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On the possible role of antiferro-magnetic short range order in quasi one dimensional organic superconductors

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Abstract. The possible influence on superconductivity of short range antiferromagnetic order observed in some organic conductors is compared with the case of cuprates.

PACS. 74.70.Kn Organic superconductors – 74.72.-h Cuprate superconductors (high-T_c and insulating parent compounds)

1 Introduction

In a recent review paper on quasionedimensional organic superconductors, Bourbonnais and Jérome [1] stress the fact that the superconductive state, first observed in that family of organic compounds [2], can coexist with antiferromagnetism (AF). This coexistence takes the form of an equilibrium mixture of two macroscopic phases over some range of the temperature T versus pressure P diagram. But, beyond a critical pressure, where the AF long range order becomes unstable and disappears, there then remains a *short range* AF order which coexists with superconductivity [3]. This short range order is observed over a large region of the (T, P) diagram, of which the superconductive phase only occupies a small fraction.

This is in a way similar to what is observed in cuprates [4] where, as here, the short range AF is observed to much higher temperatures than superconductivity. Also short range AF is observed in cuprates up to all dopings where superconductivity occurs, as is the case with pressure for quasi $1d$ organic compounds: as stated by Bourbonnais and Jérome, short range AF not only coexists with superconductivity but surrounds it to a large extent in the (T, P) diagram.

Short range AF was first observed in cuprates by neutron scattering methods; it strongly influenced early models of high T_c superconductivity, especially by Schrieffer but also by Anderson, in terms of fluctuating localised magnetic atomic moments. When it became clear, from electron photo-emission spectra and resonance techniques, that a delocalised picture of the electrons should be used, with a well defined Fermi level, the possible role of short range AF was minimized or neglected, even if strong electron charge correlations were considered. A few years ago, Friedel and Kohmoto [5] pointed out that the short range AF, when analysed in a delocalised electrons picture, could have important and perhaps essential effects, as far as the value of T_c, the symmetry of supercondive gap Δ_c and the existence of an AF pseudogap were concerned. It is therefore natural to put the same question for the organic superconductors where, as in cuprates, short range AF is definitely more stable than superconductivity it coexists with: it must indeed be fully included from the start. We shall in fact argue that, from that point of view, quasi $1d$ organic superconductors are nearer to the case of LSCO than of the other cuprates, with a somewhat reduced role of antiferro-magnetism.

2 Magnetic gap and pseudogap

The organic compounds considered are made up of parallel rows of flat organic molecules which conduct by charge transfer to neighbouring counterion: the conduction band is 1/4 filled with holes, i.e. there is one hole per pair of molecules. A slight dimerisation of the molecules introduces a small dimerisation gap, so that the top half of the conduction band is half filled.

The *long range* AF phase observed can be viewed as a Spin Density Wave (SDW) with a period ($2k_M$, π, π), in reciprocal space, the nesting vector g_0 for a Fermi suface made of sheets perpendicular to the rows of molecules. k_M is the Fermi wave number along the rows. For electrons localised on independent rows, the Fermi surface would

be made of planes; small transfer integrals between rows distort these planes slightly. As a result, the spin modulation has a period $4a$ along a row, if a is the distance between molecules along the rows; the spin modulations are in antiphase in neighbouring rows. The magnetic exchange potential between electrons which stabilises this SDW opens a sharp gap Δ_M in the density of states at the Fermi level. For an isolated row and neglecting $1d$ magnetic fluctuations, the gap is bordered by two sharp peaks of density of states, of logarithmic divergency in energy. Sufficient transfer integrals between rows kill the $1d$ magnetic fluctuations at low temperatures and round up the peaks bordering the gap. As a result, the peaks have limited tails in the magnetic gap, which would only overlap for very weak magnetism and small gaps. In fact, the Fermi level should fall in the middle of the essentially symmetrical gap, and the compound should be an insulator for the sizeable magnetic moments expected. Indeed the SDW phase of these organic compounds are all insulators. One should also expect absorption and conduction peaks in the far infrared range, due to the excitation of electrons (or holes) from the occupied (or unoccupied) peaks of the gap to the Fermi level. The corresponding energy, of the order of $1/2\ \Delta_M$, might be at least partly responsible for deviations from the Drude law in the far infrared. Other excitations in the IR range due to charge correlations effects, have also to be taken into account [1].

But it should be stressed that in the delocalized limit considered here, both types of excitations are of the order of the Coulomb self energy U.

For a short range AF with similar wave lengths and amplitude but with finite coherence lengths ξ_a, ξ_b, ξ_c, one expects a *pseudogap* of the same order of magnitude as Δ_M, limited by two peaks somewhat broadened both by the finite coherence lengths and eventually by finite fluctuations times. Between these peaks, as first pointed out by Mott in a similar context of atomic structures, the pseudogap should have larger tails that should extend continuously through it. The states in these tails should certainly conduct near the peaks; but if the pseudogap is large enough, the magnetic disorder if frozen could localise the states near the middle of the pseudogap, by an Anderson localisation. For the organic compounds considered, there is no sign of such an effect for the Fermi electrons, in the middle of the pseudogap.

In conclusion, one expects a short range AF to *lower* the density of states at the Fermi level. This would be compensated by two fairly sharp peaks of the density of states at $+/-1/2\delta_M$, above and below the Fermi level, where δ_M is the width of the pseudogap. Such peaks seem visible in the far IR at low temperatures; they should also show up in conduction and in magnetic resonance tests at $k_BT \geq 1/2\delta_M$.

Finally, they could be responsible for finite conductivity at low temperatures.

Correlation effects should be included in this description for quantitative estimates but are not expected to change these qualitative predictions.

3 Superconductivity

The effect of short range AF should clearly be detrimental to high values of T_c and Δ_c. This is in keeping with observations in the organic compounds. The situation should be in fact rather similar to that of LSCO cuprates and some YBCO ones [7], where the period of short range AF modulations varies with doping so as to keep the nesting condition and thus keep the Fermi level in the middle of the pseudogap. Most other cuprates keep a fixed period of AF modulations, independent of doping [4]; as a result, variable doping can shift the Fermi level through a peak of the pseudogap, leading to much higher values of T_c and Δ_c.

Another aspect of superconductivity concerns the symmetry of the gap Δ_c. For cuprates [5], the local coherence expected in the scattering of electrons, near the peaks of the pseudogap, by neighbouring magnetic moments should react on the symmetry of Δ_c. Thus the wave functions $|K\rangle$ near such a peak should be linear (bonding and antibonding) combinations of the non magnetic Bloch functions $|k\rangle$ and $|k - g_0\rangle$ related by the nesting vector g_0. The non s symmetry observed for Δ_c in most cuprates can be reconciled with the isotope effect on T_c (which suggests an isotropic coupling by phonons of the Bloch states $\langle k|V|k'\rangle$, if one takes into account the asymmetry relating $\langle K|V|K'\rangle$ to $\langle k|V|k'\rangle$ when the Fermi level is near a peak of the pseudogap.

In the organic compounds (or in LSCO), the Fermi level is in the middle of the pseudo gap, where bonding and antibonding wave functions are equally mixed. This should effectively suppress any effect of coherent magnetic scattering at the Fermi level. The symmetry of Δ_c should then be directly related to that of $\langle k|V|k'\rangle$. The short range AF should *not* change by itself the symmetry of the pseudogap: the non s symmetry apparently observed in these organic compounds should then be purely due to the electronic nature of $\langle k|V|k'\rangle$. The progressing lowering of T_c with increasing pressure was indeed attributed initially to a direct coupling via not phonons but AF fluctuations, which should decrease in amplitude as the static short range AF in these compounds [1].

4 Conclusions

Because they are charge transfer compounds with fixed and simple transfers (1/2 hole per molecule), quasi $1d$ organic compounds give rise to long and short range AF modulations with wavelengths simply and rigidly related to the molecular periodicity. As a result, the Fermi level falls in the middle of the AF gap or pseudogap. In the case of short range AF, the density of states should then be depressed by the pseudogap at the Fermi level; but the Fermi states are apparently still delocalisd, leading to conducting and possibly superconducting states in the presence of short range AF. The possible superconductivity has a depressed T_c. The non s symmetry of the superconductive gap cannot be related to a specific magnetic bonding or antibonding character of the electronic states, which

only exists near the peaks of the pseudogap; it must come from an intrinsic symmetry property of the BCS potential V. Is it possible to incrrease T_c in these compounds, as in cuprates, by shifting the Fermi level towards one of the peaks of the pseudogap? This would require electron or hole doping by changing the proportion or ionicity of counterions. If that was possible without changing the geometry of the molecular rows *and* if the AF modulation still occured and kept blocked on the same period, this could raise T_c considerably and would change somewhat the symmetry of the superconductive gap.

It might happen however that the AF modulation kept long range or kept perfect nesting conditions; but T_c, if maintained, would not increase. If doping killed the short range AF, only a moderate increase of T_c could at best be hoped for, due to the disappearance of the pseudogap.

Finally, as stressed in the case of cuprates, the exact nature of the short range AF order should not play a decisive role, as long as its coherence lengths ξ are of nanodimensions. The actual structure would play on the form of the peaks in the density of states. It is also clear that corrections for electron charge correlations could affect numerically the results, without probably changing the general effects and orders of magnitude.

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