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Phase Diagram of the One-Dimensional Extended Hubbard Model at Quarter-Filling.

F. MILA(*) and X. ZOTOS(**)

(*) *Institut de Physique, Université de Neuchâtel*
1 rue Breguet, CH-2000 Neuchâtel, Switzerland
(**) *Institut Romand de Recherche Numérique en Physique des Matériaux*
PHB-Ecublens - CH-1015 Lausanne, Switzerland

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Abstract. – We used exact diagonalization of small clusters and exact results in various limits to determine the phase diagram and the critical exponents of the one-dimensional (1D) U-V model at quarter-filling. We found an instability of the Luttinger liquid to a charge density wave (CDW) insulator across a boundary going from $(U, V) = (+\infty, 2t)$ to $(4t, +\infty)$. In the metallic phase, the dominant fluctuations are superconducting if V is large enough and spin density wave (SDW) otherwise. In the latter case, the critical exponent α of the momentum distribution does not exceed 9/16. The relevance of these results to 1D organic conductors is discussed.

The standard description of the low-energy electronic properties of quasi-1D compounds is based on the 1D Fermi-gas model often referred to as g-ology [1-3]. This model describes fermions with a linear dispersion interacting through four scattering processes of strength g_i ($i = 1, ..., 4$). At higher energies (of the order of the bandwidth or larger), such a description is no longer possible, and one has to turn to models that have a non-linear dispersion, like, *e.g.*, the Hubbard model. A consistent explanation of the electronic properties of a given compound requires the two descriptions to be compatible, *i.e.* that their low-energy sectors coincide for the parameters deduced from high- and low-energy data, respectively. Now, the low-energy properties of a model with a non-linear dispersion are usually quite difficult to understand and can be obtained analytically in only two cases: if the interaction terms are small, or if the model has an exact solution (in most cases of the Bethe ansatz form). Hopelessly, these models are not always able to account for the properties of real materials. A very important example is the case of the organic conductors of the $(TMTSF)_2X$ family. In a large temperature range, they exhibit low-energy properties that have a clear one-dimensional character and that are compatible with the Luttinger-liquid picture [4-6] if the exponent α defined by $n(k) - n(k_F) \propto \mathrm{sign}(k_F - k)|k - k_F|^\alpha$ is slightly larger than 1, where $n(k)$ is the momentum distribution function. Such an exponent is easy to get with a g-ology model, but not with a model with a non-linear dispersion: small interactions always yield

$\alpha \ll 1$, while for the two prominent examples of strongly correlated models that are soluble by Bethe ansatz (Hubbard [7] and t-J [8-10] models) $\alpha \leqslant 1/8$. So, one clearly has to turn to other models to have a chance to get large values of α.

In this paper, we analyse the possibility of getting such a large exponent within the context of purely electronic interactions. Such systems are characterized by the band filling n and by the form of the interaction term. In the temperature range where one-dimensional properties have been reported for $(TMTSF)_2X$, the dimerization is believed to be unimportant, and the band is 3/4-filled [3]. By electron-hole symmetry, this is equivalent to quarter-filling ($n = 1/2$), and we will concentrate on that case. For the interaction, one has to go beyond on-site repulsion to get $\alpha \geqslant 1/8$. As such models do not have in general an exact solution, one has to resort to approximations, and the choice of a particular form of the interaction should be guided by the possibility of making contact with exact results. In that respect, by far the best choice is the U-V model defined by

$$H = -t\sum_{i,\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma} + \text{h.c.}) + U\sum_{i} n_{i\uparrow}\, n_{i\downarrow} + V\sum_{i} n_i n_{i+1}\,, \tag{1}$$

because exact results can be obtained in three limits ($V = 0$, $U = +\infty$, $V = +\infty$). Note that this model is also quite reasonable from a physical point of view, U and V being *a priori* the largest coupling constants. So, we will concentrate on the analysis of Hamiltonian (1) at quarter-filling in the rest of this paper. Some remarks on the possible effect of further coupling are given at the end.

Let us start with a short summary of what is already known about this model. For $V = 0$, we recover the regular Hubbard model. At quarter-filling, it is known to be metallic [7], and its low-energy excitations are of the Luttinger-liquid [11] type, with an exponent α that goes from 0 ($U = 0$) to 1/8 ($U = +\infty$). For $U = +\infty$, we learn from the equivalence of the charge degrees of freedom to spinless fermions [6, 12] that, upon increasing V, the quarter-filled system undergoes a phase transition from a Luttinger-liquid phase to a CDW insulator at $V = 2t$. The critical exponents for spinless fermions have been calculated by Haldane [11], and from them one can deduce that α increases from 1/8 at $V = 0$ to 9/16 at $V = 2t$. These results suggest two things about the general case: first, the system is probably a Luttinger liquid for any U as long as V is not too large; second, there should be an insulating phase with a boundary terminating at $(U, V) = (+\infty, 2t)$.

Before we can say anything about the Luttinger-liquid exponents, we have to know the range of parameters for which the system is metallic. So, our first task is to determine the boundary of the insulating region. This can be done by a finite-size analysis of the gap function $\Delta(L; N)$ defined by

$$\Delta(L; N) = E_0(L; N+1) + E_0(L; N-1) - 2E_0(L; N)\,, \tag{2}$$

where $E_0(L; M)$, the ground-state energy of M particles on L sites, can be obtained by exact diagonalization of small clusters using Lanczos algorithm. Such a procedure has been used by Spronken *et al.* [13] for the case of spinless fermions with nearest-neighbour repulsion, and the critical value $V_c = 2t$ could be reproduced quite accurately by fitting $\Delta(L; N)$ with polynomials of $1/L$. In our case, the Hilbert space is much larger, and we have results for 3 sizes only ($L = 8, 12, 16$). So we cannot expect a very good accuracy. In fact, we could not get meaningful results by fitting these 3 values with $A + B/L + C/L^2$. However, fitting any pair of values with $A + B/L$, gives reasonable results that do not depend too much on the pair chosen to do the fit. Besides, as far as the large-U case is concerned, the best result is obtained by fitting the results for $L = 8$ and 16. This is probably due to the fact that the 12-site system is quite different from the other two: to get smooth results as a function of L

one must choose the boundary conditions so that k_F is one of the allowed k values, that is periodic ones for 8 and 16 sites, and antiperiodic ones for 12 sites [13]. The points obtained with $L = 8$ and 16 are given in fig. 1 (open circles).

In view of the uncertainties of the finite-size analysis, it would be good to know another point besides $(U, V) = (+\infty, 2t)$ that lies on the boundary. It turns out that the exact value of U for $V = +\infty$ can be obtained quite easily. A detailed discussion will be given elsewhere. The calculation relies on the fact that for $V = +\infty$ the pairs (if any) cannot move, while the unpaired particles have the same kinetic energy as spinless fermions interacting with an infinite V, a problem that has a Bethe ansatz solution [14, 15]. Then, for U large enough, it is quite easy to see that $E_0(L; L/2) = 0$ and $E_0(L; L/2 + 1) = U$, while $\lim_{L \to +\infty} E_0(L; L/2 - 1) = -4t$. So $\lim_{L \to +\infty} \Delta(L; L/2) = U - 4t$ vanishes when $U = 4t$, which proves that $(U, V) = (4t, +\infty)$ lies on the boundary. Our numerical results are in good agreement with this value. It seems that the boundary is horizontal between $V = 4t$ and $V = +\infty$, although a weak dependence on V cannot be excluded.

We now turn to the analysis of the metallic phase. In the weak-coupling limit, the model can be mapped onto a g-ology model with a cut-off procedure [1, 2]. At quarter-filling, the coupling constants are $g_1 = U$, $g_2 = U + 2V$, $g_{4\parallel} = 2V$ and $g_{4\perp} = U + 2V$. For $U > 0$, the system scales to the Tomonaga-Luttinger fixed point $g_1^* = 0$, $g_2^* = g_2 - g_1/2$. So, the long-wavelength properties depend on 3 parameters only. One usually chooses the velocities of the charge (respectively spin) density oscillations u_ρ (respectively u_σ) and a parameter K_ρ that determines the exponent of the correlation functions. In particular, the exponent α is given by $\alpha = (K_\rho + 1/K_\rho - 2)/4$.

In the strong-coupling limit, the perturbation theory cannot be invoked to prove that the long-wavelength physics can be described by the Tomonaga-Luttinger fixed point. However, assuming this to be the case, one can deduce the parameters of the model from the low-energy part of the spectrum [11, 16] (which can be obtained numerically for small clusters, as suggested by Schulz [6]) and check *a posteriori* if these parameters are consistent with the hypothesis. One can estimate the ratio u_ρ/K_ρ by using its relation to the

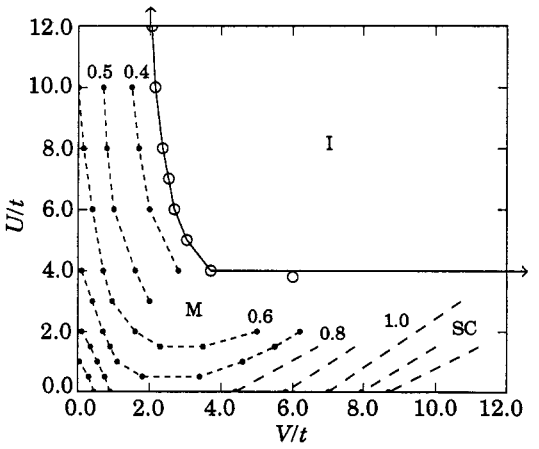

Fig. 1. – Phase diagram of the U-V model at quarter-filling. M: metal, I: insulating, SC: superconducting phases. Solid line and open circles: M-I transition; arrows: exact limiting values of the M-I boundary; dashed lines and full circles: constant-K_ρ curves.

compressibility κ:

$$\frac{\pi}{2}\frac{u_\rho}{K_\rho} = \frac{1}{n^2\kappa}, \tag{3}$$

$$\kappa = \frac{L}{N^2}\left(\frac{E_0(N+2)+E_0(N-2)-2E_0(N)}{4}\right)^{-1}. \tag{4}$$

Equation (4) is the finite-size approximation to the compressibility, $E_0(N)$ being the ground-state energy calculated with suitable boundary conditions. The charge velocity can be obtained from the low-energy spectrum as

$$u_\rho = (E_{1\rho} - E_0)/(2\pi/L). \tag{5}$$

The analysis of the t-J model by Ogata *et al.* [17] was based on these equations.

In our study, we have also used another relation that holds for Luttinger liquid, namely

$$\sigma_0 = 2u_\rho K_\rho, \tag{6}$$

where σ_0 is the weight of the Drude peak of the conductivity. In 1D systems, σ_0 can be obtained simply from [18-20]

$$\sigma_0 = \frac{\pi}{L}\frac{\partial^2 E_0(\phi)}{\partial\phi^2}\bigg|_{\phi=0}, \tag{7}$$

where $E_0(\phi)$ is the ground-state energy as a function of a phase ϕ due to the flux through the ring. Equations (3)-(7) provide us with 3 independent conditions on u_ρ and K_ρ. This is very useful for several reasons. First, the conductivity is much simpler to evaluate numerically than the compressibility, which involves systems with $N+2$ particles. Besides, we have good reasons to believe that eq. (4) does not give a reliable estimate of the compressibility when V is large, and it is important to be able to determine K_ρ without its help.

We can use the consistency of these equations to check the assumption that the system is a Luttinger liquid: eqs. (3), (4) and (6), (7) are typical of Luttinger liquids will be violated if we have an instability to another phase (*e.g.*, CDW insulator). A convenient way to measure the consistency of the three conditions is to calculate the ratio $\sigma_0/\pi n^2\kappa u_\rho^2$ which equals 1 for a Luttinger liquid. We have performed a systematic evaluation of this ratio along the lines in the (U, V)-plane. In the region where eq. (5) can be used, *i.e.* when V is not too large, we found that, to a good accuracy, this ratio equals 1 in the metallic phase, that it drops rapidly when one enters the insulating phase, and that the transition point was in good agreement with our previous determination of the phase boundary.

Another way to check that we have a Luttinger liquid is to extract the central charge from the finite-size scaling of the ground-state energy density [16]

$$e_0(L) = e_0(+\infty) - \frac{\pi(u_\rho + u_\sigma)}{6L^2}c + o(1/L^2); \tag{8}$$

u_σ was obtained from $u_\sigma = (E_{1\sigma} - E_0)/(2\pi/L)$, where $E_{1\sigma}$ is the energy of the first excited state with total spin $S \neq 0$. Comparing our results for $L = 8$, 12 and 16, we found that this scaling form was accurate except when V is too large, and that the central charge c

determined in this way equals 1 within 2%, in good agreement with the exact value $c = 1$ for Luttinger liquids.

Let us next discuss the exponents in this Luttinger-liquid phase. We have performed a systematic determination of u_ρ and K_ρ with the help of eqs. (5)-(7) for clusters of 8, 12 and 16 sites by Lanczos diagonalization. The constant K_ρ curves obtained for 16 sites are plotted in fig. 1 (dashed curves). When V is not too large, a meaningful extrapolation to the thermodynamic limit is possible, and the values obtained for $L = 16$ are quite close to the extrapolated ones. This corresponds to the short-dashed curves. However, when V gets large, various finite-size effects are present (see below), and the curves for $K_\rho \geq 0.8$ (long-dashed lines) are only indicative.

The qualitative features that emerge are the following. As long as V is not too large, K_ρ decreases when V increases. So, the exponent α effectively increases with V. The largest values are obtained close to the CDW boundary and do not exceed, say, 0.6. For $U < 4t$, K_ρ is non-monotonic and starts increasing when V is large enough. This results into a region where $K_\rho > 1$, *i.e.* where superconducting fluctuations are dominant. By increasing V even further, the $L = 16$ results suggest that the compressibility diverges, *i.e.* that there is a phase separation. This can be confirmed by looking again at the $V = +\infty$ case. When U decresaes below $4t$, local pairs are formed. In the thermodynamic limit, the Bethe ansatz results [15] can be used to show that the density n_p of paired particles is given by

$$n_p = (1/2\pi) \arccos (U/4) \tag{9}$$

and that in the ground state all the pairs sit together, resulting in a phase separation with a region where $n = 1$ and a region where $n < 1/2$. Although it is impossible to extrapolate to the thermodynamic limit on the basis of the $L = 8$, 12 and 16 results, due to the abrupt change of the number of pairs that occurs for different values of U in each case, the existence of a region of dominant superconducting fluctuations between the SDW phase and the phase separation is unambiguous. The instability of the Luttinger liquid toward a phase separation corresponds to $\kappa = +\infty$, *i.e.* $K_\rho = +\infty$. But when V is small, $K_\rho < 1$. By continuity, there has to be a line $K_\rho = 1$ and a region where $K_\rho > 1$ before the phase separation, *i.e.* a region where superconducting fluctuations dominate. Physical applications of this result are not clear yet. We just note that, although Coulomb interactions alone cannot yield effective parameters satisfying $V > U$, bipolaronic effects are known to produce strong local attraction, hence a negative contribution to U, and that the combination of both effects can be described by a U-V model with $V > U$.

Finally, coming back to the original problem of finding a microscopic model with α slightly larger than 1 at quarter-filling, we have shown that this is not possible within the model of eq. (1). Large values of α, that are possible away from quarter-filling [11, 6], cannot be obtained when $n = 1/2$ because of the CDW instability. This does not exclude the possibility that other models with longer-range interactions can do the job. However, a remarkable property of our results suggests that this will not be the case: the boundary between the insulating and the metallic phases corresponds, within the accuracy of our results, to the curve α maximum. So, one may conjecture that the CDW instability is related to the value of α, in which case other models will *not* be able to produce larger values of α before the CDW phase is reached. This property is consistent with the observation that the $4k_F$ fluctuations [21, 22] become divergent along a line α constant ($\alpha = 1/8$). The metal-insulator transition, *i.e.* the opening of a gap in the charge excitation spectrum, is a different effect, however, which, according to our results, occurs at a considerably larger value of α (9/16). So far as we know, a weak-coupling theory of commensurability effects has been worked out for

half-filling only [1], and more work is needed to confirm or dismiss our conjecture about the quarter-filled case. We are currently working on this problem.

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[1] With the noticeable exception of the $U = +\infty$ model at quarter-filling, where the transition is effectively a $2k_F$ CDW instability of spinless fermions, see [23].

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