \epsilon_k - \Sigma(k, \omega) + i\delta} \] (1)
In DMFT we derive a local effective action for a single site where the function $\zeta^{-1}(t)$ is the bare Green function of the auxiliary effective theory (not to be confused with the non-interacting one of the lattice model), and is the quantum generalization of the Weiss field in classical mean field theory.

$$S_{\text{eff}}[c, c^\dagger] = - \int_0^\beta \int_0^\beta dt \, dt' \sum_\sigma c^\dagger_{i\sigma}(t) \zeta^{-1}(t - t') c_{i\sigma}(t') + U \int_0^\beta \frac{dt}{\beta} n_{i\uparrow}(t)n_{i\downarrow}(t).$$

At variance with the classical case, however, the function $\zeta(t)$ depends on (imaginary) time.

Then we seek for an approximate form of $\Sigma(\omega)$ by mean of a self-consistency relation given by the Dyson equation

$$\Sigma^{DMFT}(\omega) = \zeta^{-1}(\omega) - \sum_k G(k, \omega)$$

$$G(k, \omega) = \frac{1}{\omega - \epsilon_k - \Sigma^{DMFT}(\omega)}.$$
Remarks

- $\Sigma^{DMFT}(\omega)$ does not depend on $k$, but the frequency dependence of the self-energy implies that the effective theory is still interacting and non trivial, although simpler than the original lattice model.
- nothing was said about the value of the coupling constant(s): DMFT is a non-perturbative method.

Due to this characteristics, DMFT has been successfully employed to study, for example, the BCS-BEC crossover in attractive Hubbard model, which is believed to capture some of the physics of the cuprates.

When DMFT is exact?

- Independent electrons: no resistance to propagation, the self-energy $\Sigma$ vanishes.
- $t_{ij} = 0$, i.e. no hopping: the system is formed by many independent atoms $\rightarrow \zeta^{-1}(\omega) = 0$
- infinite dimensionality, or full connectivity: no notion of distance, no fluctuations to be neglected
Another way to tackle with strongly interacting systems is the so-called Slave-Particle approach. The general idea is to enlarge the Hilbert space by introducing a set of auxiliary fields to represent the fermionic operators, and then to impose constraints on these fields to eliminate unphysical states. This allows to derive a mean-field approach valid in the strong-correlation regime.

In a nutshell

**very strong interaction ↔ constraints**

One of the most successful representation of fermionic operators is that by means of slave spin variables.
One introduce a spin operator $I$, 

$$I^z |\pm\rangle = \pm \frac{1}{2} |\pm\rangle$$

where $|\pm\rangle$ represents doubly occupied and empty sites, and $|\mp\rangle$ single occupied sites. Consequently the eigenvalue of $I$ reflect the presence or the absence of a local magnetic moment. Then introduce auxiliary fermion operators $f_\sigma$ to preserve canonical anticommutation relations. The physical operators of the original model are then 

$$c_\sigma^\dagger = 2I^x f_\sigma^\dagger$$

It turns out that the physical subspace is selected by the requirement that

$$I_i^z + \frac{1}{2} - (n_i - 1)^2 = 0$$

and that underlying the above representation there is a $U(1)$ gauge redundancy, which is broken to $Z_2$ when we consider the mean field approximation.

- many spin representation of fermion operators have been proposed
- in general a gauge redundancy is present
- many few auxiliary particles are needed with respect to other slave particle approach (slave bosons)
- still need extension to the superconducting phase.
Experimental measurement of mass enhancement in a typical pnictide (doped $BaFe_2As_2$), showing a different (monotonically decreasing) trend for several method of probing, thus indicating increasing selective Mottness by decreasing doping:
There is evidence that the Hund term of the Hamiltonian acts as a band decoupler:

- Different orbitals reach half filling at very different rate, thus experiencing different amounts of correlation; in particular some orbitals appear to be close to a Mott insulating state already in the stochiometric compound (6 electrons per Iron atom).
- Each orbital is sensitive only to its own filling, behaving as a single band Mott insulator.

What are the consequences on the superconducting state?
Non-perturbative treatment of multi-band superconductivity in simple models: we will use DMFT to study a simple model with attractive and repulsive interactions between different orbitals. In this way we can single out the effects of strong/intermediate coupling superconductivity in the experiments in order to filter out the effects of strong Coulomb repulsion.

Diagrammatic Theory of Superconductivity with orbital selectivity: we will identify what is the effect of the orbital selective physics on superconductivity within a weak-coupling framework.

Extension of the Slave-Spin method to the Superconducting State: We will extend the Slave-spin approach in order to treat broken-symmetry phases and in particular to the superconducting state, in order to develop a simple and effective tool to study superconductivity in a multi-orbital Hubbard model which will guide our DMFT investigation.

DMFT phase diagram from simple models to real systems: we will combine the information from Diagrammatic Theory and from the DMFT on attractive models in order to build a comprehensive understanding of simplified models for iron superconductors. This investigation is expected to shed light on the main questions about the superconducting phase of iron superconductors, including the symmetry and the origin of pairing.