I. INTRODUCTION AND SCOPE OF THE PAPER

The nature of the metallic phase of interacting electron systems depends strongly on dimensionality. The interplay between interactions and dimensionality is an important issue for a large number of materials, ranging from cuprate superconductors to low-dimensional organic conductors. For quasi-one dimensional conductors (such as the Bechgaard salts, which will be the main subject of this paper), these issues become crucial. Indeed in three dimensions, Fermi liquid (FL) theory applies, whereas in one dimension a different kind of low-energy fixed point known as a Luttinger liquid (LL) is found, with physical properties quite different from that of a FL. By varying the anisotropy of the system, or the energy scale at which it is probed, one can thus expect drastic changes in the physical properties.

This is even more true when the filling of the system is commensurate. In that case, interactions can lead to an insulating behavior via the Mott transition. This phenomenon occurs in all dimensions but the one-dimensional case is particularly favorable. In quasi one-dimensional (Q1D) systems, interchain hopping can induce a (deconfinement) transition from the Mott insulating (MI) state to a metallic state, and crossovers between different metallic behaviors. Understanding how such a deconfinement transition can take place and what are the properties of the metallic phases is a particularly challenging problem, for reasons explained below.

This paper is organized as follows:

• In Sec. I, some physical properties of the TMTSF and TMTTF organic compounds will be briefly reviewed, with an emphasis on those related to the above issues. As described there, these compounds are three dimensional stacks of quarter-filled chains, which makes them wonderful laboratories, in which all the questions above can be addressed. Along the way, we shall point out some open questions and puzzles associated with the physics of these materials.

• In Sec. II, we turn to theoretical models, and explain why non-perturbative methods are required to deal with interchain hopping. We shall review an extension of the dynamical mean-field approach designed to deal with this problem (chain-DMFT), and describe its recent application to coupled Hubbard chains and its bearing on the above issues.

II. QUASI ONE-DIMENSIONAL ORGANIC CONDUCTORS: SOME PHYSICAL PROPERTIES

The Bechgaard salts TMTSF$_2$X were the first organic compounds to exhibit superconductivity, and have thus been the focus of intense experimental and theoretical studies. In addition to the superconducting phase, these materials have a remarkably rich phase diagram (cf. Fig. 1) and exhibit a host of remarkable properties (e.g non-FL metallic behaviour, quantized Hall conductance, Fröhlich conductivity), many of which are still poorly understood.

![Phase Diagram](https://example.com/phase_diagram.png)

**Fig. 1.** Unified experimental phase diagram for the TM compounds (from [4]). Either pressure or chemical changes (increasing pressure corresponds to going from the TMTTF to the TMTSF family and changing the anions) yields the same phases [MI: Mott insulator, LL: Luttinger liquid metal, FL: Fermi liquid metal, SP: spin-Peierls, AF: antiferromagnetic spin-density wave, SC: superconducting]. The TMTTF family is insulating at ambient pressure whereas the TMTSF family shows good metallic behavior at room temperature.

Reviewing all these properties goes far beyond the scope of this lecture: we shall restrict ourselves to a discussion of the crossovers observed in the high-temperature regime, above the ordered phases. For more
extensive reviews of the physical properties of quasi one-dimensional organics, see e.g.18,6.

A. Structure

The basic building block of the Bechgaard salts (Fig. 2) is the flat molecule TMTSF (tetramethyltetraselenafualene), which contains four selenium atoms, surrounded by four methyl groups in a fulvalene type double ring structure.

FIG. 2. Structure of the Bechgaard salts (TMTSF)\(_2\)X (after6). Electronic transport takes place preferentially along the stacks of TMTSF molecules (vertical, \(a\)-axis). The horizontal axis (\(c\)-axis) for which the stacks are separated by the counter-ions is the least conducting one.

Also shown in Fig. 2 are the orbitals giving rise to the double bonds between the carbon atoms and the \(\pi\) orbitals of the selenium atoms. In the TMTTF compounds (Fabre salts), the selenium atoms are replaced by sulphur ones.

All these compounds crystallize in stacks of TM (short for TMTSF or TMTTF) molecules separated by the counter-ions X (for example PF\(_6\) or ClO\(_4\)). The counter-ions are here to provide the charge neutrality, as in a standard salt. The transfer of charge between the ion and the TM stacks is total. Since there is one ion for two TM molecules, the chains are quarter filled. In addition the chains are slightly dimerized. This raises the important question whether these systems should be considered as half-filled, rather than quarter-filled, to which we shall come back in section II B. It is important to note that the commensurate filling is fixed by the chemistry of the compound, and so far it has not been possible to move away from such a commensurate filling. No doubt that if this could be done (through e.g. a field effect transistor geometry21), this would prove very interesting.

The overlap of the \(\pi\)- orbitals of the selenium or sulphur atoms leads to a high mobility of electrons along the stacking direction; the hopping integrals in the perpendicular directions are indeed smaller by more than one order of magnitude. Estimated values of the hopping integrals along the stack direction (\(a\)-axis) and the two perpendicular axes pointing towards neighboring stacks (\(b\)-axis) and towards the anions (\(c\)-axis) respectively are: \(t_a : t_b : t_c = 1000K : 100K : 30K\). 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. At very low temperatures the system has various ordered phases (spin-Peierls (SP), antiferromagnetic (AF), spin-density wave(SDW)) and superconducting (SC)). The nature of the molecule (TMTTF vs TMTSF) or of the ions slightly changes the interchain hopping and the dimerization. Such changes can also be induced by applying pressure to the system. This modifies the relative importance of the kinetic energy and Coulomb interaction and leads to a very rich phase diagram. The chemical and pressure changes have similar effects, which can be summarised by the unified phase diagram of Fig. 4.

B. Mott insulators and Luttinger liquids

At ambient pressure, the (TMTTF)\(_2\)PF\(_6\) compound displays insulating behavior (MI). Upon increasing pressure, a transition to a metallic phase is found, and the properties of the TMTTF compounds evolve toward those of the compounds of the TMTSF family, which are good conductors. This evolution is clear from the \(a\)-axis resistivity measurements in Fig. 3.

FIG. 3. Resistivity along \(a\)-axis for a series of compounds showing the gradual evolution to metallic behavior as pressure is increased (from21).
The minimum of the resistivity (followed by an activated law as temperature is lowered) defines the onset of the MI regime in Fig. 1. Such an insulating behavior in a quarter (or half filled) system suggests that it is due to the interactions and that the TMTTF family is a Mott-Hubbard insulator. It is thus clear that the interactions play a crucial role in the TMTTF family even at relatively high energies. For the TMTSF the question is more subtle in view of the metallic behavior at ambient pressure and it was even suggested that such compounds could be described by a FL behavior with weak interactions. 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.

A blatant proof of the importance of interactions for both the TF and SF compounds is provided by the optical conductivity, as shown in Fig. 4.

The optical conductivity clearly shows that the high energy structure is the one of a Mott insulator, with a decreasing gap (of the order of 2000 cm\(^{-1}\)) to 200 cm\(^{-1}\) for TMTTF\(_2\)(PF\(_6\)) to 200 cm\(^{-1}\) for TMTSF\(_2\)(PF\(_6\)). Nearly all (99\%) of the spectral weight is in this high energy structure. In the metallic compounds there is in addition a very narrow Drude peak. The optical conductivity shows thus clearly that these compounds are very far from simple Fermi liquids. In addition one can compare the optical data with the theoretical predictions for a LL. The data above the gap fits very well the power law LL behavior and thus shows quite convincingly that these compounds are indeed well described by a LL theory down to a scale of a few hundred Kelvin (temperature or frequency). This is also consistent with the optical data along the c-axis, depicted in Fig. 5. These measurements directly probe the density of excited states in the \(a \sim b\) plane. We note however that, although clearly revealing that electrons are confined in the chains above \(\approx 100\) K, the measurements of dc transport along the c-axis do not yet fully understood theoretically from a LL picture (see [11] for a discussion). The a-axis optical measurements described above even allow for a quantitative determination of the LL parameter \(K_\rho\), yielding \(K_\rho \approx 0.23\), indicating very strong electron interactions. This estimate of the LL parameter agrees reasonably well with measurements of the longitudinal resistivity in the range 100 – 300 K. Photoemission data are also consistent with this value.

In addition to providing strong evidence for the Luttinger liquid behavior, the optical data and its comparison to the theoretical predictions force one to reinvestigate the standard interpretation for the difference between TMTTF and TMTSF compounds. Indeed the commonly accepted point of view since the pioneering work of Ref. 9 was that the insulating behaviour of the TMTTF family is due to the stronger dimerization of these compounds, which effectively changes the band filling. As mentioned above, on average two TMTSF or TMTTF molecules donate one electron to the (monovalent) anion, so that the conduction band is nominally a quarter filled hole band. However, the dimerization between neighboring molecules opens a dimerization gap in the middle of the band. When this dimerization is large, the system might best be thought of as half-filled (TMTTF) rather than quarter-filled (TMTSF). From this point of view the Mott insulating behavior comes from the half filled nature of the system.

However the optical data are inconsistent with a half filled description in the SF family. A more satisfactory explanation is thus to consider both series of compounds as quarter-filled, and the Mott insulator to be due to the quarter filled commensurability. Increasing pressure or changing the chemistry reduces the relative strength of Coulomb interactions with respect to hopping, hence suppressing Mott localization. For this interpretation to be tenable, these compounds must be very close to the Mott transition point, which is indeed supported by the measured values of the LL parameter (indeed, \(K_\rho^c = 0.25\) is the critical value for the opening of a Mott gap in a quarter-filled chain).

\(^1\)We use the conventions of Ref. 9. see also section II below. \(K_\rho = 1\) corresponds to non-interacting electrons.
C. Dimensional crossover and deconfinement

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 (because $K_\rho$ is so small), 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. 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.

A dimensional crossover is indeed observed in the transport along the $c$ axis shown in Fig. 5.

![FIG. 5. Transport along the least conducting axis. This is in effect a tunnelling experiment between the $ab$ planes and thus a measure of the density of states in such planes. In the 1d regime there are no single particle excitations and the resistivity increases with decreasing temperature, whereas when the chains couple coherently one recovers a more conventional (metallic) behavior. The maximum in resistivity thus measures the scale for the dimensional crossover (from 20).](image)

From this experiment, we see that the dimensional crossover takes place around 100K in (TMTSF)$_2$PF$_6$. This is in agreement with the change of behavior from $T$ (LL behavior) to $T^2$ observed in dc transport along the $a$ axis, and with the change of behavior in the transverse optical conductivity (see Fig. 6).

The interpretation that the change of behavior between the insulating and metallic regimes is indeed due to such deconfinement transition can be strengthened by the optical data (see Fig. 7). The change of behavior from insulating to metallic occurs when the two quantities are of the same order of magnitude showing that the difference between the various members of the TM families is indeed linked to a deconfinement transition (from 27).

![FIG. 6. Optical conductivity along the three axis, at various temperatures. Depending on the temperature a different behavior is observed along the $b$ direction which signals a dimensional crossover from essentially uncoupled chains to coherent planes. (from 16)](image)

![FIG. 7. A comparison of the measured gap in the optical conductivity with the interchain hopping. The change of behavior from insulating to metallic occurs when the two quantities are of the same order of magnitude showing that the difference between the various members of the TM families is indeed linked to a deconfinement transition (from 27).](image)
D. Summary of some open issues and questions

To summarize the experimental situation, here are some key questions raised by the physical properties of the TM family:

1. Are TMTSF strongly correlated systems? What is the strength of interactions?
2. What causes the difference between the various members of the organic families (TMTSF and TMTTF)?
3. Is the high temperature metallic regime a Luttinger liquid?
4. At what energy scale does the dimensional crossover take place?
5. What is the nature of the metallic state of the TMTSF series in the temperature range from 10 to 100 K?
6. What are the physical properties of the low-T (Fermi-liquid?) metallic regime?

As we have seen, one is now in a position to have satisfactory answers to questions 1-4. In doing so one had to reexamine most of the commonly accepted point of views. The optical data shows that the dimerization plays little role and that the Mott insulating behavior is due to the *quarter filled* nature of the compounds. The estimate of the crossover scale of ∼100 K questions early interpretations of measurements of the NMR relaxation time on (TMTSF)$_2$ClO$_4$. These showed the Korringa law typical of FL behavior $1/(T_1 T) = \text{const}$ at very low temperatures. However, strong deviations from the Korringa law are observed already around ∼10 K, which is considerably smaller than the onset of FL behavior estimated from optics and transport. This makes question 5) particularly puzzling, since the NMR is anomalous in a temperature range for which one now knows that the compounds are not in a one-dimensional regime.

III. MODELING QUASI-ONE-DIMENSIONAL SYSTEMS

A. Non-perturbative effects of inter-chain hopping

We now turn to simplified models in which one-dimensional chains of interacting electrons are coupled by an inter-chain hopping $t_{\perp}$. Later on we shall concentrate on the simplest case of the Hubbard model, but at this stage we would like to make some remarks with a broader degree of validity.

Let us consider first the case of a commensurate filling. For a single chain, strong enough interactions will then open a Mott gap, leading to an insulating state in which the electrons are confined on the chains. Technically, this is due to umklapp scattering processes being relevant. This will actually happen for arbitrarily small repulsive interactions in the half-filled Hubbard model, while at quarter-filling a strong enough nearest-neighbour interaction is needed, in addition to a local Hubbard term. (This is one of the reasons why a simple Hubbard model is insufficient to describe the organic compounds, another one being the small values of $K_{\rho}$ needed to fit the data). The interchain hopping will tend to delocalise the electrons, resulting in an insulator to metal transition at zero-temperature for a critical value of the interchain hopping. The generic situation is depicted on the schematic phase diagram of Fig. 8.

In addition to the $T = 0$ insulator to metal (“deconfinement”) transition, finite-temperature crossovers have been depicted on this diagram. For temperatures smaller than the one-dimensional bandwidth (i.e. the high-energy cutoff of the problem), but higher than the crossover scales depicted in the figure, the system is essentially insensitive to the interchain hopping. In this regime, the system is expected to behave as a Luttinger liquid (LL), which is the generic state for interacting one-dimensional electrons. However, one should bear in mind that, at least for small $t_{\perp}$, the Luttinger liquid parameter $K_{\rho}$ will be gradually renormalized downwards by the (relevant) umklapp scattering as temperature is reduced. The temperature scale at which the effective $K_{\rho}$ approaches zero signals the low-T Mott insulating regime: this is the first crossover line depicted in the figure. To the
hopping is a relevant perturbation and line starts at a metallic LL regime. Only the LL to FL crossover survives, and the decoupled chain is always in the FL. The crossover separates a high-T Luttinger liquid regime into a low-T Fermi liquid regime (FL). The crossover will occur when this effective inter-chain hopping grows as the energy scale is reduced: the crossover will occur when this

\[ E^* \sim t_\perp (t_\perp/t)^{\alpha/(1-\alpha)} \]  

(3.1)

where \( \alpha = \frac{1}{4}(K_\rho + 1/K_\rho) - \frac{1}{4} \) is the exponent associated with the one-electron Green’s function in the LL state. The important physical content of this expression is that interactions can significantly reduce the crossover scale \( E^* \) as compared to the non-interacting estimate \( t_\perp \). We note that (see Sec. II) for the TMTSF Bechgaard salts, \( \alpha \) appears to be close to 1/2. Since \( t_\perp \approx 300K \) and \( t_\perp/t_0 \approx 10 \), this would place \( E^* \) in the 10-30 K range according to the above RG estimate. Experimentally however, interchain coherence appears to set in at a significantly higher temperature, in the 100 K range: this is one of the puzzles in the field.

While this perturbative RG analysis allows to estimate a scale for the dimensional crossover, it breaks down for \( T < E^* \) since the effective \( t_\perp \) flows to large values. In particular, it does not provide informations 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. The competition between these two relevant perturbations will determine the crossovers described above.

Non-perturbative studies are thus needed to investigate both the deconfinement transition and the dimensional crossover. Several authors have developed such methods in the case of a finite number of coupled chains. Below, we present a recently developed approach designed to handle an infinite array of coupled chains in a non-perturbative manner.

**B. The chain- Dynamical Mean Field Theory approach**

This non-perturbative method is inspired by the success of dynamical mean field theory (DMFT) in the description of lattice models of correlated fermions. Ordinary DMFT maps a lattice model of interacting fermions onto a single site model in an effective time-dependent mean field, which has to be determined self-consistently. Thus the problem becomes equivalent to an Anderson impurity model in a self-consistent bath. It can be shown that in the limit of an infinite coordination number of
the lattice, all quantum fluctuations become local and the dynamical mean field description is exact.

Very anisotropic systems of coupled one-dimensional chains lend themselves to a very natural extension of this approach (dubbed “chain-DMFT”), in which the array of chains is replaced by an effective chain in a self-consistent bath. It is crucial to retain a one-dimensional geometry of the effective problem, if the limit of decoupled chains (and hence 1D physics) is to be treated properly. The self-consistent bath describes the influence of all neighboring chains on the "impurity chain", thus freezing all quantum fluctuations that are non-local in the transverse direction, but retaining spatial and dynamical fluctuations along the chains. By the same arguments as in ordinary DMFT, the chain-DMFT approach becomes exact in the limit of an infinite transverse coordination number of the array. In the limit of decoupled chains chain-DMFT reduces to the single chain problem, which is solved numerically exactly.

Consider a system of coupled chains described by the Hamiltonian

$$H = \sum_m H^{(m)}_{1D} - \sum_{\langle m, m' \rangle} t^{m'm'}_{\perp} \sum_{i\sigma} (c^+_i n_{\sigma} c_{i m'\sigma} + h.c) \tag{3.2}$$

where $H^{(m)}_{1D}$ is the Hamiltonian for a single isolated chain and the sum in the second term runs over neighboring chains $m, m'$, which are coupled by the transverse hopping $t^{m'm'}_{\perp}$. Chain-DMFT maps this system onto a single-chain system described by the effective action

$$S_{\text{eff}} = -\int \int_{0}^{\beta} d\tau d\tau' \sum_{i, j, \sigma} c^+_i n_{\sigma} \mathbb{G}^{-1}_0(i-j, \tau-\tau') c_{j\sigma}(\tau') + \int \int_{0}^{\beta} d\tau H^{\text{int}}_{1D}\{c_{i\sigma}, c^+_i n_{\sigma}\} \tag{3.3}$$

where $H^{\text{int}}_{1D}$ is the interacting part of the on-chain Hamiltonian. $\mathbb{G}_0$ is the effective propagator describing hopping processes, that destroy a fermion on site $j$ at time $\tau'$ and create one at site $i$ at time $\tau$. In analogy to usual DMFT $\mathbb{G}_0$ has to be determined from a self-consistency condition that imposes that the Green’s function $G(i-j, \tau-\tau') \equiv -\langle c(i, \tau) c^+(j, \tau') \rangle_{\text{eff}}$ calculated from $S_{\text{eff}}$ coincides with the on-chain Green’s function of the original problem. Since the self-energy is $\Sigma = \mathbb{G}^{-1}_0 - G^{-1}$, this condition reads:

$$G(k, i\omega_n) = \int d\epsilon_\perp i\omega_n + \mu - \epsilon_k - \Sigma(k, i\omega_n) - \epsilon_\perp \tag{3.4}$$

where $\epsilon_\perp(k) = \mu - \epsilon_k - \Sigma(k, i\omega_n)$ denotes the Fourier transform of the inter-chain hopping $t^{m'm'}_{\perp}$, $D(\epsilon_\perp) = \sum_{k, \perp} \delta[\epsilon_\perp - \epsilon_\perp(k)]$ the corresponding density of states, $k$ the momentum in chain direction and $\omega_n$ the Matsubara frequencies. The chain-DMFT equations (3.3,3.4) fully determine the self-energy and Green’s function of the coupled chains. In particular, once $\Sigma$ has been calculated, the full Green’s function for the coupled chains is obtained from:

$$G(k, i\omega_n)^{-1} - (i\omega_n + \mu - \epsilon_k - \Sigma(k, i\omega_n) - \epsilon_\perp) \tag{3.5}$$

We note that a key approximation of this approach is that the self-energy is considered to be independent of the transverse component of the momentum. In the following we specialize the discussion to a model of Hubbard chains coupled by a perpendicular hopping $t_{\perp}$. Then the Hamiltonian is of the form $\Sigma(k, i\omega_n) = t_{\perp}$ and $H^{(m)}_{1D}$ being the Hamiltonian of the one-dimensional Hubbard model.

Different choices of the lattice are possible. Choosing a semi-circular density of states

$$D(\epsilon) = \frac{1}{2\pi^2} \sqrt{\epsilon^2 - 4t^2} \tag{3.6}$$

in Eq. (3.4) corresponds to a Bethe lattice with infinite coordination number, in which each lattice site is replaced by a one-dimensional chain and hopping between the chains follows the topology of the Bethe lattice. This choice is particularly appealing, since the chain-DMFT formalism is exact in this case.

Another possibility is to consider a two dimensional array of chains with the square lattice geometry. In this case, each chain has exactly two nearest neighbors and chain-DMFT must be viewed as an approximation. The transverse dispersion becomes:

$$\epsilon_\perp(k) = -2t_{\perp} \cos k_{\perp} \tag{3.7}$$

and the corresponding density of states is the one of a one-dimensional lattice:

$$D(\epsilon) = \frac{1}{\pi \sqrt{\epsilon^2 - 4t^2}}. \tag{3.8}$$

As for the Bethe lattice, the self-consistency condition simplifies in the 2D geometry in such a way that the Weiss field can directly be written in terms of the Green’s function:

$$\mathbb{G}^{-1}_0(k, i\omega_n) = i\omega_n + \mu + G^{-1}(k, i\omega_n) - \sqrt{G^{-2}(k, i\omega_n) + 4t^2_{\perp}} \tag{3.9}$$

This model does not provide a controlled limit, in which chain-DMFT becomes exact. Still, from a conceptual point of view, a two-dimensional picture seems more appealing if one aims at a comparison with the experimental situation in the Bechgaard salts. Therefore the calculations presented below were performed for this choice of the model. We stress, however that in practice, the specific choice of the transverse dispersion does not have a significant qualitative influence (as long as one does not address long-range ordering).

A practical implementation of the chain-DMFT approach requires to solve the effective one-dimensional interacting problem described above. This is a rather formidable task, and numerical methods are required. Even though other techniques are conceivable, we have
chosen to use a Quantum Monte Carlo algorithm, which is a straightforward generalization of the Hirsch-Fye algorithm used in single-site DMFT. It relies on a Trotter discretization of the effective action in imaginary time, and on a discrete Hirsch transformation of the interaction term:

\[ e^{-\Delta \tau U_{n_i n_{i'}}} = \frac{1}{2} \sum_{s=\pm 1} e^{\lambda_s (n_i - n_{i'}) - \Delta \tau U_s (n_i + n_{i'})} \]  

with \( \lambda = \arccosh \left( e^{\Delta \tau U_s \rho} \right) \). An Ising field \( s \) is introduced at each time slice and each site of the chain. Monte Carlo sampling of the Ising fields then allows for the direct calculation of the on-chain Green’s function and on-chain correlation functions. In practice, chains of 16 to 32 sites with periodic boundary conditions are sufficient to access the 1d Luttinger Liquid regime.

In the following we will present numerical evidence for the deconfinement transition at half filling and the dimensional crossover as a function of temperature in the doped case.

C. Luttinger-liquid to Fermi-liquid crossover

We summarize some of our QMC results for an array of coupled Hubbard chains in the chain-DMFT approach, starting with the doped (incommensurate) case. At high temperature, the model is expected to display LL behaviour. In order to measure numerically the LL behaviour, in imaginary time, and on a discrete Hirsch transformation of the in-

D. Deconfinement transition

We now turn to the half-filled case. In Fig. 10 we display the effective \( K_\rho \) (determined as above) as a function of interchain hopping, for \( U/W = 0.92 \) and at a rather low temperature \( T/W = 0.025 \).

\[ \chi_s(\tau) = \chi_s(\beta/2) \left( \frac{1}{\sin \pi \tau/\beta} \right)^{1+K_\rho} \]  

valid for \( \beta, \tau \) and \( \beta - \tau \) larger than the inverse of the high-energy cutoff (i.e. in some range around \( \tau = \beta/2 \)). We emphasize that this is a much better manner of accessing \( K_\rho \) in a QMC simulation than by looking at the single-electron Green’s function, whose asymptotics involves the exponent \( \alpha = (K_\rho + 1/K_\rho)/4 - 1/2 \) which is never very large for the Hubbard model. This makes it very hard numerically to distinguish LL from FL behavior at the level of one-electron Green’s functions.

\[ \chi_s(\tau) = \chi_s(\beta/2) \left( \frac{1}{\sin \pi \tau/\beta} \right)^{1+K_\rho} \]
For small $t_\perp/W$, the value $K_\rho = 0$ indicating a Mott insulating behaviour (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 (Fig. 8) is clearly revealed by our calculations. In principle, it should be possible to identify first a Luttinger Liquid phase and then, with increasing interchain coupling, a Fermi Liquid phase. However, in this parameter range the Luttinger Liquid phase is too narrow to become visible. The location of the deconfinement transition is in reasonable agreement with the naive criterion $\Delta_{\perp} \sim e^{t_\perp/W}$, with $t_\perp^{\text{eff}}$ the renormalised inter-chain hopping.

**E. Interchain optical conductivity**

Inter-chain optical conductivities within chain-DMFT can be obtained from the one-particle Green’s functions. Vertex corrections drop out for analogous reasons as in single-site DMFT, and therefore:

\[
\text{Re} \sigma_\perp(\omega, T) \propto t_\perp^2 \int \frac{dk_\perp}{2\pi} \sin^2 k_\perp \int \frac{dk}{2\pi} \int d\omega A(\epsilon_\perp, k, \omega') \times A(\epsilon_\perp, k, \omega + \omega') f(\omega') - f(\omega' + \omega) \frac{1}{\omega}
\]

where $A(\epsilon_\perp, k, \omega) = -\frac{1}{\pi} \text{Im} G(\epsilon_\perp, k, \omega)$ is the single-particle spectral function of the coupled chains system. Note that we have taken into account the $k_\perp$-dependence of the current vertex in this formula.

**F. The low-temperature Fermi Liquid regime**

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 $K_\rho$ (see Fig. 10) 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. 12 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. 12) is very
close to the one of non-interacting (U = 0) coupled
chains (dotted line in Fig. 12).

![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-). The solid line depicts schematically the FS obtained within the RPA ($\Sigma = \Sigma_{1d}$).](image)

This is in striking contrast with predictions of an RPA
approach, as pointed out in [10]. The RPA consists of re-
placing the self-energy of an interacting coupled system
by the self-energy of a 1d chain. Since the 1d chain is a
Mott insulator at half-filling, $\Sigma$ diverges at low frequency
for $k = \pi/2$ and the above equation has no solution for
this $k$-value. Thus, within the RPA the Fermi surface
cannot cross the points $(\pm \pi/2, \pm \pi/2)$ but consists of dis-
connected pockets as depicted schematically in Fig. 12
(solid lines). The feedback of the effects of the interchain
hopping on the self-energy, which is taken into account by
chain-DMFT, regularizes the behavior of the self-energy
near these points, leading to an open Fermi surface.

The QP residue $Z_{k_\perp}$ calculated within chain-DMFT
depends only very weakly on the Fermi surface point (Ta-
ble I).

| $k_\perp/\pi$ | 0.23 | 0.38 | 0.50 | 0.62 | 0.77 |
|-------------|------|------|------|------|------|
| $Z(k_\perp)$ | 0.79 | 0.77 | 0.76 | 0.77 | 0.79 |

Again, this shows that the regularization by interchain
hopping feedback effects is very efficient: a nearly di-
vergent self-energy as could be imagined to result from
an only slightly regularized 1d self-energy would lead to
very small $Z(k_\perp)$ close to $\pm \pi/2$. Therefore approxima-
tions based on the 1D self-energy are likely to predict
“hot spots” at those FS points corresponding to a vanish-
ing inter-chain kinetic energy. Our results, in agreement
with those of Arrigoni, do not support such a picture.
Rather, the $k_\perp$-dependence of $Z(k_\perp)$ is very weak, with
very shallow minima at $k_\perp \sim \pm \pi/2$. This small variation
is however on the scale of our error bars.

IV. OUTLOOK

In these lecture notes, we have reviewed a few of the
fascinating physical properties of quasi one-dimensional
organic conductors. Our point of view has been that
a unified description of both the TMTTF and TMTSF
compounds is possible, as strongly interacting quarter-
filled chains with weak interchain couplings. In that
picture, the physical changes under pressure (or from
TMTTF to TMTSF) are viewed as a deconfinement tran-
sition from a Mott insulating regime to a metallic regime.
Still, we have emphasized that it is hardly possible to understand these compounds using a purely one-dimensional picture. Inter-chain coherence sets in at
low energy in the metallic compounds, and this leaves us
with a quite difficult theoretical problem, which cannot
be handled by perturbative techniques in the inter-chain
hopping.

We have reviewed the recently developed chain-DMFT
approach which is in our opinion a promising route to
handle these issues. QMC calculations on weakly cou-
pled Hubbard chains have clearly demonstrated that this
method is able to reproduce both the deconfinement tran-
sition and the dimensional crossover from a LL to a FL
as the energy scale is reduced. We have also emphasized
that a purely local Hubbard interaction is not appro-
priate for modelling quasi one-dimensional organics.
Indeed, the phenomenology requires i) the possibility of a
Mott insulating state at quarter filling and ii) rather
small values of $K_\rho$ ($\simeq 0.23$) which cannot be reached in
the Hubbard model. A minimal theoretical model obey-
ing these requirements is that of weakly coupled quarter-
filled chains with both an on-site and a nearest-neighbour
interaction. We hope to be able to deal with this model
in the chain-DMFT framework in the near future.

Many outstanding questions on the physics of organ-
ics remain unanswered at this stage. We have tried to
emphasize some of these puzzles in this paper.
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