Deconfinement Transition and Luttinger to Fermi Liquid Crossover in Quasi-One-Dimensional Systems

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We investigate a system of one-dimensional Hubbard chains of interacting fermions coupled by interchain hopping. Using a generalization of the dynamical mean-field theory we study the deconfinement transition from a Mott insulator to a metal and the crossover between Luttinger and Fermi liquid phases. One-particle properties, local spin response, and interchain optical conductivity are calculated. Possible applications to organic conductors are discussed.

The nature of the metallic phase of interacting electron systems depends strongly on dimensionality. 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. For commensurate electron fillings, strong enough repulsive interactions destroy the metallic state altogether by opening a Mott gap. This phenomenon exists in all dimensions but the one-dimensional case is particularly favorable [1]. 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 (Fig. 1). These phenomena play a key role in organic compounds such as the Bechgaard salts, which are three-dimensional stacks of quarter-filled chains [2]. Some of their low-temperature properties are well described by FL theory, whereas optical [3] and transport measurements [4] have shown that the high-temperature phase is either a LL or a MI.

Describing Q1D systems is not an easy task. The transverse hopping $t_\perp$ is a relevant perturbation on the LL [5–7]. Hence, perturbative renormalization group calculations yield an estimate of the crossover scale [5,8] but fail below that scale. In the MI state, electrons are confined on the chains by the Mott gap. A finite critical value of $t_\perp$ is needed to induce an insulator-to-metal transition. In the Bechgaard salts, the change in conductivity when increasing pressure or going from the tetramethyltetrathiafulvalene to the tetramethyltetraselenafulvalene family may be [9,10] associated with such a transition. Thus the effects of the interchain hopping that are the most important physically *cannot be handled reliably by perturbative methods*. Although some nonperturbative studies of deconfinement have been made for a finite number of chains [11] the case of an infinite system is still open. Some of the key questions yet to be answered are: (i) What is the crossover scale from the LL to MI, or from the LL to FL (Fig. 1), and is there only one crossover scale for the different physical properties (transport, spin response, single-particle proper-

ties, etc.)? (ii) What is the nature of the low-temperature FL state, and is the shape of the Fermi surface (FS) affected by interactions? Do quasiparticle (QP) properties, such as the QP residue $Z(k)$, vary significantly as the wave vector k moves along the FS?

In order to deal with these questions, a new method has been proposed [12,13], which generalizes the single site dynamical mean-field theory (DMFT) [14] and replaces the Q1D system by a single *effective chain* from which electrons can hop to a self-consistent bath. We thus nickname it *chain-DMFT* (ch-DMFT). It is exact in the limit of decoupled chains, while it reduces to usual DMFT in the opposite limit of zero hopping along the chains. In this Letter, the first quantitative solution of the ch-DMFT equations is presented. We show that the above issues can be addressed, and some of the above questions answered. In view of the difficulty of the problem only the Hubbard model is considered here, but more realistic extensions are in sight, as discussed below.
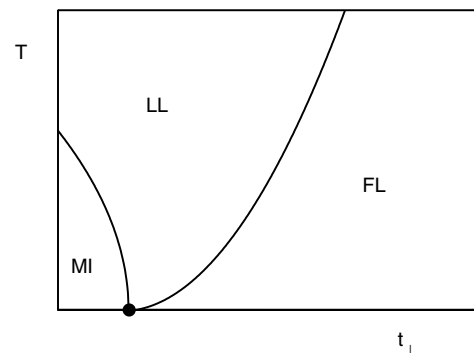

FIG. 1. Schematic phase diagram of a Q1D system, as a function of temperature T and interchain hopping $t_\perp$. The Mott insulator (MI), Luttinger liquid (LL), and Fermi liquid (FL) regimes are displayed. All lines are crossovers, except for the $T = 0$ transition from a MI to a FL. The MI phase is present only for commensurate fillings. Possible phases with long-range order have been omitted.

Let us consider a system of coupled chains described by a sum of Hamiltonians of the isolated chains plus a hopping term between neighboring chains. The ch-DMFT approximates this system by the effective action:

$$S_{\text{eff}} = -\iint_0^\beta d\tau \, d\tau'$$
$$\times \sum_{ij,\sigma} c_{i\sigma}^+(\tau) \mathcal{G}_0^{-1}(i-j, \tau-\tau') c_{j\sigma}(\tau')$$
$$+ \int_0^\beta d\tau \, H_{1D}^{\text{int}}[\{c_{i\sigma}, c_{i\sigma}^+\}], \qquad (1)$$

where H_{1D}^{int} is the interacting part of the on-chain Hamiltonian. $\mathcal{G}_0$ is an *effective propagator* determined from a self-consistency condition: the Green's function $G(i - j, \tau - \tau') \equiv -\langle c(i,\tau) c^+(j,\tau') \rangle_{\text{eff}}$ calculated from S_{eff} should coincide with the on-chain Green's function of the original problem, with the same self-energy $\Sigma = \mathcal{G}_0^{-1} - G^{-1}$. This reads

$$G(k, i\omega_n) = \int d\epsilon_\perp \frac{D(\epsilon_\perp)}{i\omega_n + \mu - \epsilon_k - \Sigma(k, i\omega_n) - \epsilon_\perp}, \qquad (2)$$

where $\epsilon_\perp(k_\perp)$ denotes the Fourier transform of the interchain hopping $t_\perp^{mm'}$, $D(\epsilon_\perp) = \sum_{k_\perp} \delta[\epsilon_\perp - \epsilon_\perp(k_\perp)]$ denotes the corresponding density of states, k denotes the momentum in chain direction, and ω_n denotes the Matsubara frequencies. The ch-DMFT equations (1),(2) fully determine the self-energy and Green's function of the coupled chains $G(k, k_\perp, i\omega_n)^{-1} = i\omega_n + \mu - \epsilon_k - \epsilon_\perp(k_\perp) - \Sigma(k, i\omega_n)$. The ch-DMFT approach can be rigorously justified in the formal limit where the lattice connectivity in the transverse direction is taken to infinity. In systems with finite transverse connectivity it can be viewed as an approximation neglecting the dependence of the self-energy on transverse momentum, keeping both frequency and in-chain momentum dependence: $\Sigma = \Sigma(k, i\omega_n)$. In our numerical calculations we adopt this latter point of view and consider a two-dimensional array of chains forming a square lattice with nearest neighbor hopping, so that $\epsilon_\perp(k_\perp) = -2t_\perp \cos k_\perp$. We specialize to the Hubbard model, i.e., for each chain,

$$H_{1D} = -t \sum_{i\sigma} [c_{i\sigma}^+ c_{i+1\sigma} + \text{H.c.}] + U \sum_i n_{i\uparrow} n_{i\downarrow}. \qquad (3)$$

We solve the effective chain problem for chains of 16 or 32 sites with periodic boundary conditions using the quantum Monte Carlo Hirsch-Fye algorithm [15]. Using 32 time slices in imaginary time allows us to reliably access temperatures down to $T/W \simeq 0.02$ with $U/W \simeq 1$, where $W = 4t$ is the bandwidth of the one-dimensional chain. Typically, about 5000 QMC sweeps and 10 to 15 ch-DMFT iterations are sufficient to reach convergence. The main quantities that we calculate and analyze are (a) on-chain (i.e., summed over $k_\perp$) single particle Green's functions: $G(k, i\omega_n)$, and self-energies $\Sigma(k, i\omega_n)$ (ob-

tained from $\mathcal{G}_0^{-1} - G^{-1}$ [16]). This allows us to identify the location of the FS $k_\perp^F(k)$ by solving $\epsilon_\perp(k_\perp^F) = \mu - \text{Re}\Sigma(k, i\omega_{n=1}) - \epsilon_k$ and the QP residue $Z = Z(k_\perp^F)$ by fitting the slope $(= 1 - Z^{-1})$ of Σ vs $i\omega_n$ at a specific FS point. (b) On-chain spin and charge response functions, in particular, the local spin response function: $\chi_s(\tau) = \langle S^z(j,0) S^z(j,\tau) \rangle = \sum_{k,k_\perp} \chi_s(k, k_\perp, \tau)$. Indeed, in a LL (or with $K_\rho = 1$ in a FL) we have $\chi_s(\tau) = \chi_s(\beta/2) \times (\sin \pi \tau/\beta)^{-(1+K_\rho)}$ in the asymptotic regime where β, τ are larger than some coherence scale. By fitting our results to this form, we can define an effective K_ρ. Furthermore, the temperature dependence of $\chi_s(\beta/2)$ is related to the NMR relaxation rate $1/T_1 \equiv \lim_{\omega \to 0} \chi_s''(\omega)/\omega$. In a FL liquid at low-enough temperature [17], $1/T_1 = \beta \chi_s(\beta/2)/2\pi^2$. In a LL $1/T_1$ and $\beta \chi_s(\beta/2)$ have the same T dependence (albeit with a proportionality factor depending on K_ρ). (c) Interchain optical conductivity. Within ch-DMFT vertex corrections drop out [13] and the conductivity is given by

$$\sigma_\perp(i\omega) \propto \frac{t_\perp^2}{\omega} \int \frac{dk_\perp}{2\pi} \sin^2 k_\perp \int \frac{dk}{2\pi} \frac{1}{\beta} \sum_m G(k, k_\perp, i\omega_m)$$
$$\times G(k, k_\perp, i\omega_m + i\omega). \qquad (4)$$

Note that we have taken into account the $k_\perp$ dependence of the current vertex in (4). In practice, we perform analytically the $k_\perp$ integration in (4) and numerically the k integration and Matsubara summation. We then use the maximum entropy algorithm [18] to continue $\sigma_\perp(i\omega)$ to the real axis and obtain the interchain optical conductivity $\text{Re}\sigma_\perp(\omega, T)$.

We first discuss our results away from half filling, for $U/W = 1$ and $\mu = 0.2$ (corresponding to a total density $n \simeq 0.8$). The numerical method was tested for decoupled chains ($t_\perp = 0$), for which our fitting procedure of χ_s yields $K_\rho \simeq 0.7$, in agreement with the exact result [19]. We then study how interchain coherence develops as temperature is lowered for coupled chains with $t_\perp/W = 0.14$. Figure 2 displays the effective K_ρ as a function of temperature: a crossover from a LL (with $K_\rho \simeq 0.7$) to a
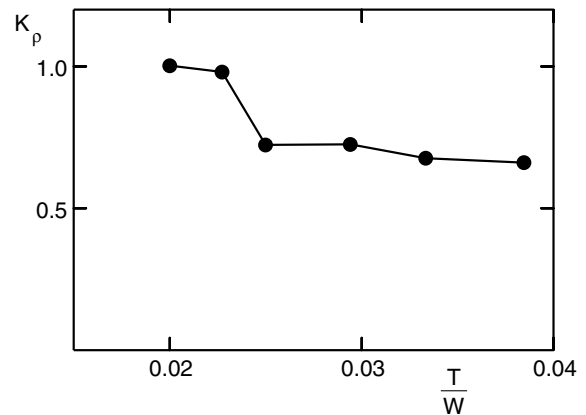

FIG. 2. Effective K_ρ vs temperature in the doped case (filling $n \simeq 0.8$) for $U/W = 1.0$, $t_\perp/W = 0.14$.

TABLE I. QP weights $Z(k_\perp)$ for different points on the FS (doped case: $n \simeq 0.8$, $U/W = 1.0$, $t_\perp/W = 0.14$).

$k_\perp/\pi$	0.19	0.36	0.50	0.62	0.74	0.91
$Z(k_\perp)$	0.62	0.65	0.69	0.72	0.75	0.78

FL ($K_\rho = 1$) is seen as temperature is lowered below $T^*/W \simeq 1/44$. According to [5,8], the crossover scale is given by $T^* = \frac{t_\perp}{\pi} C (t_\perp/t)^{\theta/(1-\theta)}$, with $\theta = (K_\rho + 1/K_\rho)/4 - 1/2$ ($\simeq 0.03$ here). The interactions reduce its value compared to the naive one $t_\perp/\pi$. We cannot test this renormalization effect because of the small values of θ in the Hubbard model. Our results are consistent with $T^* \simeq C t_\perp/\pi$ with $C \simeq 0.5$. In the low temperature FL regime, we find that the location of the FS is essentially unaffected by interactions. The QP residue Z is not uniform along the FS. Its dependence on $k_\perp^F$ is displayed in Table I. Z is larger for $k_\perp$ close to π, while it is somewhat smaller for small $k_\perp$. This is not a big effect however, and it would be inappropriate to speak of "hot spots" [20] (even though it may suggest that such a phenomenon appears for larger U). Note that, in agreement with Arrigoni [12], we find that Z is more uniform along the FS than suggested by the single-chain approximation $\Sigma = \Sigma_{1D}$ used by many authors. We now turn to the commensurate (half-filled) case and present results for $U = 0.65W$. By fitting the self-energy to an analytical form, we first checked that our numerical results are consistent with a MI state with a gap $\Delta_{1D}/W = 0.1$, in agreement with exact results. Turning on $t_\perp$, we estimate the $t_\perp$ dependence of the gap by performing simulations at one of the lowest accessible temperatures $T/W = 1/40$. The gap vanishes for $t_\perp/W \simeq 0.07$. Hence our method captures the insulator-to-metal transition induced by transverse hopping. The effective K_ρ, shown in Table II, is also a clear indicator of the MI ($K_\rho = 0$) to FL ($K_\rho = 1$) transition, in agreement with the qualitative expectations of Fig. 1. At this low temperature, the intermediate LL regime is too narrow to be visible. The location of the transition is in reasonable agreement with the naive criterion $\Delta_{1D} \sim t_\perp^*$ [9–11]. Figure 3 displays the interchain optical conductivity for several values of $t_\perp$. In the MI phase, $\sigma_\perp(\omega)$ shows a gap, followed by an onset of absorption starting at approximately the gap and extending up to a scale of order U, where a broad second peak is apparent. A low-frequency Drude peak develops as the insulator-to-metal transition is crossed. Close to the transition, the weight in the Drude peak is small, while the Hubbard band feature is still visible and carries a significant part of the spectral weight. The results for the NMR relaxation rate $1/T_1$ are

TABLE II. Effective K_ρ at half filling, as a function of $t_\perp/W$ for $U/W = 0.65$ and $T/W = 1/40$.

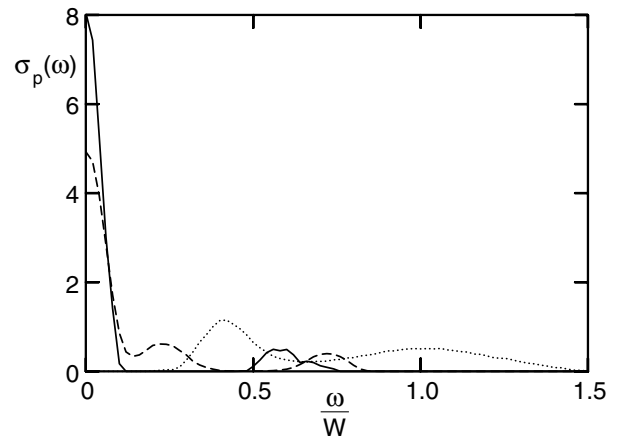| $t_\perp/W$	0.00	0.04	0.07	0.11	0.14	0.16	0.18
K_ρ	0.00	0.02	1.01	1.09	1.07	1.06	1.04

FIG. 3. Interchain optical conductivity at half filling for $U = 0.65W$, $\beta = 40/W$, and $t_\perp = 0.14$ and 0.07 (solid and dashed lines) and for $U = 1.0W$, $\beta = 40/W$, and $t_\perp = 0$ (dotted line).

displayed in Fig. 4 for a value of $t_\perp/W = 0.11$. At low temperatures the Korringa law $1/(T_1 T) = $ const is recovered, while at higher temperatures $1/T_1 T$ is temperature dependent. The observed T dependence is consistent with $1/(T_1 T) \simeq T^{K_\rho - 1}$ [5] with a T-dependent exponent $K_\rho \le 1$, indicative of a LL evolving gradually into a FL (cf. Fig. 1). As for the doped case, the FS is nearly indistinguishable from the noninteracting case (see Fig. 5). The QP residue $Z_{k_\perp}$ depends only very weakly on the Fermi surface point (Table III). The $k_\perp$ dependence of $Z(k_\perp)$ is quite different from the doped case, with very shallow minima at $k_\perp \sim \pm \pi/2$, corresponding to a vanishing interchain kinetic energy. This small variation is however on the scale of our error bars. We contrast our findings with the conclusions drawn from the "single-chain" (RPA) approximation [6,21]: $\Sigma = \Sigma_{1D}$. As recently pointed out [21], RPA predicts that the FS close to the transition should consist of disconnected electron and hole "pockets," as depicted schematically in Fig. 5. This is because the self-energy of a MI diverges at low frequency for $k = \pi/2$, so that no FS point can correspond to this value of k. In contrast, our data find a conventional connected FS
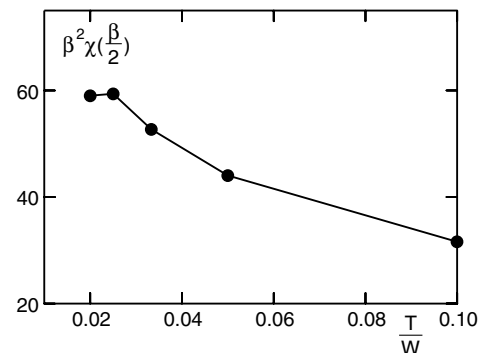

FIG. 4. $1/(T_1 T)$ versus T in the half-filled case with $t_\perp/W = 0.11$, $U/W = 0.65$. The crossover from a FL at low T to a LL for $T/W \gtrsim 0.025$ is clearly apparent.
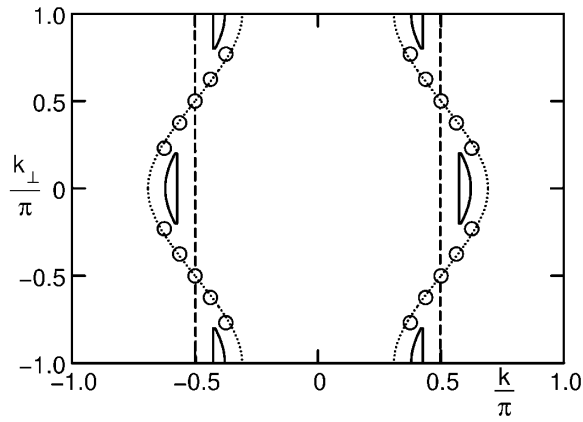
FIG. 5. FS in the half-filled case with $t_\perp/W = 0.14$, $U/W = 0.65$ (circles), compared to the FS of the noninteracting case (dotted line) and of the purely 1D case ($t_\perp = 0$, dashed line). The solid line depicts schematically the FS obtained within the RPA ($\Sigma = \Sigma_{1D}$) [21].

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

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

down to the transition point (up to our numerical accuracy). This shows that it is crucial, as done in ch-DMFT, to take into account the feedback effects of the interchain hopping in the self-energy.

In conclusion, we have shown in this Letter that the ch-DMFT approach is a tool of choice for the study of the crossovers and insulator-to-metal transitions induced by transverse hopping in Q1D systems. Our results are qualitatively reminiscent of experimental observations on organic conductors, such as the deconfinement transition itself, the crossover from a LL at high T to a FL at low T (as revealed, e.g., in NMR), and most significantly the coexistence of a Drude feature with small spectral weight and of a Hubbard-band feature in the optical conductivity. We believe that the ch-DMFT approximation (i.e., neglecting the interchain momentum dependence of Σ) is reasonable for temperatures such that the interchain correlation length is small. Extensions of the model including on-site and nearest neighbor interactions would allow us to study the deconfinement transition at quarter filling and thus to make a more realistic [3,9] comparison with experimental results. We hope to address this problem in future work.

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