STRONGLY CORRELATED ELECTRONS IN SOLIDS - II

Superconductivity and electron-phonon interaction

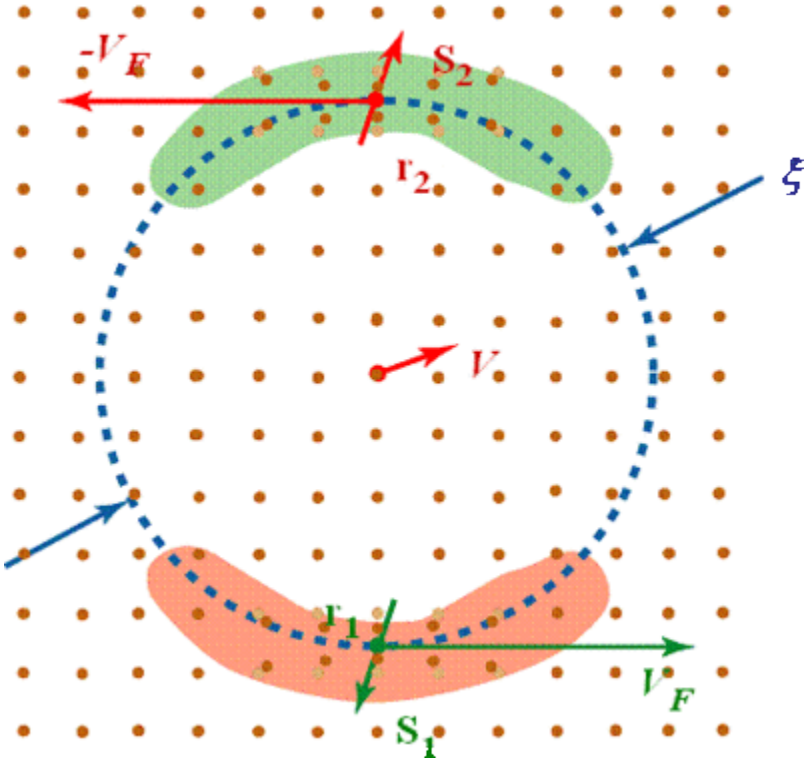

Figure 3: Spatial representation of a Cooper pair. The lattice distortions shown by pink and green shadings have been produced by the electrons at $\mathbf{r}_2$and $\mathbf{r}_1$ respectively and trap the electrons with opposite spins in a singlet state.

So far we have seen that the original properties of electronic matter are mostly governed by the magnitude of the Coulomb repulsion between electrons which is essential in the magnetic properties and in promoting localized electronic states rather than extended states. But, although we mentioned it at many places already, we did not consider so far one of the most important correlated electronic states which has been studied at length during most of the last century, that is superconductivity. This electronic state of matter is by no way an independent electron case, as the basic feature of this state is an electronic organisation which emphasizes pairs of electrons, the Cooper pairs. This has been highlighted in classical metals by the development of the Bardeen Cooper Schrieffer (BCS) theory which states that in the presence of an attractive interaction between electrons, no matter how weak it may be, the electron gas becomes unstable.

The beauty of this unexpected physical situation is that the lower energy condensed electronic state is a quantum state of electronic matter in which the correlations between electrons extend on macroscopic distances.The mystery which prevented the actual understanding of superconductivity during the first half of the 20th century concerned the actual possibility of such an attractive interaction between electrons. This has only been understood when it had been noticed that the electrons do attract the ions of the atomic background, and that their displacements (the phonons) being slow due to the large ionic masses provide a memory effect which mediates an attractive interaction between electrons. If that electron-phonon interaction dominates the electronic Coulomb repulsion, then the net attractive interaction favors the pairing of electrons which is qualitatively depicted in **Fig. 3**. The pairing of electrons results in the many body electronic states which is the basis of the electronic properties of the superconductors. One of the main unexpected behaviors which could be explained by the BCS theory is the existence of a gap between the electronic superconducting ground and excited states. The occurrence of such a gap has been initially ascertained by NMR experiments.

From Mott Insulators to Metallic Magnetism and Superconductivity

We have examined so far two completely different limiting descriptions of electronic states in a solid. In the band structure approach we have described the case of electrons considered as independent, their interactions being restricted to an averaged potential. The delocalisation of these electrons between the atomic sites driven by the transfer integrals may yield metallic states. In contrast we have considered the specific situation for which electrons localized on ionic states lead to local atomic magnetic moments. Those arise when the Pauli principle and on site inter-electronic Coulomb repulsion are taken into account properly. We have assumed implicitly that these electrons do not delocalise when the transfer integrals between electrons on neighboring ions are small enough in such solids. This then corresponds to an insulating magnetic state quite different from the band insulating states considered so far in the independent electron band approach.

The actual situation in real materials does indeed sometimes correspond to these limiting cases, but a wide variety of solids correspond to intermediate situations, like that of ferromagnetic metals such as Fe or Ni. But the correlated electron physics is now rich with examples of such intermediate cases which are quite important both for the fundamental questions raised and for the applications of the novel physical effects which come into play.

From Mott insulators to metal insulator transitions

In a Mott-Hubbard insulator, if we increase t (or if we consider compounds with lower values of U), for a certain critical value of t/U, the upper and lower Hubbard bands begin to overlap (see **Fig. 2 right**), causing the band gap to disappear and leading to a metallic state. Such an increase in t can be produced by bringing the atoms closer together. This was first achieved in the case of doped semiconductors by increasing the donor concentration, e.g., by increasing the concentration of phosphorus in silicon. This causes the hydrogen-like orbitals of P to move much closer together and increases the hopping integrals, while remaining in a configuration corresponding to one electron per donor atom. A simpler way to achieve this situation directly without changing the number of electrons in a material is to apply an external pressure. This increases the hopping integrals t by bringing the atoms closer together, provided that the material is compressible. In the metallic state thereby induced, one then observes magnetic and thermodynamic properties which require taking into account the existence of the strong coulomb repulsion U.As for the Mott-Hubbard insulator, let us point out that it looks at first glance like a band insulator, the only difference being that here each Hubbard band contains only N_n states rather than $2N_n$ states in the case of the band theory of **section 2**.

Doping a Mott insulator: the cuprate problem

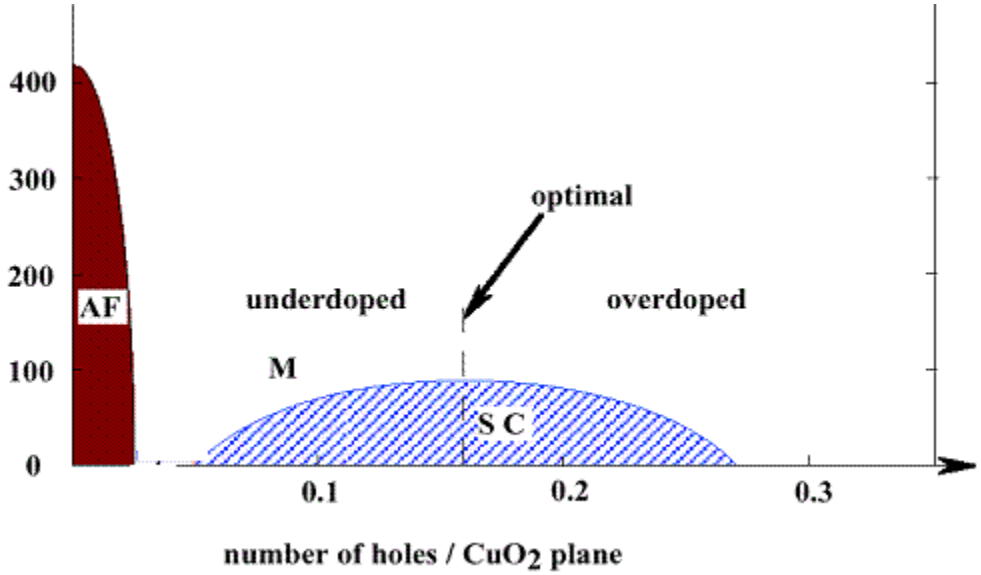

Figure 4: Elementary phase diagram of the cuprates obtained by hole doping the AF Mott insulating state. The AF state is rapidly destroyed by hole doping beyond 0.05 and opens the way to a metallic state which becomes superconducting at

low T. One observes a SC T_c dome shape as a function of the hole doping. The highest T_c occurs for optimal doping and one speaks of underdoped and overdoped states.

Chemical treatment may be envisaged to change the number of electrons in a Mott insulator. For example, it can be doped with holes, reducing the number of electrons in the lower Hubbard band to a number N_e smaller than N_n. This is exemplified by the case of cuprates such as $YBa_2Cu_3O_6$ or La_2CuO_4which are antiferromagnetic Mott insulators. In the latter, the Cu are in a $3d^9$ state with spin 1/2, which order antiferromagnetically below 340K. By chemical exchange of a fraction x of La^{3+} by Sr^{2+} one can typically reduce the number of Cu electrons to become $N_e = (1-x)N_n$. This reduction of the number of electrons in the lower Hubbard band suggests that the doped Mott-Hubbard insulator is expected to be a metal. Experimental investigations carried out on the cuprates, and also on certain other classes of doped Mott insulators, have shown that doping gradually reduces the Néel temperature of the antiferromagnetic state. This AF state is completely suppressed for a low level of doping, of the order of $x \approx 0.05$, as can be seen in the phase diagram for $La_{2-x}Sr_xCuO_4$ displayed in **Fig. 4.**

Superconductivity in correlated electronic systems

The importance of the cuprates in the physics of correlated systems has resulted from the discovery that when the AF is suppressed by hole doping, the doped metallic state which results has a SC ground state and displays strange metallic and magnetic properties. The most surprising feature has been the fact that the superconductivity discovered in these materials has the highest critical temperatures T_c found so far in any superconducting material, and exceeds any T_c which could be expected within the BCS approach known to apply in classical metallic states. This has immediately led to the idea that SC in the cuprates has an exotic origin linked with electron-electron interactions rather than the classical electron-phonon driven superconductivity which prevails in classical metals. An important observation in the cuprates has been the fact that the phase diagram with increasing hole doping displays a dome shaped SC regime, that is SC disappears for dopings beyond about 0.3. While the cuprates are certainly exotic superconductors, let us state that many other materials have been shown to display situations where magnetism and SC are proximate to each-other in phase diagrams. In pnictides those are sometimes spanned by doping as in the cuprates, but in other families of compounds the phase diagrams are spanned by pressure control of the overlap integrals as for organic, heavy fermions or Cs_3C_{60} compounds. The author shall present many examples of such families in the Scholarpedia article NMR in strongly correlated materials.

Experimental techniques

Such original states have been revealed initially by experimental techniques which were quite adapted at the time of the discovery of the cuprates to studies of their electronic properties. Among those, Nuclear Magnetic Resonance (NMR) is a technique which is quite essential as it permits local measurements in the materials. This gives precious information which goes beyond the first indications given by the macroscopic magnetic measurements as they permit one to differentiate the properties of the materials which can be attributed to specific phases or sites in the structure. Also, as usual for magnetic materials, inelastic and elastic Neutron scattering techniques reveal the occurrence of magnetic responses and of their k-dependence.

Significant effort has been invested to improve the quality of single crystals which are essential for the studies of the transport properties in these exotic metals and SC. Static or pulsed high magnetic field sufficiently large to suppress the superconducting state have been achieved, though this not yet possible for samples with high optimal Tc.

Other new specific techniques for studies of surfaces of 2D compounds have been developed during the last decades. The Angular Resolved Photoemission Spectroscopy (ARPES) uses X-rays generated by synchrotrons to perform k-space resolved spectroscopy of the occupied electron states. This permits determination of the band structures of these correlated electron materials. Deviations with respect to simple band calculations permit determination of the incidence and strength of the electronic correlations. Also Scanning Tunneling Microscopy experiments reveal spatial inhomogeneities of the gaps and of the electronic structures at surfaces in these materials. Some experimental groups have developed Fourier transformations at a level of refinement which allowed them to reproduce some of the ARPES spectral information. The existence of charge density wave transitions is also detected by Resonant Inelastic X-ray Scattering (RIXS) or Resonant Elastic X-ray Scattering (REXS).

Many of these novel techniques have been improved by recent technical developments, but their input on the physics of correlated electron systems are still far from being fully understood at this time and will be introduced in dedicated Scholarpedia articles.

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