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Abstract. The Bechgaard salts are made of weakly coupled one dimensional chains. This particular structure gives the possibility to observe in these systems a dimensional crossover between a high temperature (or high energy) one dimensional phase and a two or three dimensional system. Since the filling of the chains is commensurate the system thus undergoes a deconfinement transition from a one dimensional Mott insulator to a two (or three) dimensional metal. Such a transition has of course a strong impact on the physical properties of these compounds, and is directly seen in transport measurements.

In order to describe such a transition a dynamical mean field method has been introduced (chain-DMFT). Using this method we investigate a system of coupled Hubbard chains and show that we can indeed reproduce the deconfinement transition. This allows to determine physical quantities such as the transport transverse to the chains and the shape of the Fermi surface and quasiparticle residues in the low temperature phase.

Keywords. Organic conductors – Luttinger liquid – Deconfinement

1. INTRODUCTION

The Bechgaard salts TMTSF_2X were the first organic compounds to exhibit superconductivity, and have thus been the focus of intense experimental and theoretical studies [1, 2]. These systems are highly anisotropic crystals that consist of parallel conducting chains. The electron transfer integrals along the chains (in the a direction) and transverse to the chains (in the b and c directions) are typically $t_a = 3000$ K, $t_b = 300$ K, and $t_c = 10$ K. Therefore one can think of these materials as one-dimensional chains coupled by small inter-chain hoppings. Given the hierarchy of transverse coupling the system is first expected to become two dimensional and then three dimensional at low temperatures.

Despite the fact that they have been studied for more than twenty years, these compounds are still largely not understood. Some of the most important open questions are: (i) the nature and properties of the the high temperature “normal” phase. (ii) what happens when the energy (temperature, frequency, etc.) is lowered and one can expect the various hopping integrals to play a role. We will briefly review in this paper the recent progress that have been made to understand these two questions.

2. “Normal” state

Since the interchain hopping are so widely separated one would expect that when the temperature or energy (frequency, etc.) is higher than t_b the interchain hopping cannot occur coherently and the systems are in a one dimensional limit. In that case one would expect due to interactions a Luttinger liquid behavior [3]. However, although the Bechgaard salts themselves are metallic, the parent compounds TMTTF (Fabre salts) show a marked insulating behavior. Such a behavior is obviously due to interactions and related to Mott physics. Indeed, by chemistry both TMTTF and TMTSF compounds are quarter filled. Such insulating behavior is thus the proof of the importance of interactions in TMTTF, even at relatively high energies. For the TMTSF the question is more subtle in view of the metallic behavior at ambient pressure and whether such compound is a Luttinger liquid or a Fermi liquid was the subject of considerable debate [4]. Another important question is of course the reason for such a difference between the very close families TMTTF and TMTSF, for which the various characteristics (bandwidth, dimerization, interactions) vary relatively little.

One possible interpretation of this difference was suggested a long time ago [5] and attributed to the dimerization of the chains. Indeed because of the existence of a slight dimerization, the effective band is half filled and not quarter filled and one is now in the standard situation to get a Mott insulator (one particle per site). In such a case it is well known that in one dimension any repulsive interaction leads to a Mott insulating state. The accepted idea was thus that in the TMTSF family, dimerization being much smaller, the system would be viewed as quarter filled and thus could not be a Mott insulator. The commonly adopted point of view to describe these systems would thus be to describe them by a Hubbard like model, where the insulating character would mostly depend on the local interaction U and on the dimerization Δ_d .

However this point of view had to be seriously reexamined in the recent years. On the experimental side, optical data [6, 7] shows quite clearly that even the TMTSF family exhibits strong interaction effects. Indeed, although such compound seems to have a rather “standard” d.c. conductivity, all the d.c. transport is in fact due to a very narrow Drude peak containing only 1% of the spectral weight, whereas 99% of the spectral weight is above an energy gap (of the order of 200 cm^{-1}), and is reminiscent of a Mott insulating structure. On the theory side, it was shown that the Mott insulating state could exist for higher commensurabilities than one particle per site [8, 9] for strong enough and *non on-site* interactions. Physical quantities such as the optical conductivity were computed for such one dimensional Mott insulators [10, 11]. Since even purely quarter filled systems could be Mott insulators, this prompted for the question of which mechanism was dominant for the gap observed in the TMTSF optical data: (i) the “half filled” nature of the band, due to the weak dimerization of the band; (ii) the direct mechanism responsible for the Mott insulating behavior of a quarter filled interacting system (no dimerization is needed).

Let us examine the two mechanisms (for more details see [11, 7]). In order to get an insulator in one dimension one has to consider the interaction processes that do not conserve momentum (so called Umklapp processes). For a system at half filling the umklapp takes two electrons from the left part of the Fermi surface (i.e. with momenta close to $-k_F$) and transfers them to the right part of the Fermi surface (i.e. with momenta close to $+k_F$). The total momentum transferred is thus $4k_F$ and for a half filled band this is 2π , i.e. a vector of the reciprocal lattice. For a half filled system any interaction process is thus able to lead to an umklapp process, and thus the strength of the umklapp is of order U if U is the interaction. If the band is quarter filled such a process is inefficient since the transferred momentum would be $4k_F = \pi$, and thus different from a vector of the reciprocal lattice. However in the presence of a slight dimerization of the chains one should diagonalize the kinetic energy and the eigenstates of the system are now mixtures of states containing k and $k + \pi$. In the presence of a dimerization Δ_d it is thus easy to show that an umklapp process should exist and that its strength is given by $g_{3,1/2} \sim U\Delta_d/W$ where W is the bandwidth of the system. Thus if the dimerization is zero one recovers that no umklapp process corresponding to half filling exists. In one dimension such an umklapp is relevant for any repulsive interactions and would open a gap in the spectrum of order $\Delta_{1/2} \sim W(g_{3,1/2}/W)^{1/(2-2K_\rho)}$, where K_ρ is the so-called Luttinger liquid parameter. $K_\rho < 1$ corresponds to repulsive interactions. $g_{3,1/2}$ is thus relevant for $K_\rho < 1$. However an umklapp process can also exist directly for a quarter filled system, if one transfers *four* electrons from one side of the Fermi surface to the other. Since an interaction process only scatters two electrons, such a process can only be generated at the third order in perturbation theory. The corresponding umklapp strength is of order $g_{3,1/4} \sim U(U/W)^2$. This process is only relevant if the Luttinger parameter is smaller than $K_\rho < 1/4$. Note that to obtain such a value it is necessary in addition to having strong interactions to have finite range (i.e. more than on site) interactions. Indeed for the Hubbard model the smallest possible value of the Luttinger parameter is $K_\rho > 1/2$.

Thus in the organic compounds, both processes are present and the question is whether one of the two is dominant [11]. Clearly this depends on the interactions: if the interactions are weak then the $g_{3,1/4}$ can obviously be neglected. Not only the coupling constant is small since it contains the factor $(U/W)^2$ but the process is also irrelevant. On the other hand, if the interactions are strong (i.e. of the order of the bandwidth), then $g_{3,1/4}/W \sim 1$ whereas $g_{3,1/2}/W \sim \Delta_d/W$ which is quite small (a few percents). Estimates of the interactions in the TM family suggests rather strong interactions, a sign that the system could be dominated by quarter filled umklapps. A clear answer to this question is provided by the optical conductivity [7]. For a Mott insulator in one dimension, the behavior of the conductivity above the Mott gap

should be $\sigma(\omega) \propto \omega^{4K_\rho-5}$ for half filling and $\sigma(\omega) \propto \omega^{16K_\rho-5}$ for quarter filling. The observed behavior fits well a power-law $\omega^{-1.3}$. If one tries to fit this behavior to an half filled process this leads to exceedingly weak interactions $K \sim 1 - U/(\pi v_F) \sim 0.93$. Using the expression for the Mott gap would lead to a gap which is orders of magnitude smaller than the observed optical gap $\Delta \sim 200\text{cm}^{-1}$. Thus the only possibility to fit the optical data is to assume that for the TMTSF family the conductivity is in fact dominated by the quarter filled umklapp. The value of K_ρ extracted from the optics $K_\rho \sim 0.23$ corresponds indeed to quite strong interactions and thus leads to a consistent description.

This prompts for several conclusions: (i) In order to modelize the TMTSF it is thus necessary to include in addition to a local interaction U a quite strong nearest neighbor (at least – and possibly longer range) repulsion V . Although one can show the importance of this term for TMTSF, given the similarities between the two systems such a term need also to be taken into account for TMTTF also. (ii) Given the proximity of $K = 0.23$ to the value at which the quarter filled umklapp is irrelevant, the observed decrease of the gap under pressure could be attributed to the proximity of this quantum critical point. Indeed applying pressure increases the hoppings, therefore reducing the interactions compared to the bandwidth and making K_ρ larger. One can thus expect the gap to vary rapidly with pressure. (iii) Although dimerization is clearly present and certainly plays a role in some of the physical quantities, most of the physics seems to be directly controlled by the quarter filled nature of the band. This strongly suggests that most of the physics of the TMTSF family should also be observed in a purely quarter filled compound. Compounds without dimerization have been synthesized and have been showed to be (quarter-filled) insulators (see e.g. [12]). The existence of such insulators confirms the above description. It would be extremely interesting to carefully study these systems under pressure, since they should exhibit most of the properties of the Bechgaard salts, including most probably the superconductivity.

3. Deconfinement transition

Let us now move to the effects of interchain hopping. Due to the interchain hopping a dimensional crossover will take place at low energy between decoupled chains and a higher- dimensional behavior. Since the isolated chains would be insulators, the interchain hopping can induce a deconfinement transition provided that it becomes larger than the Mott gap. The system will thus crossover from a regime where one has essentially uncoupled (insulating) chains to that of metallic planes. The interpretation that the change of behavior between the insulating and metallic regimes is indeed due to such deconfinement transition [11] can be strengthened by the optical data. A measure of the gap extracted from the optical conductivity shows that the change of nature occurs when the observed gap is roughly of the order of magnitude of the interchain hopping [13]. Understanding the characteristics of such a transition (energy scale, critical values of the hopping, physical nature of the various phases) is one of the most challenging questions on these systems, on which we shall focus in the following (for more details see [14, 15]).

Perturbation theory in the interchain hopping t_\perp is only of limited use for the study of the crossovers. For incommensurate fillings a perturbative RG treatment indicates that this effective inter-chain hopping grows as the energy scale is reduced: the crossover will occur when this running coupling reaches kT . While this perturbative RG analysis allows to estimate a scale E^* for the dimensional crossover [16, 17], it breaks down for $T < E^*$ since the effective t_\perp flows to large values. In particular, it does not provide information on the detailed nature of the low-T Fermi liquid regime. Thus, a proper handling of the dimensional crossover in quasi one-dimensional systems has to resort to techniques which are not perturbative in t_\perp . This is even clearer in the case of a commensurate filling. If one starts from the 1D Mott insulator fixed point, the deconfinement transition is clearly a non-perturbative phenomenon since the inter-chain hopping is an irrelevant perturbation at this fixed point. If, on the other hand, one starts with the LL fixed point associated with the high-T regime, then one has to deal simultaneously with *two* relevant perturbations: the umklapp scattering (responsible for Mott physics) and the interchain hopping. Non-perturbative studies are thus needed to investigate both the deconfinement transition and the dimensional crossover. Recently we have developed a mean field approach designed to handle *an infinite array of coupled chains* in a non-perturbative manner [18, 19, 14]. The details of the method [14, 15] can be found elsewhere and we

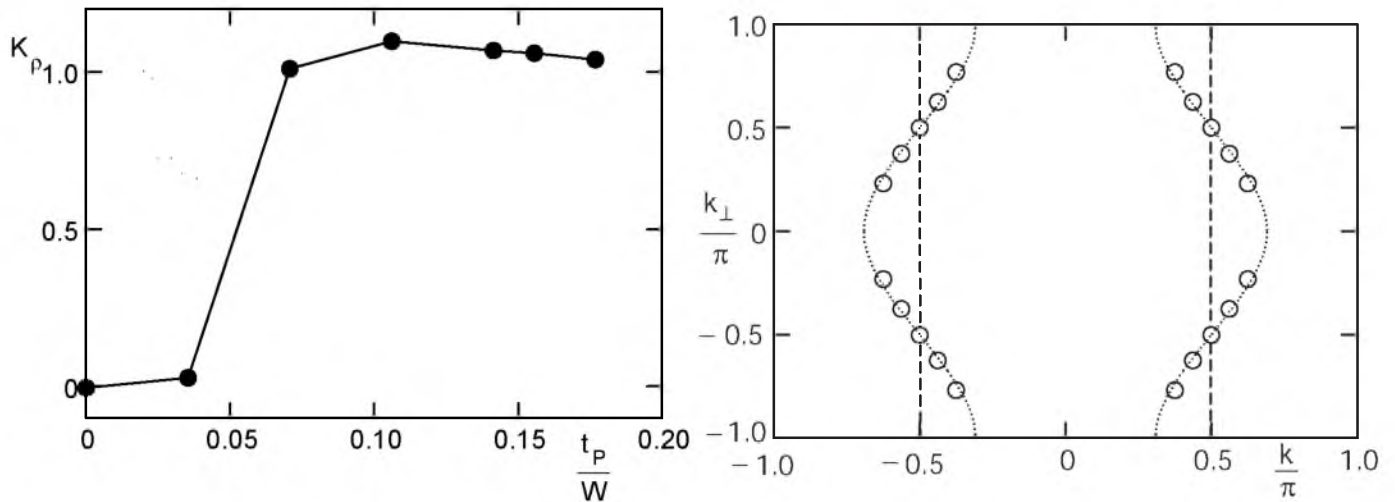


Figure 1: (left) K_ρ as a function of the perpendicular hopping t_\perp for a half filled system. The deconfinement transition is clearly visible. (right) Fermi surface (FS) in the half-filled case with $t_\perp/W = 0.14$, $U/W = 0.65$ (circles), compared to the FS of the non-interacting case (dotted line) and of the purely 1d case ($t_\perp = 0$ -dashed-). After [14, 15].

focus here on some of the results that could be extracted.

An analytical solution of the mean field equations is impossible. Thus only few quantities such as the Drude weight of the transverse conductivity could be obtained analytically [19]. In order to see whether our mean field approximation was able to capture the deconfinement transition we used it on a simpler model, namely a model of coupled Hubbard chains at half filling. Let us point out that this is only a toy model, the proper model for the organics being a U, V model at quarter filling. Nevertheless, as far as the deconfinement transition is concerned, this toy model should contain most of the necessary ingredients and is simpler to simulate, in order to test the method. More complicated calculation on the more realistic model being necessary as a second step to confirm the results of the toy model.

In Fig. 1, we display the effective K_ρ as a function of interchain hopping, for $U/W = 0.65$ and at a rather low temperature $T/W = 0.025$. For small t_\perp/W , the value $K_\rho = 0$ indicates a Mott insulating behavior (with a decay of the spin-spin correlation similar to that of a Heisenberg spin chain). In that regime, the calculated charge correlation function (not shown) clearly displays the exponential decay associated with a finite charge gap. Beyond a critical value of t_\perp/W , we find $K_\rho \simeq 1$, signalling a FL regime (and a corresponding behavior for the charge correlation function). Hence, the expected deconfinement transition is clearly revealed by our calculations. The location of the deconfinement transition is in reasonable agreement with the naive criterion $\Delta_{1D} \sim t_\perp^{\text{eff}}$, with t_\perp^{eff} the renormalized inter-chain hopping. [11, 13, 20]. At strong enough transverse coupling the system becomes a FL. In our numerical simulations, the onset of the FL regime is identified from the behavior of K_ρ (see Fig. 1) and from a linear behavior of the imaginary part of the self-energy in Matsubara space: $\Sigma(k, i\omega) \sim i\omega$. The equation defining the Fermi surface $\mu - \epsilon_k - \Sigma(k, 0) - \epsilon_\perp = 0$ then yields a relation $k_\perp(k)$ for the points (k, k_\perp) that lie on the Fermi surface. These are visualized in Fig. 1 for the half-filled case. For the uncoupled (1d) system the Fermi surface consists of straight lines (dashed lines in the figure); the transverse hopping induces some cosine-like modulation but does not change the topology drastically. Indeed, the Fermi surface of the interacting coupled system (circles in Fig. 1) is very close to the one of non-interacting ($U = 0$) coupled chains (dotted line in Fig. 1).

A very interesting question, is whether the strong interactions can lead to the existence of “hot spots” (see e.g. [21, 22]) on the Fermi surface of the system at low energy. Clearly this question needs to be investigated further but our calculation can bring some answers to this question. If one looks inside the 3D metallic regime ($K_\rho = 1$) and computes the QP residue Z_{k_\perp} then only a very small dependence on the Fermi surface points is seen (Table I), with very shallow minima at $k_\perp \sim \pm\pi/2$. This small variation is however on the scale of our error bars. This is true even for the closest point to the transition. Therefore

Table 1: QP weights $Z(k_{\perp})$ for different points on the FS (half-filled case, $t_{\perp} = 0.14W$, $U/W = 0.65$).

k_{\perp}/π	0.23	0.38	0.50	0.62	0.77
$Z(k_{\perp})$	0.79	0.77	0.76	0.77	0.79

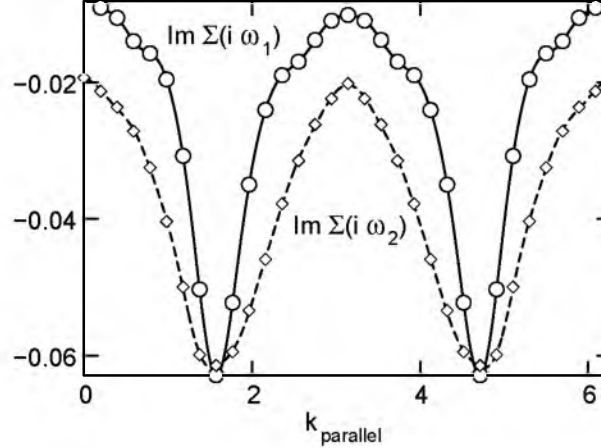


Figure 2: Imaginary part of the self energy as a function of k along the chains for $\beta = 40$, $U = 0.65$, $t_{\perp} = 0.05/\sqrt{2}$. $\omega_1 = \pi/\beta$ denotes the lowest Matsubara frequency and $\omega_2 = 3\pi/\beta$ the second one.

in the metallic regime we do not find signs of “hot spots” within our approximation. On the other hand the situation is quite different if one is close to the transition but on the $K_{\rho} = 0$ side (see Fig. 2) In that case the imaginary part of the self energy shows a strong dip. In the insulator this dip would signal the divergence $\Sigma \sim \Delta/(i\omega_n)$ for $\beta \rightarrow \infty$ and $k_{\parallel} = \pm\pi/2$ characteristic of an insulator. At finite temperature, the ratio of the imaginary part of the self-energy for the two lowest Matsubara frequencies would be $\sim \omega_2/\omega_1 = 3/2$. However close to the transition this ratio is much closer to one, as can be seen on the figure. Whether the fact that it seems to be still greater than one is simply a finite size artefact, and the system is in reality in an intermediate metallic regime with very small quasiparticle residue around the points $k_{\parallel} = \pm\pi/2$ is an interesting open issue that clearly deserves further investigation.

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Dimensional crossover and deconfinement in Bechgaard salts

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