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Breakdown of the Luttinger sum rule at the Mott-Hubbard transition in the one-dimensional t_1-t_2 Hubbard model

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Abstract. – We investigate the momentum distribution function near the Mott-Hubbard transition in the one-dimensional t_1-t_2 Hubbard model (the zigzag Hubbard chain) with the density matrix renormalization group technique. We show that for strong interactions the Mott-Hubbard transition occurs between the metallic phase and an insulating dimerized phase with incommensurate spin excitations, suggesting a decoupling of magnetic and charge excitations not present in weak coupling. We illustrate the signatures for the Mott-Hubbard transition and the commensurate-incommensurate transition in the insulating spin-gaped state in their respective ground-state momentum distribution functions.

Introduction. – Many aspects of the low-energy physics of an electronic system are influenced by the shape of its Fermi surface and the occupation of nearby states. Finite temperature, disorder or strong correlations may change the Fermi-surface geometry and or topology and induce magnetic and other instabilities.

The investigation of the interplay of magnetic interactions, in particular the existence of incommensurate phases, with charge excitations emerges as one of the central issues in the physics of low-dimensional electronic systems [1–7]. The nature and mechanism of the Mott-Hubbard transition, as one of its most striking manifestations, have been subject to intense investigation for many years. It is therefore important to study the renormalization of individual Fermi-surface sections under the influence of electron-electron correlations in competition with frustrating interactions.

Recent investigations suggested a spontaneous, interaction-induced deformation of the Fermi surface of the 2D (extended) Hubbard model close to half-filling, indicating in part a violation of the Luttinger sum rule [8–10]. The possibility of a relevant Fermi-surface renormalization near the Mott-Hubbard (MH) transition in one-dimensional generalized Hubbard

models has been raised on the basis of a DMRG study [11], drawing on arguments from results obtained for the Fermi-surface flow by RG [12,13].

In this letter we examine this Mott-Hubbard transition in one of the prototypical frustrated one-dimensional models: the half-filled zigzag Hubbard ladder. For appropriate choices of the parameters this model describes either the low-energy properties of Hubbard ladders [12] or half-filled edge-sharing double-chain materials like $SrCuO_2$ [14] or LiV_2O_5 [15] for which the next-nearest-neighbor hopping is expected to be substantial. The study of this system permits both the consideration of incommensurate phases and strong interactions. The former are difficult to study in the limit of infinite dimensions, where part of our present understanding of the Mott-Hubbard transition orginates. The latter can now be treated adequately for one-dimensional systems using the density matrix renormalization group (DMRG), which emerged in the last decade as a reliable tool to investigate the electronic structure of quasi–one-dimensional systems [16,17].

We find no renormalization to perfect nesting of the Fermi surface in the metallic state as the Mott-Hubbard transition is approached. We explicitly demonstrate that the dimerized state on the insulating side of the Mott-Hubbard transition has gaped incommensurate spin excitations, which only later give way to an insulating phase with commensurate spin excitations. Our results indicate that perfect nesting is not a prerequisite for the Mott-Hubbard transition at finite values of the interaction. The opening of the charge gap decouples from changes in the nature of magnetic excitations, in stark contrast to the weak-coupling scenario, where Umklapp scattering becomes relevant at perfect nesting and leads to the opening of a charge gap. We report the characteristic signatures of the incommensurate insulating state in momentum distribution functions for future experimental analysis.

Model. – The Hamiltonian of the zigzag Hubbard ladder is given as

$$H = -\sum_{\substack{n,\sigma \\ \Delta n=1,2}} t_{\Delta n}\left(c^{\dagger}_{n+\Delta n,\sigma}c_{n,\sigma} + \text{H.c.}\right) + U\sum_{n} n_{\uparrow}n_{\downarrow}\,, \tag{1}$$

where the $c^{\dagger}_{n,\sigma}$ ($c_{n,\sigma}$) are Fermion creation (destruction) operators on site n and spin $\sigma =\uparrow,\downarrow$ and $n_{\sigma} = c^{\dagger}_{n,\sigma}c_{n,\sigma}$.

Let us first discuss a few known properties of the phase diagram at half-filling, compare fig. 1. Following Balents and Fisher [18], we denote with $CnSm$ a phase with n/m *gapless* charge/spin modes. A Mott-Hubbard transition of type $C0S1$-$C2S2$ is predicted [12] by RG at half-filling for $t_2 = t_1/2$. This prediction should be valid at infinitesimal U/t_1.

In the limit of large U the model (1) transforms to the J_1-J_2 chain,

$$H_J = \sum_{\substack{n,\sigma \\ \Delta n=1,2}} J_{\Delta n}\,\boldsymbol{S}_n\cdot\boldsymbol{S}_{n+\Delta n}\,, \tag{2}$$

with $J_{\Delta n} = 4t^2_{\Delta n}/U$. The J_1-J_2 model spontaneously dimerizes [19] for big enough J_2. The critical value for $\alpha = J_2/J_1$ can be determined by examination of the nature of the lowest-lying excitation for finite clusters [20]. In the spin-fluid state $C0S1$ it is a triplet, in the dimerized state $C0S0$ it is a singlet (the dimerized state is doubly degenerate in the thermodynamic limit). One finds [20]: $\alpha_{\rm c} = 0.2411 = (0.491)^2$.

Torio *et al.* [21] have extended the level-crossing study used to determine $\alpha_{\rm c}$ for the J_1-J_2 model to finite U/t_1, see the dashed line in fig. 1. They propose that the dimerization line $C0S1$-$C0S0$ extends until $U/t_1 \to 0$ and connects to $t_2 = t_1/2$. This would consequently

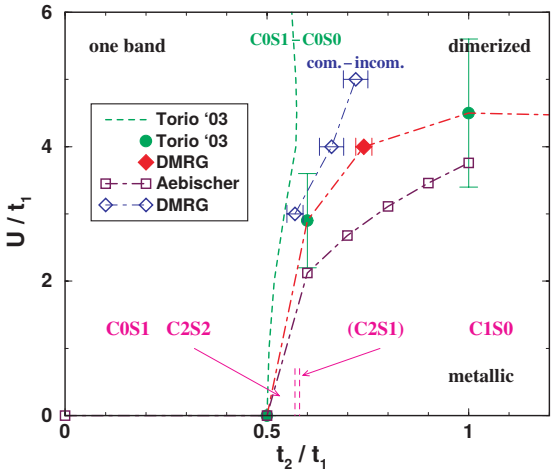

Fig. 1 – Phase diagram for the half-filled t_1-t_2 Hubbard model as explained in the text. Included are the DMRG result for the Mott-Hubbard transition at $U = 4t_1$ (filled diamonds) and for the commensurate-incommensurate transition in the insulating state (open diamonds). The dash-dotted lines are guides to the eye. The states $CnSm$ predicted by weak-coupling RG are denoted at the bottom of the phase diagram.

invalidate the weak-coupling RG prediction of a Mott-Hubbard transition of type $C0S1$-$C2S2$. It seems, presently, more likely that the transition is of $C0S0$-$CnSm$ type, with $n > 0$.

The Majumbdar-Gosh point $J_2 = J_1/2$, also called disorder point, has an exact valence-bond dimer ground state. For $\alpha > 0.5 = (0.707)^2$ the short-range spin-spin correlations become incommensurable. Due to the absence of long-range order [22], the peak in the static structure factor $S(q)$ moves away from $q = \pi$ only at the Lifschitz point, which can be determined via DMRG [23] as $\alpha_{\rm L} = 0.52063 = (0.7215)^2$.

The classical spin-wave solution to (2) yields a long-ranged spiral ground state for $\alpha > 0.5$ [24,25]. Long-ranged–ordered states are unstable towards quantum fluctuations in 1D and they become short-ranged. For the J_1-J_2 model the quantum fluctuations lead to a dimerized state with finite dimerization and short-ranged spiral (incommensurate) spin-spin correlations. They show up as a peak in $S(q)$ for an incommensurate wave vector q and width $1/\xi$, where ξ is the correlations length. There has been no study so far of the extension of the dimerized phase with incommensurate excitations, realized for $\alpha > 0.5$ in the limit of large U/t_1 to finite values of U/t_1. Here we propose that it connects to the metallic state.

Also included in fig. 1 are the predictions for the critical $U_{\rm c}$ for the Mott-Hubbard transition by Torio *et al.* [21] and by Aebischer *et al.* [26]. It has turned out to be very difficult to determine numerically the location of this transition from estimates of the charge gap, extrapolated to the thermodynamic limit, due to the fact that the charge gap is exponentially small near the Mott-Hubbard transition. Here we find that a quite accurate lower bound for the Mott-Hubbard transitions can be obtained from the study of the momentum distribution function.

Method. – In the last decade the density matrix renormalization group [16] emerged as a reliable tool for the study of electronically one-dimensional models [17]. For strongly interacting fermionic systems, the evaluation of $n(k)$ as the Fourier transform of the correlation

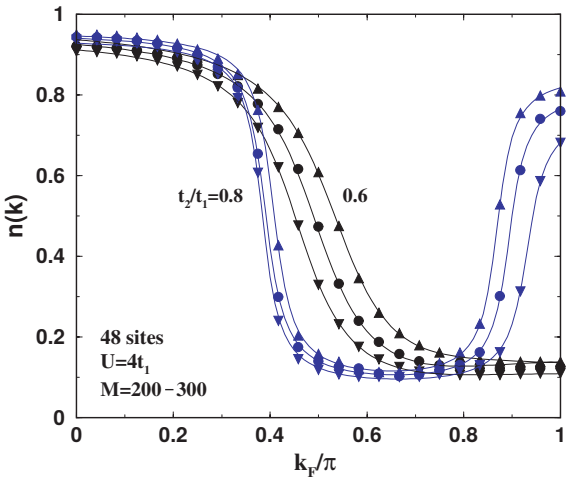

Fig. 2 – Illustration of the momentum distribution function $n(k)$ for $L = 48$ sites, $U = 4t_1$ and $t_2/t_1 = 0.6, 0.8$. DMRG results for $N_\uparrow = N_\downarrow = L/2$ (filled circles) and for $N_\uparrow = L/2+2$, $N_\downarrow = L/2-2$ (triangles-up: majority spin, triangles-down: minority spin). The lines are fits by eq. (4).

function

$$n_\sigma(k) = \frac{2}{L} \sum_{n,n'=1}^{L} \cos(k(n-n')) \langle c^\dagger_{n,\sigma} c_{n',\sigma} \rangle \tag{3}$$

is numerically difficult and costly in the framework of the DMRG [16, 17], in particular for periodic boundary conditions [27]. Here we report results from DMRG calculations on half-filled chains of length $L = 48$, 80 using up to 300 DMRG states, which we found sufficiently accurate to determine $n(k)$.

To obtain estimates for the Fermi wave vectors we have analyzed the momentum distribution function, see eq. (3), obtained by DMRG, via two smoothed step functions at $k_{\rm F1}$ and $k_{\rm F2}$ with respective widths p_1 and p_2 [11]:

$$n(k) = a_0 + a_1 \,\mathrm{atan}\, \frac{k - k_{\rm F1}}{p_1} + a_2 \,\mathrm{atan}\, \frac{k - k_{\rm F2}}{p_2} \,. \tag{4}$$

The quality of fits by (4) to $n(k)$ is illustrated in fig. 2. We will use the so obtained estimates for the Fermi wave vectors $k_{\rm F1}$ and $k_{\rm F2}$ in the further analysis. We note that the fitting procedure is possible for all regions of parameter space, but that the interpretation of k_F as a Fermi wave vector is confined to regions where the corresponding width is small.

Results. – In order to elucidate the properties of the Mott-Hubbard transition [26] and of the incommensurate-commensurate transition in one-dimensional frustrated systems, we studied the momentum distribution function for a range of parameters that crosses all relevant phase transition lines of the phase diagram of the 1D t_1-t_2 Hubbard model [28]. In fig. 3 we present our estimates for $k_{\rm F1}$ as a function of t_2/t_1 for $U = 4t_1$, in comparison with the result for $U = 0$. We note a substantial renormalization of $k_{\rm F1}$ towards larger values below $t_2/t_1 \approx 0.74$.

In the metallic state the Luttinger sum rule states that the total volume of both Fermi seas together equals the number of electrons. At half-filling this statement is equivalent to

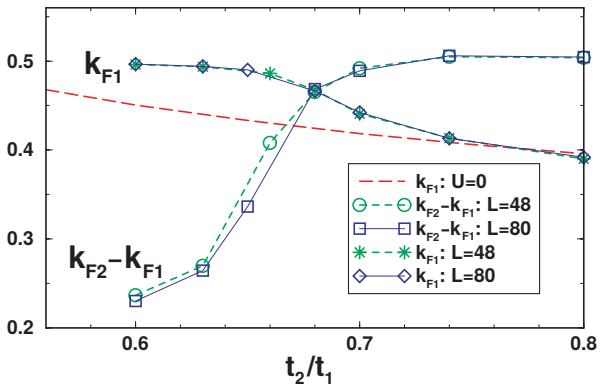

Fig. 3 – For $U = 4t_1$ and $L = 48$, 80 sites the DMRG results for $k_{\mathrm{F}1}$ and the difference $k_{\mathrm{F}2} - k_{\mathrm{F}1}$ (both in units of π) as obtained by fitting the DMRG results for $n(k)$ by eq. (4), compare fig. 2. The lines are guides to the eye. Below $t_2/t_1 \approx 0.74$ two things happen: $k_{\mathrm{F}1}$ renormalizes substantially with respect to its $U = 0$ value (dashed line) and $k_{\mathrm{F}2} - k_{\mathrm{F}1}$ deviated from its Luttinger sum rule value of 0.5.

$k_{\mathrm{F}2} - k_{\mathrm{F}1} = \pi/2$. Our DMRG data for $(k_{\mathrm{F}2} - k_{\mathrm{F}1})/\pi$ presented in fig. 3 indicates a violation of the Luttinger sum rule below $t_2/t_1 \approx 0.74$. We therefore conclude that the Mott-Hubbard transition occurs in the vicinity of this point (as indicated in fig. 1 by the filled diamonds) and that the system is insulating for $t_2/t_1 < 0.74$. Due to the exponentially small gap in this region our result for the position of the Mott-Hubbard transition is in fact a lower bound (in terms of t_2/t_1) for the exact transition point, as we would not be able to resolve numerically a possible exponentionally small departure from the Luttinger-liquid sum rule for $t_2/t_1 > 0.74$.

Next we turn to an analysis of the nature of the spin excitation in the vicinity of the Mott-Hubbard transition. The spin excitations in the insulating state correspond to renormalized particle-hole excitations with a spin-flip. They correspond therefore to states with $N_\uparrow = L/2 + \Delta N/2$ and $N_\downarrow = L/2 - \Delta N/2$. Using for numerical convenience $\Delta N = 2$, we have calculated the respective Fermi wave vectors for the majority $k_{\mathrm{F}1,\uparrow}$ and minority $k_{\mathrm{F}1,\downarrow}$ spins.

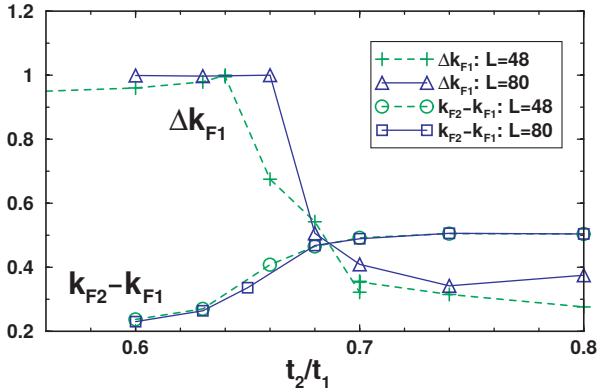

Fig. 4 – The normalized shift $\Delta k_{\mathrm{F}1}$, see eq. (5) for $L = 48$, 80 sites and $U = 4t_1$. The lines are guides to the eye. For comparison, we have reproduced the results for $k_{\mathrm{F}2} - k_{\mathrm{F}1}$ from fig. 3.

We define the normalized shift for the Fermi wave vector as

$$\Delta k_{\mathrm{F}1} = (k_{\mathrm{F}1,\uparrow} - k_{\mathrm{F}1,\downarrow})\, L/(\pi \Delta N). \tag{5}$$

The normalization in eq. (5) is chosen such that $\Delta k_{\mathrm{F}1} = 1$, independent of the system size L, for the case of a single Fermi sea. In the limit $t_2/t_1 \to \infty$, the Hubbard zigzag chain has two equally large Fermi seas, with equal Fermi velocities, and $\Delta k_{\mathrm{F}1} \to 0.5$ in this limit, as we have verified numerically for large t_2/t_1.

We have obtained $\Delta k_{\mathrm{F}1}$ by fitting the respective momentum distribution functions for the majority and minority spins, see fig. 2, by eq. (4). The results are presented in fig. 4. We notice that $\Delta k_{\mathrm{F}1} \approx 1$ for small t_2/t_1, implying commensurated spin excitations. A well-defined kink in $\Delta k_{\mathrm{F}1}$ at $t_2/t_1 \approx 0.64$–0.66 indicates a second-order transition to a state with incommensurate spin excitations (denoted by the open diamond in fig. 1).

These results imply that the Mott-Hubbard transition takes place for Fermi wave vectors at arbitrary, incommensurate values, and the Fermi wave vectors do not renormalize towards perfect nesting $k_{\mathrm{F}1} \to \pi/2$ and $k_{\mathrm{F}2} \to \pi$. In weak coupling, Umklapp scattering becomes relevant at perfect nesting and leads to the opening of a charge gap. Our results indicate, that effective perfect nesting is not necessary for the Mott-Hubbard transition for finite values of the interaction strength.

Discussion. – The interplay between magnetic order and carrier mobility in strongly interacting systems, with the Mott-Hubbard transition as one important manifestation, has long been subject to intense investigation. For the two-dimensional (2D) case, important for experimental realizations, exact analytical or numerical techniques are still lacking. It is known that in 2D the commensurate ordered phase for the nearest-neighbor Hubbard model is unstable with respect to helical fluctuations [1, 2] either upon doping or in the presence of frustrating next-nearest-neighbor interactions. Other, even more exotic phases [3, 4] have also been proposed, in particular in the context of studies into the mechanism of high-temperature superconductivity. Our investigation of the one-dimensional case offers new insight into driving forces behind the MH transitions: nesting, *i.e.* the divergence of the magnetic susceptibility due to special features of the Fermi-surface geometry emerges as sufficient, but apparently not necessary condition of the MH transition [29]. This result is inaccessible by weak-coupling theory and indicates the existence of a generic mechanism for charge carrier freezing that is independent of dominant Umklapp-scattering processes. Spin-charge separation in Luttinger liquids may enhance this effect in one dimension, but similar strong-coupling scenarios must be present also in higher dimensions to explain the MH transition between incommensurate insulators and metals in doped or frustrated 2D systems.

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