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Emergence of Irrationality: Magnetization Plateaux in Modulated Hubbard Chains

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Abstract

Hubbard chains with periodically modulated coupling constants in a magnetic field exhibit gaps at zero temperature in their magnetic and charge excitations in a variety of situations. In addition to fully gapped situations (plateau in the magnetization curve *and* charge gap), we have shown [Phys. Lett. **A268**, 418 (2000)] that plateaux also appear in the presence of massless modes, leading to a plateau with a magnetization m whose value depends continuously on the filling n. Here we detail and extend the arguments leading to such doping-dependent magnetization plateaux. First we analyze the low-lying excitations using Abelian bosonization. We compute the susceptibility and show that due to the constraint of fixed n, it vanishes at low temperatures (thus leading to a magnetization plateau) even in the presence of one massless mode. Next we study correlation functions and show that one component of the superconducting order parameter develops quasi-long-range order on a doping-dependent magnetization plateau. We then use perturbation theory in the on-site repulsion U to compute the width of these plateaux up to first order in U. Finally, we compute groundstate phase diagrams and correlation functions by Lanczos diagonalization of finite clusters, confirming the presence of doping-dependent plateaux and their special properties.

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I. INTRODUCTION

Strongly correlated electron systems in low dimensions are presently a subject of intense research. In particular, the magnetism of such systems has revealed very interesting properties and it is by now well established that spin chains and spin ladders present plateaux in their magnetization curves. It has been shown theoretically that plateaux occur in general at *rational* fractions of the saturation magnetization. The position of these plateaux is subject to a quantization condition that involves the volume of a translationally invariant unit cell (see *e.g.* [1–7]). From the experimental side, different materials have been found which exhibit plateaux. One example is a dimerized spin-1 chain [8] which exhibits a plateau at half the saturation magnetization as predicted in [3]. A good candidate for a plateau at one third of the saturation magnetization is $Cu_3Cl_6(H_2O)_2 \cdot 2H_8C_4SO_2$ [9], though it is not yet fully clear whether the proposed frustrated trimer chain model is really appropriate or which parameters should be used [10].

The most striking examples of plateaux have so far been observed experimentally in the materials $SrCu_2(BO_3)_2$ [11] and NH_4CuCl_3 [12] and both constitute again challenges for theory. There is generally agreement that $SrCu_2(BO_3)_2$ is a predominately two-dimensional material and how it should be modeled theoretically. Though some progress has been made in understanding the origin of some of the observed plateaux [13], it remains a difficult problem to compute the complete magnetization process within this model. On the other hand, the high-temperature crystal structure of NH_4CuCl_3 suggests a one-dimensional model, but nevertheless it remains unclear what really is the appropriate theoretical model for this compound.

Materials with a ladder structure (see *e.g.* [14]) are further good candidates for exhibiting magnetization plateaux. However, since the copper-oxide related materials are strongly coupled, plateaux with non-zero magnetization are predicted in a magnetic field range which causes difficulties with the present experimental tools. A mechanism yielding plateaux at lower values of magnetic fields would therefore be very attractive. As we have shown in the case of modulated Hubbard chains [15], doping may actually provide such a mechanism since it allows a continuous variation of the plateau magnetization m with the filling n – extending in this particular case also into the low-field region. Doping-dependent magnetization plateaux have recently been also theoretically studied in a different system, namely an integrable spin-S generalization of the $t - J$ chain doped with $(S - 1/2)$ carriers [16] where, however, the appearance of plateaux is restricted to large magnetization values. Another example of such a situation occurs in the one-dimensional Kondo lattice model [17] where unpaired spins behave ferromagnetically thus giving rise to a spontaneous magnetization of a value controlled by doping.

Here we detail and extend our previous study [15] of the effect of a magnetic field and a periodic modulation (*p*-merization) of the hopping amplitude or the on-site energy on a *doped* one-band Hubbard chain whose Hamiltonian is given by

$$H = -\sum_{x,\alpha} t(x) \, (c^\dagger_{x+1,\alpha} c_{x,\alpha} + H.c.) + U \sum_{x=1}^{L} c^\dagger_{x,\uparrow} c_{x,\uparrow} c^\dagger_{x,\downarrow} c_{x,\downarrow}$$

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$$+ \sum_{x,\alpha} \mu(x) \, c_{x,\alpha}^\dagger c_{x,\alpha} - \frac{h}{2} \sum_{x=1}^{L} (c_{x,\uparrow}^\dagger c_{x,\uparrow} - c_{x,\downarrow}^\dagger c_{x,\downarrow}) \; . \tag{1.1}$$

Here $c_{x,\alpha}^\dagger$ and $c_{x,\alpha}$ are electron creation and annihilation operators at site x, $\alpha = \uparrow, \downarrow$ the two spin orientations and h the external magnetic field. The hopping amplitude $t(x)$ and the chemical potential $\mu(x)$ are taken as periodic in the variable x with period p.

The one-dimensional Hubbard model with dimerized coupling constants ($p = 2$) is realized in a number of real compounds like the organic (super)conductors [18] and the ferroelectric perovskites [19]. While some materials in the former class come at quarter filling, one frequently finds also realizations of the half-filled Hubbard model. In this case, the model (1.1) is in the same universality class as a modulated spin-1/2 Heisenberg chain. Realizations of the latter exist also at periods $p > 2$: Some examples of trimerized chains ($p = 3$) have been studied in [20,21,9].

A technical motivation for resorting to the one-dimensional Hubbard model is that the uniform chain is exactly solvable by Bethe Ansatz (BA) for arbitrary values of the on-site repulsion U, filling and magnetic field [22]. The exact solution can then be used to construct a low energy bosonized effective field theory [23–25] which can in turn be used to study perturbations of this model (see *e.g.* [26]). Here we first review some aspects of the bosonization description of the Hubbard chain [27,28] and extend it for the case of a finite magnetic field $h \neq 0$.

Focusing on the case of constant chemical potential $\mu(x) = \mu$, we have shown in [15] that magnetization plateaux can appear for the model (1.1) if the density of particles n and magnetization m [29] satisfy

$$\frac{p}{2} (n \pm m) \in \mathbb{Z} \; . \tag{1.2}$$

These conditions are commensurability conditions for the up electrons $n_\uparrow = (n + m)/2$ and down electrons $n_\downarrow = (n - m)/2$, respectively. More precisely, if both conditions are simultaneously satisfied, the system has both charge and spin gaps. On the other hand, if only one of these conditions is fulfilled, the filling has to be kept fixed in order to have a magnetization plateau. A simple explanation of the conditions (1.2) can be given [15] in the non-interacting limit ($U = 0$). Then, the Hamiltonian (1.1) can be easily diagonalized and is found to have p bands $\varepsilon^\lambda(k)$ (see section III for more details). The magnetic field breaks the symmetry between up- and down-spin electrons by shifting their chemical potentials by opposite amounts. It is then possible that one chemical potential (say for the up electrons) lies in one of the $p - 1$ band gaps while the other (for the down electrons) is in the middle of a band. This situation leads to a doping-dependent plateau, if one imposes the constraint of fixed filling n (and only in this case). Then the magnetization can be increased only by moving an electron from the down-spin band into the up-spin band which requires a finite energy or equivalently a finite change of magnetic field, leading to a plateau. However, since the filling of the down-spin electrons remains adjustable, one obtains a doping-dependent value of the magnetization at the plateau.

Finally, we have also shown [15] that a charge gap opens if the combination $pn \in \mathbb{Z}$ of the two conditions (1.2) is satisfied. The latter case generalizes the well known charge gap at half filling ($n = 1$) as well as the charge gap at quarter filling in the dimerized Hubbard chain ($n = 1/2$, $p = 2$) [30–33].

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The plan of this paper is as follows: In subsection II A we briefly review the bosonization approach for the Hubbard chain for arbitrary filling and on-site Coulomb repulsion U in the presence of an external magnetic field (our conventions are summarized in appendix A and details on the bosonization approach in appendix B) [23,25]. In subsection II B we then use this bosonization scheme to study the effect of a modulation of the hopping amplitudes and the on-site energy $\mu(x)$ and find the conditions under which a plateau is present. The appearance of plateaux for irrational values of the magnetization and superconducting correlations are analyzed in subsections II C and II D, respectively. In section III we study the limit of small U perturbatively and show that the doping-dependent plateaux are also present there. Then we study the groundstate phase diagram (subsection IV A) and correlation functions (subsection IV B) numerically on finite size systems by means of Lanczos diagonalization. Finally, we summarize our results in section V, discuss some experimental settings where the features presented in this paper could be observed and point out open routes for further research.

II. BOSONIZATION APPROACH

A. Field theory description of the Hubbard chain in a magnetic field

In this section, we summarize the analysis of the Hubbard model in a magnetic field using Abelian bosonization. For further details see Ref. [25]. The lattice Hamiltonian is the standard one, *i.e.* (1.1) with constant $t(x) = t$, $\mu(x) = \mu$:

$$H = -t \sum_{x,\alpha}(c^\dagger_{x+1,\alpha}c_{x,\alpha} + H.c.) + U \sum_x c^\dagger_{x,\uparrow}c_{x,\uparrow}c^\dagger_{x,\downarrow}c_{x,\downarrow}$$

$$+\mu \sum_x (c^\dagger_{x,\uparrow}c_{x,\uparrow} + c^\dagger_{x,\downarrow}c_{x,\downarrow}) - \frac{h}{2}\sum_x (c^\dagger_{x,\uparrow}c_{x,\uparrow} - c^\dagger_{x,\downarrow}c_{x,\downarrow}) \ . \tag{2.1}$$

This model has been exactly solved by BA already in 1968 [22] but it took until 1990 for the correlation functions to be computed by combining BA results with Conformal Field Theory (CFT) techniques [23]. Spin-charge separation is a well known feature of the Hubbard chain at zero magnetic field. Interestingly, it is no longer spin and charge degrees of freedom that are separated if an external magnetic field is switched on [23]. Nevertheless it has been shown that in the presence of a magnetic field, the spectrum of low energy excitations can be described by a semi-direct product of two CFT's with central charges $c = 1$ [23]. This in turn implies that the model is still in the universality class of the Tomonaga-Luttinger (TL) liquid and therefore allows for a bosonization treatment.

In order to proceed, we write the fermion operator as

$$c_{x,\alpha} \rightarrow \psi_\alpha(x) \sim e^{ik_{F,\alpha}x}\ \psi_{L,\alpha}(x) + e^{-ik_{F,\alpha}x}\ \psi_{R,\alpha}(x) \ + \ldots \tag{2.2}$$

$$= e^{ik_{F,\alpha}x}\ e^{-i\sqrt{4\pi}\phi_{L,\alpha}(x)} + e^{-ik_{F,\alpha}x}\ e^{i\sqrt{4\pi}\phi_{R,\alpha}(x)} \ + \ldots \ , \tag{2.3}$$

where $k_{F,\alpha}$ are the Fermi momenta for up and down spin electrons and $\phi_{R,L,\alpha}$ are the chiral components of two bosonic fields, introduced as usual in order to bosonize the spin up and down chiral fermion operators $\psi_{R,L,\alpha}$. (Our conventions are settled in appendix A). The

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dots stand for higher order terms some of which are written explicitly in appendix B. They take into account the corrections arising from the curvature of the dispersion relation due to the Coulomb interaction. For non-zero Hubbard repulsion U and magnetic field h, the low energy effective Hamiltonian corresponding to (2.1) written in terms of the bosonic fields $\phi_\uparrow$ and $\phi_\downarrow$ has a complicated form, mixing up and down degrees of freedom. The crucial step to obtain a simpler bosonized Hamiltonian is to consider the Hamiltonian of a generalized (two component) TL model and identify the excitations of the latter with the exact BA ones for the model (2.1), providing in this way a *non-perturbative* bosonic representation of the low energy sector of the full Hamiltonian (2.1). This program has been carried out in Ref. [25] and we just quote here the final result. The fixed point (*i.e.* neglecting all irrelevant terms) bosonized Hamiltonian reads

$$H = \int dx \left[\frac{u_c}{2} \partial_x \vec{\Phi}^t \mathcal{A}_c \, \partial_x \vec{\Phi} + \frac{u_s}{2} \partial_x \vec{\Phi}^t \mathcal{A}_s \, \partial_x \vec{\Phi} \right] \ , \tag{2.4}$$

where $\vec{\Phi}^t = (\phi_{R,\uparrow}, \phi_{L,\uparrow}, \phi_{R,\downarrow}, \phi_{L,\downarrow})$. The matrices $\mathcal{A}_{c,s}$ have the following form:

$$\mathcal{A}_{c,s} = \begin{pmatrix} a_{c,s} + b_{c,s} & a_{c,s} - b_{c,s} & c_{c,s} + d_{c,s} & c_{c,s} - d_{c,s} \\ a_{c,s} - b_{c,s} & a_{c,s} + b_{c,s} & c_{c,s} - d_{c,s} & c_{c,s} + d_{c,s} \\ c_{c,s} + d_{c,s} & c_{c,s} - d_{c,s} & e_{c,s} + f_{c,s} & e_{c,s} - f_{c,s} \\ c_{c,s} - d_{c,s} & c_{c,s} + d_{c,s} & e_{c,s} - f_{c,s} & e_{c,s} + f_{c,s} \end{pmatrix} \ , \tag{2.5}$$

where

$$\begin{cases} a_c = (Z_{cc}^{-1})^2 & b_c = (Z_{cc} - Z_{sc})^2 & c_c = Z_{cc}^{-1}(Z_{cc}^{-1} + Z_{cs}^{-1}) \\ d_c = Z_{sc}(Z_{cc} - Z_{sc}) & e_c = (Z_{cc}^{-1} + Z_{cs}^{-1})^2 & f_c = Z_{cs}^2 \end{cases} \tag{2.6}$$

$$\begin{cases} a_s = (Z_{sc}^{-1})^2 & b_s = (Z_{cs} - Z_{ss})^2 & c_s = Z_{sc}^{-1}(Z_{ss}^{-1} + Z_{sc}^{-1}) \\ d_s = Z_{ss}(Z_{cs} - Z_{ss}) & e_s = (Z_{ss}^{-1} + Z_{sc}^{-1})^2 & f_s = Z_{ss}^2 \end{cases} \tag{2.7}$$

In these expressions Z_{ij} (resp. Z_{ij}^{-1}), $i, j = c, s$, are the entries of the dressed charge matrix Z (resp. its inverse Z^{-1}) taken at the Fermi points

$$Z = \begin{pmatrix} Z_{cc} & Z_{cs} \\ Z_{sc} & Z_{ss} \end{pmatrix} \ . \tag{2.8}$$

These matrix elements are solutions of a set of coupled integral equations obtained from the BA [23] and depend on the coupling U, the chemical potential μ and the magnetic field h. They can be in turn related to physical thermodynamic quantities [23].

Substituting for the bosonic fields

$$\begin{pmatrix} \phi_c \\ \phi_s \end{pmatrix} = \frac{1}{\det Z} \begin{pmatrix} Z_{ss} & Z_{ss} - Z_{cs} \\ Z_{sc} & Z_{sc} - Z_{cc} \end{pmatrix} \begin{pmatrix} \phi_\uparrow \\ \phi_\downarrow \end{pmatrix} \ , \tag{2.9}$$

and for their dual fields

$$\begin{pmatrix} \theta_c \\ \theta_s \end{pmatrix} = \begin{pmatrix} Z_{cc} - Z_{sc} & Z_{sc} \\ Z_{ss} - Z_{cs} & -Z_{ss} \end{pmatrix} \begin{pmatrix} \theta_\uparrow \\ \theta_\downarrow \end{pmatrix} \ , \tag{2.10}$$

the Hamiltonian takes the form

$$\sum_{i=c,s} \frac{u_i}{2} \int dx \ \left[(\partial_x \phi_i)^2 + (\partial_x \theta_i)^2 \right] \ , \tag{2.11}$$

where $\phi = \phi_R + \phi_L$ and $\theta = \phi_R - \phi_L$.

At zero magnetic field, the matrix Z reduces to

$$Z(h=0) = \begin{pmatrix} \xi & 0 \\ \xi/2 & 1/\sqrt{2} \end{pmatrix} \ , \tag{2.12}$$

with $\xi = \xi(\mu, U)$. In this case we recover the well known expressions for the charge and spin fields

$$\phi_c = \frac{1}{\xi} \left(\phi_\uparrow + \phi_\downarrow \right) \ , \quad \phi_s = \frac{1}{\sqrt{2}} \left(\phi_\uparrow - \phi_\downarrow \right) \ , \tag{2.13}$$

where the compactification radius of the spin field (*i.e.* the parameter which indicates the period of ϕ_s, $\phi_s = \phi_s + 2\pi R_s$, $R_s = 1/\sqrt{2\pi}$) [34] is fixed by the $SU(2)$ symmetry of the spin sector. The radius for the charge field, on the other hand, depends on the chemical potential μ and the Coulomb coupling U. Furthermore, for $h = 0$ the charge and spin degrees of freedom are completely decoupled.

It should be noted that for $m \neq 0$, the fields arising in the diagonalized form of the bosonic Hamiltonian (2.11) are no longer the charge and spin fields even though they have been labeled by 'c' and 's'. For example, the charge field is in general given by $\phi_\uparrow + \phi_\downarrow = Z_{cc}\phi_c - Z_{cs}\phi_s$.

For generic values of the parameters of the model (2.1), we can now write down for example the bosonized expression for the charge density operator:

$$\begin{aligned}
\rho(x) &= \psi_\uparrow^\dagger \psi_\uparrow(x) + \psi_\downarrow^\dagger \psi_\downarrow(x) \\
&= \frac{1}{\sqrt{\pi}} \partial_x \left(Z_{cc}\phi_c - Z_{cs}\phi_s \right) + a_\rho \ \sin[k_+ x - \sqrt{\pi}\left(Z_{cc}\phi_c - Z_{cs}\phi_s \right)] \\
&\quad \times \cos[k_- x - \sqrt{\pi}\left((Z_{cc} - 2Z_{sc})\phi_c - (Z_{cs} - 2Z_{ss})\phi_s \right)] \\
&\quad + b_\rho \sin(2k_+ x - \sqrt{4\pi}(Z_{cc}\phi_c - Z_{cs}\phi_s)) \ , \tag{2.14}
\end{aligned}$$

where a_ρ, b_ρ are non-universal constants, whose numerical values are known only in special cases. Details on how such expressions are obtained are given in appendix B. Formulae of the type (2.14) are our fundamental bosonization rules.

B. Space dependent modulations

In the present subsection we study two different perturbations of the Hubbard chain (2.1), which consist in space dependent modulations of certain parameters. In particular we shall consider a space dependent modulation of the hopping amplitude $t(x)$ and of the on-site energy $\mu(x)$.

1. Modulated hopping amplitude

In this case, the Hamiltonian reads as in eq. (1.1) with $\mu(x) = const$ and $t(x) = t$ if $x \neq lp$ and $t(lp) = t' = t + \delta$, with p, l integers and p fixed. This is equivalent to the uniform Hubbard Hamiltonian (2.1) perturbed by the term

$$H_{pert} = -\delta \sum_{x'=lp,\alpha} (c_{x',\alpha}^\dagger c_{x'+1,\alpha} + H.c.) \;. \tag{2.15}$$

At half filling and for large U, a standard second order perturbative computation in $1/U$ shows that the effective Hamiltonian is given by

$$\tilde{H} = \sum_x \frac{4t^2(x)}{U} \; \vec{S}_x \cdot \vec{S}_{x+1} \;, \tag{2.16}$$

thus leading to the p-merized Heisenberg chain studied in [6]. It was predicted there that magnetization plateaux occur when the condition $\frac{p}{2}(1-m) \in \mathbb{Z}$ is satisfied [29]. We use now Abelian bosonization techniques to analyze the more general case of the model (1.1) in the small δ (weak p-merization) limit.

Using the bosonization dictionary given in appendix B, we find the expression for the continuum limit of the lattice perturbation (2.15)

$$
\begin{aligned}
O_{pert} = \;& \lambda_1 \sin[k_+/2 + pk_+x - \sqrt{\pi}\,(Z_{cc}\phi_c - Z_{cs}\phi_s)] \\
& \times \cos[k_-/2 + pk_-x - \sqrt{\pi}\,((Z_{cc} - 2Z_{sc})\phi_c - (Z_{cs} - 2Z_{ss})\phi_s)] \\
& + \lambda_2 \sin[k_+ + 2pk_+x - \sqrt{4\pi}(Z_{cc}\phi_c - Z_{cs}\phi_s)] \;,
\end{aligned}
\tag{2.17}
$$

where $\lambda_1, \lambda_2 \propto \delta$ and the Fermi momenta are $k_+ = k_{F,\uparrow} + k_{F,\downarrow} = \pi n$, $k_- = k_{F,\uparrow} - k_{F,\downarrow} = \pi m$, where n is the filling and m is the magnetization. The presence of a factor p in the oscillating part will play an important role in the following.

The operator

$$\lambda_3 \cos[k_- + 2pk_-x - 2\sqrt{\pi}\,((Z_{cc} - 2Z_{sc})\phi_c - (Z_{cs} - 2Z_{ss})\phi_s)] \;, \tag{2.18}$$

with $\lambda_3 \propto \delta^2$ is radiatively generated from the first term in (2.17) and must therefore be included as well.

In the case of zero magnetic field the dressed charge matrix is given by (2.12) and we have then a neat separation between charge and spin fields. The most relevant perturbation takes the form

$$O_{pert} = \lambda_1 \sin[\frac{\pi n}{2} + pn\pi x - \sqrt{\pi}\xi\phi_c]\cos[\sqrt{2\pi}\phi_s] + \lambda_2 \sin[\pi n + 2pn\pi x - \sqrt{4\pi}\xi\phi_c] \;. \tag{2.19}$$

The marginal operator associated with λ_3 contains only the spin field, its dimension (fixed by the $SU(2)$ symmetry) is 2 and it is marginally irrelevant. A term like this is already present in the original model and is also marginally irrelevant. Hence, for δ small enough, this term can be absorbed in the original marginally irrelevant perturbation term without changing its relevance character.

The λ_2 term affects only the charge degrees of freedom and its dimension runs from 1, for $U \to \infty$ to 2, for $U = 0$, being then always relevant for the cases of interest. We can therefore conclude that the charge field is massive whenever this operator is commensurate, which in turn happens if the condition $pn \in \mathbb{Z}$ is satisfied.

If this happens, we can integrate out the massive charge degrees of freedom which leaves us with an effective theory for the spin degrees of freedom. This effective theory is massless except when the operator associated with λ_1 becomes also commensurate, i.e. if the condition $\frac{pn}{2} \in \mathbb{Z}$ is satisfied. In that case, we have also a spin gap in the system.

These considerations are easily generalized to the case of non-zero magnetization as long as the condition $pn \in \mathbb{Z}$ is satisfied. In this case, the λ_2 term in (2.17) is always commensurate. Since it contains only the proper charge field $\phi_\uparrow + \phi_\downarrow$, a charge gap opens for all values of m at these commensurate values of the filling. The condition $pn \in \mathbb{Z}$ is also satisfied when the two conditions (1.2) are simultaneously satisfied. In this case, also the λ_1 term in (2.19) becomes commensurate thus leading also to a spin gap.

In particular for $p = 2, 3$, we predict the following fully gapped situations:

$p = 2$: Half filling ($n = 1$): gap for the charge, and plateau for $m = 0$.
Quarter filling ($n = 1/2$) (and also $n = 3/2$): gap for the charge [30–33], and plateau for $m = \pm 1/2$.

$p = 3$: $n = 1$, $n = 1/3$ and $n = 5/3$: gap for the charge, and plateau for $m = \pm 1/3$.
$n = 2/3$ and $n = 4/3$: gap for the charge, and plateau for $m = \pm 2/3, 0$.

The final case where only one of the conditions (1.2) holds is more complicated since then the charge and spin degrees of freedom can no longer be separated. We therefore postpone discussion of this case a little.

2. Modulated on-site energy

Now we consider the Hubbard chain (1.1) with a uniform hopping amplitude $t(x) = t$ but a periodic modulation of the chemical potential $\mu(x) = \mu$ if $x \neq lp$ and $\mu(lp) = \mu + \delta\mu$, with p, l integers, p fixed. This is equivalent to the uniform chain (2.1) plus an on-site energy term which reads

$$H'_{pert} = \delta\mu \sum_{x'=lp,\alpha} c^\dagger_{x,\alpha} c_{x,\alpha} . \tag{2.20}$$

The case $p = 2$, $h = 0$ has been studied in detail in [35].

In the continuum limit the perturbing operator (2.20) becomes:

$$O'_{pert} = \lambda_1 \sin[pk_+ x - \sqrt{\pi}\,(Z_{cc}\phi_c - Z_{cs}\phi_s)] \cos[pk_- x - \sqrt{\pi}\,((Z_{cc} - 2Z_{sc})\phi_c - (Z_{cs} - 2Z_{ss})\phi_s)]$$
$$+ \lambda_2 \sin(2pk_+ x - \sqrt{4\pi}(Z_{cc}\phi_c - Z_{cs}\phi_s)) , \tag{2.21}$$

which radiatively generates a term of the form

$$\lambda_3 \cos[2pk_- x - 2\sqrt{\pi}\,((Z_{cc} - 2Z_{sc})\phi_c - (Z_{cs} - 2Z_{ss})\phi_s)] . \tag{2.22}$$

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The only difference with respect to the previous case, eqs. (2.17), (2.18), is a phase in each of the sines or cosines, which however plays a role only at half filling and zero magnetic field (see also [35]). Apart from this particular case, the conclusions remain the same as in the previous case.

C. Partial gap: irrational plateaux

We have shown in the previous subsection that, when both commensurability conditions (1.2) are satisfied, the spectrum of the model (1.1) is fully gapped. It remains to understand what happens if only one of these conditions is satisfied. In this case, apparently one degree of freedom remains massless. We will show that the system nevertheless exhibits a gap for magnetic excitations (*i.e.* excitations changing the value of the magnetization), provided the total charge (*i.e.* the filling n) is kept fixed.

For the sake of simplicity we will restrict ourselves to the dimerized chain ($p = 2$) in this subsection though the argument can be generalized easily to $p > 2$. Suppose that

$$\frac{p}{2}(n - m) = n - m = 2n_\downarrow \in \mathbb{Z} \ , \tag{2.23}$$

but that $n + m$ is not an integer, *i.e.* the commensurability condition is fulfilled only for down electrons. Assume first that there is no interaction between up and down electrons ($U = 0$). Then we are led to analyze the excitation spectrum of the following Hamiltonian in a system of length L:

$$H = \int_0^L dx \ \frac{v_\uparrow}{2} \left[(\partial_x \phi_\uparrow)^2 + (\partial_x \theta_\uparrow)^2\right] + \frac{v_\downarrow}{2} \left[(\partial_x \phi_\downarrow)^2 + (\partial_x \theta_\downarrow)^2\right] + \lambda \cos(2\sqrt{\pi}\phi_\downarrow) \ , \tag{2.24}$$

with total magnetization

$$M = \int_0^L dx \ \frac{1}{\sqrt{\pi}} \partial_x(\phi_\uparrow - \phi_\downarrow) = \frac{1}{\sqrt{\pi}}(\phi_\uparrow - \phi_\downarrow)|_0^L \ . \tag{2.25}$$

Motivated by experimental realizations of Hubbard systems, where typically doping is fixed, we also impose the constraint that the total particle number is fixed:

$$N = \int dx \ \frac{1}{\sqrt{\pi}} \partial_x(\phi_\uparrow + \phi_\downarrow) = \frac{1}{\sqrt{\pi}}(\phi_\uparrow + \phi_\downarrow)|_0^L \ . \tag{2.26}$$

From eqs. (2.25) and (2.26) we see that the fields $\phi_{\uparrow,\downarrow}$ satisfy the following boundary conditions:

$$2\phi_\uparrow|_0^L = \sqrt{\pi}(N + M) \ , \tag{2.27}$$
$$2\phi_\downarrow|_0^L = \sqrt{\pi}(N - M) \ . \tag{2.28}$$

Notice, furthermore, that the fields $\phi_{\uparrow,\downarrow}$ are compactified, *i.e.* they satisfy the periodicity condition

$$\phi_{\uparrow,\downarrow} \to \phi_{\uparrow,\downarrow} + \sqrt{\pi}\mathbb{Z} \ . \tag{2.29}$$

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Therefore, in a semiclassical picture, the vacuum configuration for $\phi_\uparrow$ is

$$\phi_\uparrow(x) = \frac{\sqrt{\pi}}{2L}(N+M)x + const . \tag{2.30}$$

On the other hand, for $\phi_\downarrow$ the vacuum configuration is a kink

$$\phi_\downarrow(x) = k(x) , \tag{2.31}$$

where $k(x)$ is a configuration interpolating between two minima of the cosine potential in the Hamiltonian (2.24) and satisfying the boundary condition (2.28). Now we change the total magnetization keeping the total number of particles fixed. The lowest energy excitation of this type consists in reversing the spin of a particle, which corresponds to the change $M \to M+2$. The new boundary conditions become then

$$2\phi_\uparrow|_0^L = \sqrt{\pi}(N+M+2) , \tag{2.32}$$
$$2\phi_\downarrow|_0^L = \sqrt{\pi}(N-M-2) . \tag{2.33}$$

The new vacuum configuration for $\phi_\uparrow$ is therefore

$$\phi_\uparrow(x) = \frac{\sqrt{\pi}}{2L}(N+M+2)x + const , \tag{2.34}$$

and it is straightforward to show that the difference in energy with respect to the original one is linear in $1/L$. On the contrary, changing the configuration of the kink requires a finite amount of energy (proportional to λ) because the new configuration is in a different topological sector. This corresponds to the presence of a gap in the spectrum of magnetic excitations, and therefore of a plateau in the magnetization curve.

To support the previous conclusion further, we analyze the magnetic susceptibility for a chain of finite size L. It is given by the integral of the correlation function of the spin density operator $\frac{1}{\sqrt{\pi}}\partial_x(\phi_\uparrow - \phi_\downarrow)$. Since the down sector is gapped it does not contribute to the zero temperature limit of the susceptibility. Let us therefore focus on the up sector, which is apparently massless but constrained to be in a particular topological sector. One can easily see that determination of the susceptibility amounts to calculate

$$\left\langle \left(\int_0^L dx \ \partial_x \phi_\uparrow \right)^2 \right\rangle - \left\langle \left(\int_0^L dx \ \partial_x \phi_\uparrow \right) \right\rangle^2 . \tag{2.35}$$

For the free massless sector, the Hamiltonian in a finite size L can be written in Fourier space for each topological sector as (see for example [36]):

$$H_L = \frac{v}{2} \sum_{q \neq 0} \left[\frac{1}{K}q^2 \phi_{-q}\phi_q + Kq^2\theta_{-q}\theta_q \right] + \frac{\pi v}{2L}\left(\frac{1}{K}Q^2 + KJ^2 \right) , \tag{2.36}$$

where Q and J stand for the particle number and current zero modes:

$$Q = \frac{1}{\sqrt{\pi}} \ \phi_\uparrow|_0^L , \qquad J = \frac{1}{\sqrt{\pi}} \ \theta_\uparrow|_0^L ,$$

and the summation over q is for oscillatory modes. If the global constraint is not present, one has to sum over all possible values of Q, *i.e.* one has to compute

$$\chi = \frac{1}{\beta L} \left(\frac{1}{Z} \text{Tr} \left(\exp(-\beta H_L) Q^2 \right) - \left(\frac{1}{Z} \text{Tr} \left(\exp(-\beta H_L) Q \right) \right)^2 \right) . \tag{2.37}$$

The local part (the oscillator modes) decouples, and if the constraint is not imposed we obtain the standard result

$$\chi = \frac{1}{\beta L} \left(\frac{1}{Z} \sum_Q \left(\exp(-\beta \frac{\pi v Q^2}{2LK}) Q^2 \right) - \left(\frac{1}{Z} \sum_Q \left(\exp(-\beta \frac{\pi v Q^2}{2LK}) Q \right) \right)^2 \right) = \frac{K}{2\pi v} . \tag{2.38}$$

If we now impose the global constraint on N, due to the gap in the down sector as discussed above, all the sectors will be exponentially suppressed, except the sector $Q = (N+M)/2$. Therefore, for small enough temperature, the distribution $\exp(-\beta \frac{\pi v Q^2}{2LK})$ has to be replaced by a delta function in $Q = (N+M)/2$, giving

$$\chi = \frac{1}{\beta L} \left(\langle Q^2 \rangle - \langle Q \rangle^2 \right) = 0 . \tag{2.39}$$

We find then an exotic situation in which we have simultaneously algebraic decay of correlation functions, since the local dynamics is massless, but zero magnetic susceptibility, due to the global constraint imposed on the system. The only somewhat similar situations we are aware of include plateau states of strongly frustrated spin ladders with gapless non-magnetic excitations [4,37,38] as well as the large number of singlets inside the gap of the Heisenberg antiferromagnet on a Kagomé lattice [39].

D. Superconducting fluctuations

Having found a situation with a gap which can be attributed to magnetic excitations and another massless degree of freedom, one may wonder whether superconducting fluctuations develop. We therefore now briefly analyze the correlators of the superconducting order parameter. In the presence of a magnetic field, the superconducting order parameter has four components which read on the lattice:

$$\Delta_{\alpha,\beta} = c_{x+1,\alpha} c_{x,\beta} . \tag{2.40}$$

For $h = 0$, these components can be grouped in a triplet (t) and a singlet (s). On the lattice, the corresponding $S^z = 0$ components can be chosen as

$$\Delta_{t,s}^{latt} = c_{x,\uparrow} c_{x+1,\downarrow} \pm c_{x,\downarrow} c_{x+1,\uparrow} . \tag{2.41}$$

In the continuum, using eq. (A1) this leads to the following expression

$$\Delta_{t,s} = e^{-ik_- x} \psi_{R,\uparrow} \psi_{L,\downarrow} \left(e^{ik_{F\downarrow}} \mp e^{-ik_{F\uparrow}} \right) + e^{ik_- x} \psi_{L,\uparrow} \psi_{R,\downarrow} \left(e^{-ik_{F\downarrow}} \mp e^{ik_{F\uparrow}} \right)$$
$$+ e^{-ik_+ x} \psi_{R,\uparrow} \psi_{R,\downarrow} \left(e^{-ik_{F\downarrow}} \mp e^{-ik_{F\uparrow}} \right) + e^{ik_+ x} \psi_{L,\uparrow} \psi_{L,\downarrow} \left(e^{ik_{F\downarrow}} \mp e^{ik_{F\uparrow}} \right) . \tag{2.42}$$

In particular, for zero magnetic field $k_{F\uparrow} = k_{F\downarrow} = k_F$ and neglecting "$2k_F$" terms, eqs. (2.42) reduce to the standard ones (see for example Ref. [26]):

$$\Delta_t = 2i \sin k_F(\psi_{R,\uparrow}\psi_{L,\downarrow} + \psi_{R,\downarrow}\psi_{L,\uparrow}), \qquad \Delta_s = 2\cos k_F(\psi_{R,\uparrow}\psi_{L,\downarrow} - \psi_{R,\downarrow}\psi_{L,\uparrow}(x)). \qquad (2.43)$$

For general m, one finds instead

$$\Delta_t \sim \frac{1}{\pi a}e^{i\sqrt{\pi}(\theta_\uparrow + \theta_\downarrow)}\cos(\sqrt{\pi}(\phi_\uparrow - \phi_\downarrow) - k_- x), \quad \Delta_s \sim \frac{i}{\pi a}e^{i\sqrt{\pi}(\theta_\uparrow + \theta_\downarrow)}\sin(\sqrt{\pi}(\phi_\uparrow - \phi_\downarrow) - k_- x).$$
$$(2.44)$$

These expressions show that the correlators associated to the order parameters Δ_t and Δ_s decay exponentially, even in the partially massless plateau phases. Indeed, since the $S^z = 0$ components of $\Delta_{\alpha,\beta}$ are products of up and down degrees of freedom, it is sufficient that one of them is gapped in order to lead to an exponential decay of the composite object.

On the other hand, the diagonal components are bosonized as

$$\Delta_{\alpha,\alpha} \sim 2\cos(k_{F,\alpha})e^{i\sqrt{4\pi}\theta_\alpha} + e^{-ik_{F,\alpha}(1+2x)}e^{i\sqrt{4\pi}(\phi_\alpha + \theta_\alpha)} + e^{ik_{F,\alpha}(1+2x)}e^{i\sqrt{4\pi}(-\phi_\alpha + \theta_\alpha)} + ..., \qquad (2.45)$$

where the dots include terms which mix $\phi_\uparrow$ with $\phi_\downarrow$. It is then clear that on a doping-dependent plateau, where only one of the fields is gapful, only one of the correlators $\langle \Delta^\dagger_{\alpha,\alpha}\Delta_{\alpha,\alpha}\rangle$ decays exponentially, but the other exhibits *algebraic* behavior. In fact, all fields involving only the gapless spin component decay algebraically. In particular, also the two-point correlator of $c_{x,\alpha}$ decays algebraically if $\Delta_{\alpha,\alpha}$ exhibits quasi-long-range order. The algebraic decay of the latter should therefore not be taken as a sign for superconductivity, but is interesting nevertheless.

III. SMALL-U LIMIT

The previous section was dedicated to the bosonization approach to the p-merized Hubbard chain in the small p-merization limit. In the present section, we give a further argument for doping dependent plateaux, valid in the low U limit but at arbitrary p-merization strength. For the sake of simplicity, we will concentrate on the case of modulated hopping amplitude $t(x) = t'$ for x a multiple of p, otherwise $t(x) = t$ and constant $\mu(x) = \mu$, but the arguments can be generalized easily.

First we diagonalize the Hamiltonian (1.1) at $U = 0$ by a unitary transformation

$$d^\lambda_{k,\sigma} = \frac{1}{\sqrt{L}}\sum_{x=1}^{L/p}e^{ikx}\sum_{j=1}^{p}a^\lambda_{k,j}c_{xp+j,\sigma}. \qquad (3.1)$$

In order for the kinetic part of the Hamiltonian (1.1) to take the form

$$H_0 = \sum_{\lambda=1}^{p}\sum_\sigma \epsilon^\lambda(k)d^{\dagger\lambda}_{k,\sigma}d^\lambda_{k,\sigma}, \qquad (3.2)$$

the coefficients $a^\lambda_{k,j}$ have to satisfy the following eigenvalue equation:

$$-\begin{pmatrix} 0 & t & 0 & \cdots & 0 & t'\mathrm{e}^{-ik} \\ t & 0 & t & \ddots & & 0 \\ 0 & t & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & t & 0 \\ 0 & & \ddots & t & 0 & t \\ t'\mathrm{e}^{ik} & 0 & \cdots & 0 & t & 0 \end{pmatrix} \begin{pmatrix} a_{k,1}^{\lambda} \\ a_{k,2}^{\lambda} \\ \vdots \\ \\ a_{k,p}^{\lambda} \end{pmatrix} = \epsilon^{\lambda}(k) \begin{pmatrix} a_{k,1}^{\lambda} \\ a_{k,2}^{\lambda} \\ \vdots \\ \\ a_{k,p}^{\lambda} \end{pmatrix} . \tag{3.3}$$

The resulting p energy bands $\epsilon^{\lambda}(k)$ are illustrated in Fig. 2 of [30] for $p = 2$ and in Fig. 2 of [15] for $p = 3$ (note that in the latter case, the energy ϵ was plotted with the wrong sign which can be absorbed by shifting $k \to k + \pi$).

In the sequel we first work out the simpler case $p = 2$ and then generalize to $p \geq 3$.

A. Case $p = 2$

In the dimerized case, the eigenvalue equation (3.3) reduces to

$$-\begin{pmatrix} 0 & t + t'\mathrm{e}^{-ik} \\ t + t'\mathrm{e}^{ik} & 0 \end{pmatrix} \begin{pmatrix} a_{k,1}^{\lambda} \\ a_{k,2}^{\lambda} \end{pmatrix} = \epsilon^{\lambda}(k) \begin{pmatrix} a_{k,1}^{\lambda} \\ a_{k,2}^{\lambda} \end{pmatrix} . \tag{3.4}$$

The eigenvalue problem (3.4) is solved readily, yielding

$$\begin{aligned} \epsilon^{\pm}(k) &= \pm\sqrt{t^2 + t'^2 + 2tt' \cos k} \,, \\ a_1^{\pm} &= \mp \sqrt[4]{\frac{t + t'\mathrm{e}^{-ik}}{t + t'\mathrm{e}^{ik}}} \,, \\ a_2^{\pm} &= \sqrt[4]{\frac{t + t'\mathrm{e}^{ik}}{t + t'\mathrm{e}^{-ik}}} \,. \end{aligned} \tag{3.5}$$

The inverse of the transformation (3.1) is:

$$\begin{aligned} c_{2x+2,\sigma} &= \frac{1}{\sqrt{L}} \sum_k \mathrm{e}^{-ikx} \sqrt[4]{\frac{t + t'\mathrm{e}^{-ik}}{t + t'\mathrm{e}^{ik}}} \left(d_{k,\sigma}^{-} + d_{k,\sigma}^{+} \right) \,, \\ c_{2x+1,\sigma} &= \frac{1}{\sqrt{L}} \sum_k \mathrm{e}^{-ikx} \sqrt[4]{\frac{t + t'\mathrm{e}^{ik}}{t + t'\mathrm{e}^{-ik}}} \left(d_{k,\sigma}^{-} - d_{k,\sigma}^{+} \right) \,. \end{aligned} \tag{3.6}$$

Eigenstates $|\{k_{j,\sigma}^{\lambda}\}\rangle$ of the free Hamiltonian H_0 are now written down by simply specifying the momenta $k_{j,\sigma}^{\lambda}$ occupied in the various bands. Now we treat the Coulomb repulsion

$$H_I = U \sum_{x=1}^{L} n_{x,\uparrow} n_{x,\downarrow} \tag{3.7}$$

in first order perturbation theory.

To proceed further, we assume that none of the bands are half-filled. Then H_I has only diagonal terms (*i.e.* Umklapp scattering is absent) which are readily evaluated as (denoting $n_{k,\sigma}^{\lambda} = d_{k,\sigma}^{\dagger\lambda} d_{k,\sigma}^{\lambda}$)

$$\langle \{k_{j,\sigma}^\lambda\}|H_I|\{k_{j,\sigma}^\lambda\}\rangle = \frac{U}{L}\langle \{k_{j,\sigma}^\lambda\}| \sum_{k,k'}(n_{k,\uparrow}^- + n_{k,\uparrow}^+)(n_{k',\downarrow}^- + n_{k',\downarrow}^+)|\{k_{j,\sigma}^\lambda\}\rangle$$

$$= \frac{U}{L}(N_\uparrow^- + N_\uparrow^+)(N_\downarrow^- + N_\downarrow^+)$$

$$= \frac{U}{4}L(n_\uparrow^- + n_\uparrow^+)(n_\downarrow^- + n_\downarrow^+). \tag{3.8}$$

In the second line, we have defined the number of particles with spin σ in band λ by $N_\sigma^\lambda = n_\sigma^\lambda L/2$ [40]. The densities have been normalized such that $n_\sigma^\lambda = 1$ for a completely filled band.

Similarly, expectation values of the number operators $\sum_{x=1}^L n_{x,\sigma}$ give $L\left(n_\sigma^- + n_\sigma^+\right)/2$. Putting everything together, we find the energy of the Hamiltonian (1.1) to first order in U as

$$E = \sum_\lambda \sum_{k_{j,\sigma}^\lambda} \epsilon^\lambda(k_{j,\sigma}^\lambda) + \frac{U}{4}L(n_\uparrow^- + n_\uparrow^+)(n_\downarrow^- + n_\downarrow^+)$$

$$+ \frac{\mu}{2}L(n_\uparrow^- + n_\uparrow^+ + n_\downarrow^- + n_\downarrow^+) - \frac{h}{4}L(n_\uparrow^- + n_\uparrow^+ - n_\downarrow^- - n_\downarrow^+). \tag{3.9}$$

Assume now that the '$-$' bands are both partially filled. Then (3.9) specializes to

$$E/L = \frac{1}{4\pi}\sum_\sigma \int_{-n_\sigma\pi}^{n_\sigma\pi} dk\epsilon^-(k) + \frac{U}{4}n_\uparrow n_\downarrow + \frac{\mu}{2}(n_\uparrow + n_\downarrow) - \frac{h}{4}(n_\uparrow - n_\downarrow), \tag{3.10}$$

where $n_\sigma = n_\sigma^-$ [41]. Setting $n = n_\uparrow + n_\downarrow$ and fixing $n_\uparrow \approx 1$, we find from the condition that it does not require energy to flip $\uparrow$ to $\downarrow$ spins,

$$h_{c_1} = \epsilon^-(\pi) - \epsilon^-((n-1)\pi) + U\left(\frac{n}{2} - 1\right). \tag{3.11}$$

On the other hand, if we consider the case of a completely filled "$-, \uparrow$" band and partially filled "$+, \uparrow$" and "$-, \downarrow$" bands, eq. (3.9) specializes as follows:

$$E/L = \frac{1}{2\pi}\int_{(1-n_\uparrow^+)\pi}^{n_\uparrow^+\pi} dk\epsilon^+(k) + \frac{1}{2\pi}\int_0^\pi dk\epsilon^-(k) + \frac{1}{2\pi}\int_0^{n_\downarrow\pi} dk\epsilon^-(k) + \frac{U}{4}(1 + n_\uparrow^+)n_\downarrow$$

$$+ \frac{\mu}{2}(1 + n_\uparrow^+ + n_\downarrow) - \frac{h}{4}(1 + n_\uparrow^+ - n_\downarrow). \tag{3.12}$$

Setting $n = 1 + n_\uparrow^+ + n_\downarrow$ and fixing $n_\uparrow^+ \approx 0$, we find in the same way as before that

$$h_{c_2} = \epsilon^+(\pi) - \epsilon^-((n-1)\pi) + U\left(\frac{n}{2} - 1\right). \tag{3.13}$$

Using eqs. (3.13) and (3.11) we find that the width of the plateau at fixed N is not affected by the on-site Coulomb repulsion to first order in U:

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$$h_{c_2} - h_{c_1} = 2\left|t - t'\right| + \mathcal{O}(U^2). \tag{3.14}$$

This ensures the presence of a doping-dependent plateau with $m = 1 - n$ in the low U limit. The absence of a first-order correction in U to the width in (3.14) can be traced to the mean-field form (3.8) of the matrix elements of the on-site repulsion H_I. This in turn is due to the fact that $\left|a_i^{\pm}\right| = 1$ for all k as can be seen from (3.5) and is a manifestation of the symmetry between the lower and upper band. Both the mean-field form of the interaction as well as the absence of a first-order correction to the plateau width are special properties of the case $p = 2$, as will become clear in the following discussion of the case $p \geq 3$.

B. Case $p \geq 3$

For general p, the diagonalization (3.3) is more complicated leading to the absence of explicit expressions such as (3.6). Nevertheless, we can still use unitarity of the transformation (3.1) to formally invert it

$$c_{xp+j,\sigma} = \frac{1}{\sqrt{L}} \sum_k \sum_\lambda e^{-ikx} a_{k,j}^{*\lambda} d_{k,\sigma}^\lambda. \tag{3.15}$$

First, we look at the transformation of number operators $n_{x,\sigma} = c_{x,\sigma}^\dagger c_{x,\sigma} \to n_{k,\sigma}^\lambda = d_{k,\sigma}^{\dagger\lambda} d_{k,\sigma}^\lambda$:

$$\sum_x n_{x,\sigma} = \frac{1}{p} \sum_{k,\lambda} \sum_{j=1}^p \left|a_{k,j}^\lambda\right|^2 n_{k,\sigma}^\lambda = \sum_{k,\lambda} n_{k,\sigma}^\lambda. \tag{3.16}$$

Here, we have just used that $\sum_{j=1}^p \left|a_{k,j}^\lambda\right|^2 = p$.

The diagonal terms of the interaction (3.7) can now be treated similarly as for $p = 2$. Instead of (3.8) one finds for general p

$$\langle\{k_{j,\sigma}^\lambda\}|H_I|\{k_{j,\sigma}^\lambda\}\rangle = \frac{U}{pL}\langle\{k_{j,\sigma}^\lambda\}|\sum_{j=1}^p \sum_{k,\lambda} \left|a_{k,j}^\lambda\right|^2 n_{k,\uparrow}^\lambda \sum_{k',\lambda'} \left|a_{k',j}^{\lambda'}\right|^2 n_{k',\downarrow}^{\lambda'}|\{k_{j,\sigma}^\lambda\}\rangle$$

$$= \frac{U}{pL} \sum_{j=1}^p \sum_{\substack{k,\lambda \\ k_{j,\uparrow}^\lambda \text{ occupied}}} \left|a_{k,j}^\lambda\right|^2 \sum_{\substack{k',\lambda' \\ k_{j,\downarrow}'^{\lambda'} \text{ occupied}}} \left|a_{k',j}^{\lambda'}\right|^2. \tag{3.17}$$

Next we pass to the thermodynamic limit which leads to replacing sums by integrals. Due to (3.16), integrals and differentials over densities can be replaced by integrals in k-space. We work at a fixed particle number n, which implies

$$0 = dn = dn_\uparrow + dn_\downarrow \quad \Rightarrow \quad dn_\downarrow = -dn_\uparrow. \tag{3.18}$$

Now we concentrate on the situation where all bands $\lambda \leq \lambda_0$ are completely occupied with up spins and those with $\lambda > \lambda_0$ do not contain any up spins generalizing thus the reasoning of the previous section. The band λ_0' is partially occupied with down spins, those with $\lambda' < \lambda_0'$ are completely filled with down spins while those with $\lambda' > \lambda_0'$ do not contain any down spins. For a partially filled band ν denote finally the occupied states by $[k_l^\nu, k_u^\nu]$.

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Then we can generalize (3.10) to first order in U as follows [41]

$$E/L = u + v + \frac{\mu}{p}(n_\uparrow + n_\downarrow) - \frac{h}{2p}(n_\uparrow - n_\downarrow) \tag{3.19}$$

with

$$u = \frac{1}{2\pi p}\left\{\sum_{\lambda \leq \lambda_0}\int_{-\pi}^{\pi}dk\epsilon^\lambda(k) + \int_{k_l^{\lambda_0'}}^{k_u^{\lambda_0'}}dk'\epsilon^{\lambda_0'}(k') + \sum_{\lambda' < \lambda_0'}\int_{-\pi}^{\pi}dk'\epsilon^{\lambda'}(k')\right\} \tag{3.20}$$

and

$$v = \frac{U}{4\pi^2 p^3}\left\{\sum_{j=1}^{p}\sum_{\lambda \leq \lambda_0}\int_{-\pi}^{\pi}dk\left|a_{k,j}^\lambda\right|^2\left(\int_{k_l^{\lambda_0'}}^{k_u^{\lambda_0'}}dk'\left|a_{k',j}^{\lambda_0'}\right|^2 + \sum_{\lambda' < \lambda_0'}\int_{-\pi}^{\pi}dk'\left|a_{k',j}^{\lambda'}\right|^2\right)\right\}. \tag{3.21}$$

This yields for the lower boundary of the associated plateau

$$h_{c_1} = \epsilon^{\lambda_0}(k_u^{\lambda_0}) - \epsilon^{\lambda_0'}(k_u^{\lambda_0'}) + \mathcal{U}(\lambda_0) + \mathcal{O}\left(U^2\right) \tag{3.22}$$

with

$$\mathcal{U}(\nu) = \frac{U}{2\pi p^2}\left\{\sum_{j=1}^{p}\left|a_{k_u^\nu,j}^\nu\right|^2\left(\int_{k_l^{\lambda_0'}}^{k_u^{\lambda_0'}}dk'\left|a_{k',j}^{\lambda_0'}\right|^2 + \sum_{\lambda' < \lambda_0'}\int_{-\pi}^{\pi}dk'\left|a_{k',j}^{\lambda'}\right|^2\right)\right.$$
$$\left. - \sum_{j=1}^{p}\sum_{\lambda \leq \lambda_0}\int_{-\pi}^{\pi}dk\left|a_{k,j}^\lambda\right|^2\left|a_{k_u^{\lambda_0'},j}^{\lambda_0'}\right|^2\right\}. \tag{3.23}$$

For the corresponding upper boundary one finds

$$h_{c_2} = \epsilon^{\lambda_0+1}(k_u^{\lambda_0+1}) - \epsilon^{\lambda_0'}(k_u^{\lambda_0'}) + \mathcal{U}(\lambda_0 + 1) + \mathcal{O}\left(U^2\right). \tag{3.24}$$

Eqs. (3.22) and (3.24) imply that

$$h_{c_2} - h_{c_1} = \epsilon^{\lambda_0+1}(k_u^{\lambda_0+1}) - \epsilon^{\lambda_0}(k_u^{\lambda_0}) + UO_1 + \mathcal{O}(U^2) \tag{3.25}$$

with

$$O_1 = \frac{1}{2\pi p^2}\sum_{j=1}^{p}\left(\left|a_{k_u^{\lambda_0+1},j}^{\lambda_0+1}\right|^2 - \left|a_{k_u^{\lambda_0},j}^{\lambda_0}\right|^2\right)\left(\int_{k_l^{\lambda_0'}}^{k_u^{\lambda_0'}}dk'\left|a_{k',j}^{\lambda_0'}\right|^2 + \sum_{\lambda' < \lambda_0'}\int_{-\pi}^{\pi}dk'\left|a_{k',j}^{\lambda'}\right|^2\right). \tag{3.26}$$

The first-order contribution does in general not vanish (for $p > 2$). It can be estimated as

$$|O_1| \leq \frac{1}{2\pi p^2}\sum_{j=1}^{p}p\left(\int_{k_l^{\lambda_0'}}^{k_u^{\lambda_0'}}dk'\left|a_{k',j}^{\lambda_0'}\right|^2 + \sum_{\lambda' < \lambda_0'}\int_{-\pi}^{\pi}dk'\left|a_{k',j}^{\lambda'}\right|^2\right) = \frac{n_\downarrow}{p}, \tag{3.27}$$

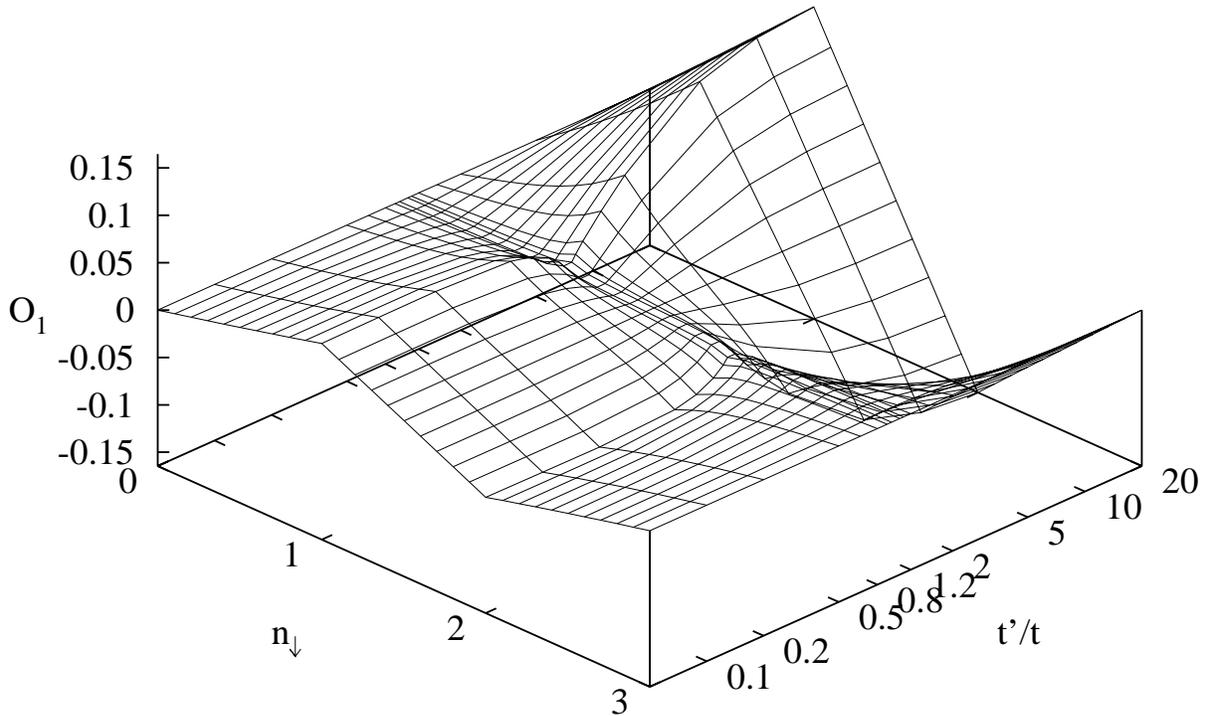which shows that in principle it can be of order one.

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FIG. 1.   Value of the first-order correction O_1 to the plateau width as given by (3.26) for $p = 3$ and $n_\uparrow = 2$.

In general, it is not difficult to evaluate the first-order contribution (3.26) to the plateau width numerically. We will illustrate this now for $p = 3$. First notice that, for the case $p = 3$, the contribution from the kinetic energy can be readily evaluated as

$$\epsilon^3(0) - \epsilon^2(0) = \epsilon^2(\pi) - \epsilon^1(\pi) = \left| \frac{\sqrt{8t^2 + t'^2} - 3t'}{2} \right| . \qquad (3.28)$$

Now we fix $n_\uparrow = 2$, *i.e.* the lowest two bands of up electrons are completely filled. Then one has that $k_u^3 = k_u^2 = 0$ in (3.26). Numerical diagonalization of (3.3) and evaluation of the remaining integrals in (3.26) then leads to Fig. 1. Note that in the conventions of the other sections (where $0 \leq n \leq 2$) this corresponds to the plateau with $m = 4/3 - n$. The numerical data satisfies $O_1 \to -O_1$ as $n_\downarrow \to 3 - n_\downarrow$. This implies in particular that the values of O_1 can be both positive and negative, corresponding to an enhancement or reduction of the plateau width, respectively. Furthermore, for $t \to 0$ and $n_\downarrow < 1$, the linear behaviour of (3.27) is reproduced, though with a coefficient which is $1/6$, *i.e.* by a factor of two smaller than in the estimate. The maximal values attained are $\pm 1/6$ for $n_\downarrow \to 1$ or 2, respectively and $t \to 0$. This shows that the doping-dependent plateaux should be stable features for $p = 3$ as well.

We conclude this section by noting that the calculations are also valid for the on-site p-merized energy. The free Hamiltonian H_0 to be diagonalized is modified, but the conclusions remain qualitatively unchanged.

IV. LANCZOS DIAGONALIZATION

Finally, we have performed Lanczos diagonalizations of the Hamiltonian (1.1) for $p = 2$ and $p = 3$ with constant $\mu(x) = \mu$ and periodic boundary conditions on finite lattices in order to further support the previous results. The particle numbers $n_\uparrow$ and $n_\downarrow$ have been used as quantum numbers and translational symmetry was exploited. Furthermore, reflection symmetry was exploited for $k = 0, \pi$ and spin inversion for $n_\uparrow = n_\downarrow$.

A. Groundstate phase diagrams

Computations have been performed mainly for one choice of parameters due to the large number of sectors for which the groundstate energy had to be found (for $p = 2$ and $L = 16$ of the order of 10^3 sectors). Keeping (2.16) in mind, we have chosen the parameters $U = 3t$ and $t' = 0.7t$ in order to look at a situation sufficiently different from the limiting cases discussed before, *i.e.* both intermediate (to strong, as compared to the band-width) on-site repulsion U and intermediate t'/t.

For the interpretation of our Lanczos results to be presented below, it is useful to remember the following consequences of particle-hole symmetry on a finite size lattice (see [22,42] and references therein): For L even, the groundstate phase-diagram of the Hubbard chain with periodic boundary conditions is symmetric under $\mu \mapsto -U - \mu$ (with our conventions), while for L odd the particle-hole transformation interchanges periodic and antiperiodic boundary conditions.

Our numerical results for the groundstate phase diagram are shown in Figs. 2 and 3 for $p = 2$ and $p = 3$, respectively. The polygons in the figures denote regions in the (μ,h)-plane where the groundstate has a fixed filling n and magnetization m at the given system size L (those values of m and n which are common to all investigated system sizes are indicated in the figures). The groundstate phase diagrams are symmetric under spin inversion ($m \to -m$ when $h \to -h$) and as mentioned before, for even L also under a particle-hole transformation ($n \to 2 - n$ when $\mu \to -U - \mu$). Therefore, for even L we show only the quadrant with $\mu \geq -U/2$, $h \geq 0$ and for odd L only the region with $h \geq 0$.

The schematic groundstate phase diagrams in [15] were in fact based on parts of these results and the reader may wish to use them as a guide to the diagrams at finite size.

We note that for the saturated case $n_\downarrow = 0$ (and by particle-hole symmetry also for $n_\uparrow = 1$), the Coulomb repulsion is not effective and the non-interacting result ($\epsilon^\pm(k)$ given by eq. (3.5) for $p = 2$) can be used to determine the transitions between different particle numbers. Complete agreement between this analytical computation and the corresponding numerical results in Figs. 2 and 3 is found. This also guides the interpretation of the finite-size data since it follows in particular that the completely gapped situations at saturation are those with $pn \in \mathbb{Z}$ in the thermodynamic limit. Such a guide is useful since the fermions behave differently for even and odd particle numbers thus yielding non-monotonic finite-size effects which can be still strong for the small systems sizes considered here. In the particular case of the gapped states with $pn \in \mathbb{Z}$ at $m = n$ (or $m = 2 - n$), the corresponding groundstate always has an even number of fermions when L/p is even while cases with an odd number occur when L/p is odd. This leads to vanishing finite-size effects for the
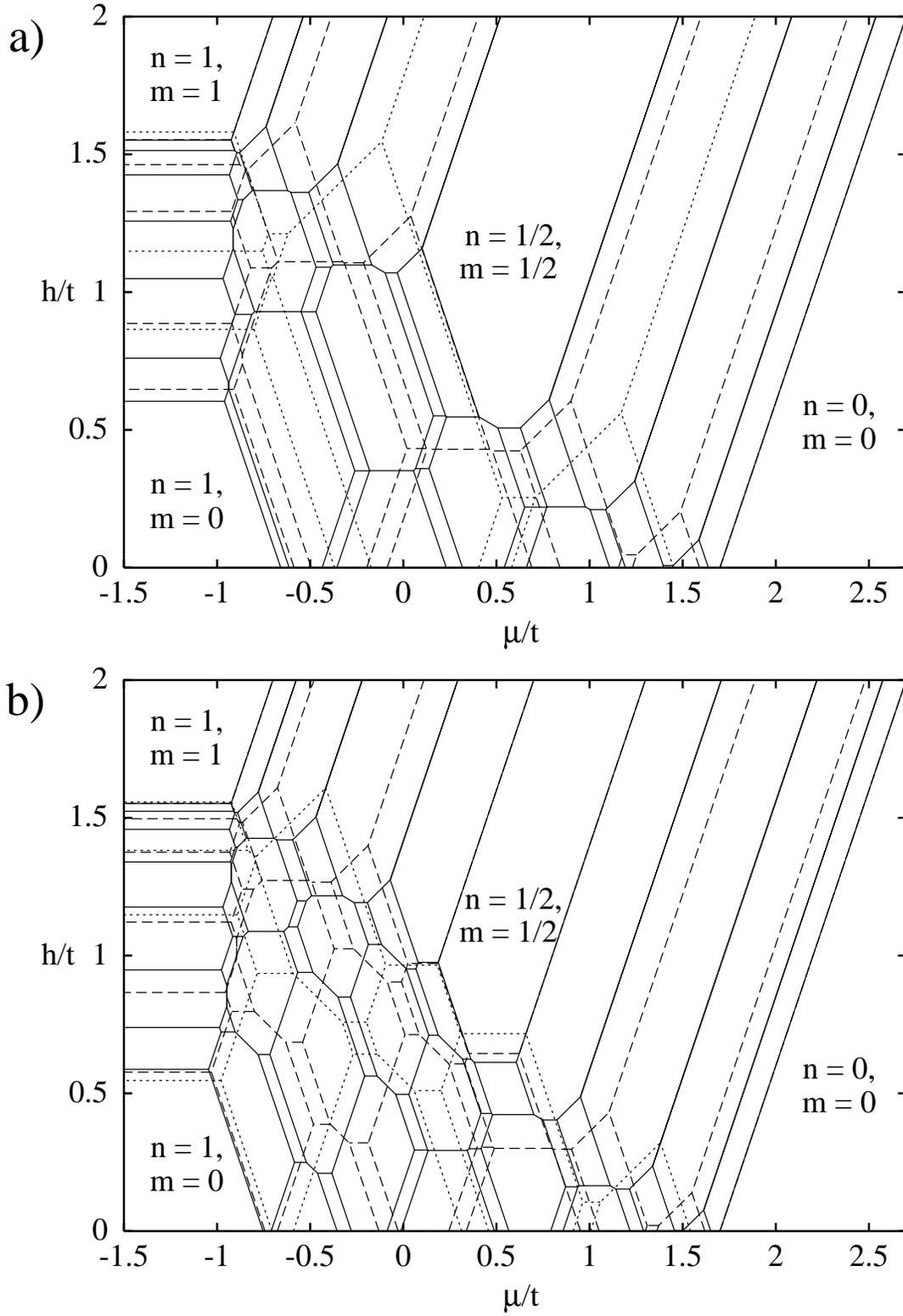
FIG. 2. Groundstate phase diagram of the dimerized chain ($p = 2$) with $U = 3t$, $t' = 0.7t$. In a) the lines are for $L = 6$ (dotted), $L = 10$ (dashed) and $L = 14$ (full) while in b) they are for $L = 8$ (dotted), $L = 12$ (dashed) and $L = 16$ (full).
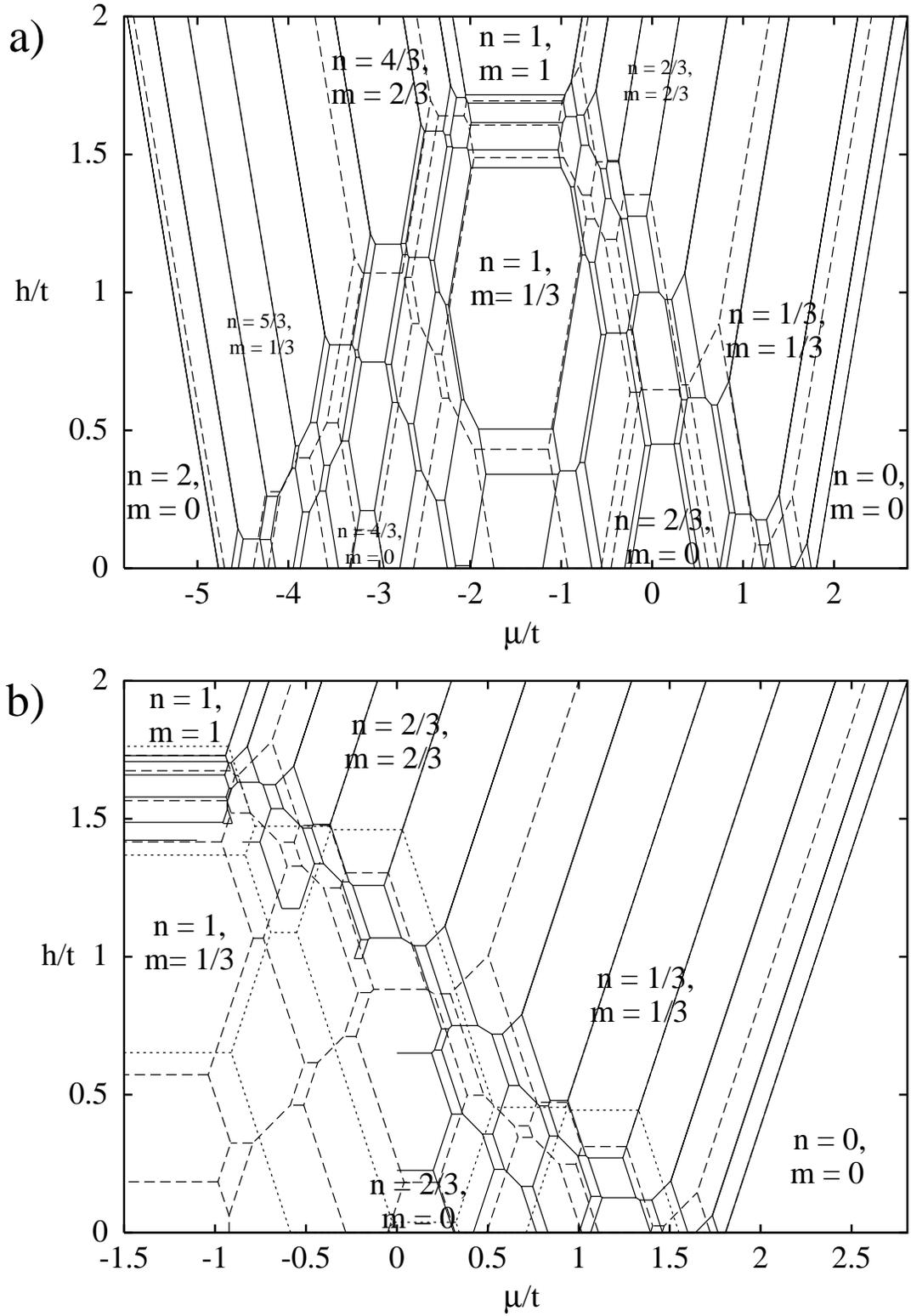
FIG. 3. Groundstate phase diagram of the trimerized chain ($p = 3$) with $U = 3t$, $t' = 0.7t$. In a) the lines are for $L = 9$ (dashed) and $L = 15$ (full) while in b) they are for $L = 6$ (dotted), $L = 12$ (dashed) and $L = 18$ (full). Note that the $L = 18$ data in b) is incomplete for $n > 2/3$ (*e.g.* only $m \geq 1/3$ for $n = 1$).

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transition lines in the former case, but not always in the latter. Since even and odd L/p behave differently, we show separate figures for the two cases.

For $p = 2$, one can quite clearly recognize the fully gapped situations at $(n, m) = (1, 0)$, $(1, 1)$, $(1/2, 1/2)$ and $(0, 0)$ from the finite-L data shown in Fig. 2. Also the charge gap at half filling $(n = 1)$ is obvious. The most interesting region is the doping-dependent plateau with $m = 1 - n$ which is a stable feature in Fig. 2a), but less clear in Fig. 2b). Still, in the latter case the region of stability of states with $m = 1 - n$ can be seen to increase with increasing system size, thus supporting the presence of a gap. Just the charge gap at quarter filling $(n = 1/2)$ is not distinct in this numerical data, but it is known to be small anyway for these parameters [30].

The case $p = 3$ is shown in Fig. 3. There is clear evidence for the expected fully gapped situations (the labeled regions in the figure) as well as the charge gap at half filling. There is also evidence for the charge gap at $n = 2/3$ and the equivalent case $n = 4/3$, just the charge gap at $n = 1/3, 5/3$ is again difficult to see. Also the expected doping-dependent magnetization plateau with $m = |n - 2/3|$ can be recognized in Fig. 3a). By particle-hole symmetry, the plateau with $m = |4/3 - n|$ must be present as well though it is more difficult to recognize. The finite-size behavior of its stability region in Fig. 3a) (and of both plateaux in the case of Fig. 3b)) can again be taken as an indication that it will indeed be present in the thermodynamic limit.

B. Correlation functions

Having provided also numerical evidence for the existence of doping-dependent magnetization plateaux, we now present a few numerical results for correlation functions at $p = 2$.

Is is technically useful to consider only objects which respect the decomposition of the Hilbert space according to symmetries of the Hamiltonian. We therefore define averages of an operator A_x as

$$\langle A_x \rangle = \begin{cases} \frac{1}{L} \langle \psi_0(k)| \sum_{x_0=1}^{L} A_{x_0} |\psi_0(k)\rangle & \text{for } k \neq 0, \pi, \\ \frac{1}{2L} \langle \psi_0(k)| \sum_{x_0=1}^{L} (A_{x_0} + A_{-x_0}) |\psi_0(k)\rangle & \text{for } k = 0, \pi, \end{cases} \tag{4.1}$$

where $|\psi_0(k)\rangle$ is the groundstate with momentum k. An additional advantage of this definition is that oscillations originating from the modulation of $t(x)$ are smoothed by taken averages of the up to $p = 2$ correlation functions at a given distance.

The connected correlation function of two quantities A and B is defined as

$$C_{A,B}(x) = \left\langle A^\dagger_{x_0+x} B_{x_0} \right\rangle - \left\langle A^\dagger_{x_0} \right\rangle \langle B_{x_0} \rangle . \tag{4.2}$$

Of particular interest are the diagonal components of the superconducting order parameter (2.40) since quasi-long-range order is expected for one of them.

Numerical results for correlation functions on an $L = 18$ system at the plateau with $m = 1 - n$ are shown in Fig. 4. Characteristic oscillations are observed in the density-density and electron-electron correlation functions. This and the finite system size make a detailed analysis of the asymptotics difficult. Nevertheless, one observes that correlation functions containing up electrons decay faster than the corresponding ones containing only
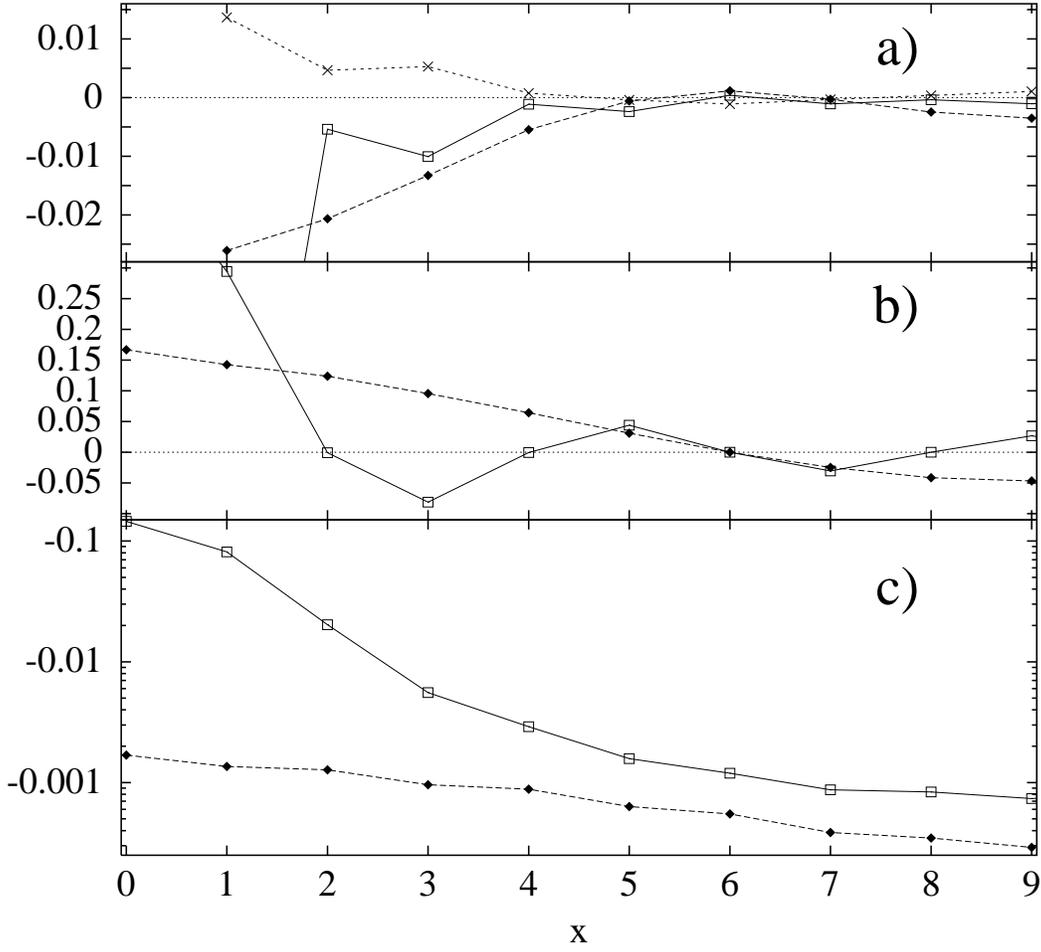
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FIG. 4. Correlation functions for the dimerized chain ($p = 2$) with $U = 3t$, $t' = 0.7t$ at $L = 18$, $n = 2/3$ and $m = 1/3$. Panel a) shows density-density correlations $C_{n_\alpha,n_\beta}(x)$, panel b) electron-electron correlations $C_{c_\alpha,c_\beta}(x)$ and panel c) superconducting correlations $C_{\Delta_{\alpha,\alpha},\Delta_{\beta,\beta}}(x)$. The symbols are for $\alpha = \beta = \uparrow$ (boxes), $\alpha = \beta = \downarrow$ (filled diamonds) and $\alpha = \uparrow$, $\beta = \downarrow$ ('×'); the lines are guides to the eye.

down electrons (the latter may still be smaller in absolute value due to a smaller overall prefactor). In fact, all correlation functions shown in Fig. 4 are very similar to those obtained in the non-interacting situation ($U = 0$) at the same L. We therefore interpret our results as support for exponential decay of all correlation functions containing $\uparrow$ operators and power-law decay for those containing only $\downarrow$ operators, as is expected according to the analysis of section II. In particular, these numerical results are compatible with quasi-long-range order in $\Delta_{\downarrow,\downarrow}$ on the $m = 1 - n$ plateau.

V. DISCUSSION AND CONCLUSIONS

We have shown that Hubbard chains with periodic hopping or on-site energy present a rich structure of magnetization plateaux. More precisely, for a periodicity p, we obtain the

conditions (1.2) for the appearance of the plateaux. If both conditions are simultaneously satisfied, both spin and charge degrees of freedom are massive. When the combination $pn \in \mathbb{Z}$ of these two conditions is satisfied, a charge gap opens irrespective of the value of m. Finally, if just one of the conditions (1.2) is satisfied, a magnetization plateau appears *if* the total filling n is kept fixed. This result has been shown first by means of bosonization techniques, valid in the regime where the differences in the modulation amplitudes δ in (2.15) and $\delta\mu$ in (2.20) are small and for arbitrary values of U. We have then shown that these results are confirmed by standard quantum mechanical arguments valid for small U and arbitrary p-merization strength and provided an expression for the width of the plateau to first order in U. We finally showed explicitly such plateaux in finite size systems by means of Lanczos diagonalization.

The combination of a gap which can be attributed to the spin degrees of freedom and gapless (charge) modes prompted us to look for superconducting correlations. Indeed, we found quasi-long-range order in one component of the superconducting order parameter in those cases where only one of the conditions (1.2) is satisfied.

In [15] it has been pointed out that the fully gapped situations can be most easily understood in the limit $t' = 0$ (the same argument applies also for $\delta\mu = \infty$). Then the chain effectively decomposes into clusters of p sites, whose magnetization curves are obviously staircase-like. The charge gap at $pn \in \mathbb{Z}$ can also be understood in the limit of $t' \ll t$ ($\delta\mu \gg \mu$), one just needs to generalize the mapping of a quarter-filled dimerized chain to an effective half-filled homogenous chain [30] to $m \neq 0$ and commensurate filling at general p. Finally, this mapping can also be adapted to provide a further complementary argument for the existence of the doping-dependent magnetization plateaux. Again, to first order in t', an effective Hamiltonian can be found in the regime of strong p-merization, *i.e.* in the limit $t' \ll t, U$ (resp. $\delta\mu \gg t, U$) for the case of modulation of the hopping amplitude (respectively of the on-site energy). When only one of the conditions (1.2) is satisfied, which amounts to a condition on the filling of spin-up or spin-down bands, this effective Hamiltonian acquires a gap in the spin sector thus leading to a doping-dependent magnetization plateau.

We would like to emphasize that such irrational plateaux are not present in systems where the doping is not fixed. Moreover, due to the remaining massless mode on such a plateau, the thermodynamical behavior of the system retains some particularities of a gapless system, such as a specific heat vanishing linearly as $T \to 0$. An important feature is that the value of the magnetization m on the plateaux at fixed n depends continuously on doping n. Analogous situations [16,17] encourage us to believe that this scenario is generic in doped systems. Doping could therefore be used as a tool to study experimentally irrational plateaux in systems whose half-filled parent compounds exhibit plateaux only at prohibitively high magnetic fields. A natural candidate are ladders systems [14] where doping can indeed be controlled. Theoretical results on doping-dependent magnetization plateaux in Hubbard ladders will be reported elsewhere [43].

There are also natural problems for further study in the case of modulated chains. For example, the large-U limit of the Hubbard model leads to the $t - J$ model. As a check of the generality of our results, one could therefore investigate the $t - J$ model which at half filling would then be exactly the situation studied in [6]. Due to the reduced Hilbert space, the $t - J$ model would be particularly well suited for further numerical checks. Another problem to be addressed is the universality class of the transitions associated to the corners

of a plateau. In the case of the BA solvable model [16], it was found that the presence of a massless mode on a doping-dependent plateau may modify the universality class of part of these transitions – a fact which would be interesting to investigate also in the present model.

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APPENDIX A: CONVENTIONS

In this short appendix, we define our conventions and notations. The continuum fermion operators read

$$\psi_\alpha(x) = e^{-ik_{F,\alpha}x}\psi_{R,\alpha}(x) + e^{ik_{F,\alpha}x}\psi_{L,\alpha}(x) \ , \tag{A1}$$

$$\psi_\alpha^\dagger(x) = e^{ik_{F,\alpha}x}\psi_{R,\alpha}^\dagger(x) + e^{-ik_{F,\alpha}x}\psi_{L,\alpha}^\dagger(x) \ . \tag{A2}$$

Using standard bosonization rules we have:

$$\psi_{R,\alpha}(x) = \frac{1}{\sqrt{2\pi a}}e^{i\sqrt{4\pi}\phi_{R,\alpha}(x)} + \dots \ , \tag{A3}$$

$$\psi_{L,\alpha}(x) = \frac{1}{\sqrt{2\pi a}}e^{-i\sqrt{4\pi}\phi_{L,\alpha}(x)} + \dots \ , \tag{A4}$$

where a is the lattice constant and $\phi_{R,L,\alpha}$ are the chiral components of two real bosonic fields:

$$\phi_\alpha(x) = \phi_{R,\alpha}(x) + \phi_{L,\alpha}(x) \ , \tag{A5}$$

whose dual fields are defined by

$$\theta_\alpha(x) = \phi_{R,\alpha}(x) - \phi_{L,\alpha}(x) \ . \tag{A6}$$

The dots in eqs. (A3) and (A4) stand for higher order terms, due to the curvature of the dispersion relation, which are discussed in the next appendix. The up and down Fermi momenta are related to filling and magnetization:

$$k_+ = k_{F,\uparrow} + k_{F,\downarrow} = \pi n \ ; \qquad k_- = k_{F,\uparrow} - k_{F,\downarrow} = \pi m \ , \tag{A7}$$

where

$$n = \frac{1}{L}\langle\sum_{x,\alpha} n_{x,\alpha}\rangle \ , \qquad m = \frac{2}{L}\langle\sum_{x} S_x^z\rangle = \frac{1}{L}\langle\sum_{x,\alpha} n_{x,\uparrow} - n_{x,\downarrow}\rangle \ , \tag{A8}$$

$n_{x,\alpha} = c_{x,\alpha}^\dagger c_{x,\alpha}$ and L is the number of sites. Note that our definition of m (which is the one used for the XXZ chains in [4]) differs by a factor of 2 from the one of Frahm and Korepin [23].

APPENDIX B: FERMION FIELD OPERATOR

In this appendix we discuss the bosonization of the fermion operator in the Hubbard model in a magnetic field starting from the exact BA solution. According to Frahm and Korepin [23], the long-distance asymptotics of zero-temperature correlation functions of physical fields is in general a sum of terms of the form

$$\frac{\exp(-i2D_c k_{F\uparrow} x) \ \exp[-i(D_c + D_s)k_{F\downarrow}x]}{(x - iv_c\tau)^{2\Delta_c^+}(x + iv_c\tau)^{2\Delta_c^-}(x - iv_s\tau)^{2\Delta_s^+}(x + iv_s\tau)^{2\Delta_s^-}} \ , \tag{B1}$$

where the scaling dimensions $\Delta_{c,s}^\pm$ are given by:

$$2\Delta_c^\pm = \left(Z_{cc}D_c + Z_{sc}D_s \pm \frac{Z_{ss}\Delta N_c - Z_{cs}\Delta N_s}{2\det Z}\right)^2 + N_c^\pm \ , \tag{B2}$$

$$2\Delta_s^\pm = \left(Z_{cs}D_c + Z_{ss}D_s \pm \frac{Z_{cc}\Delta N_s - Z_{sc}\Delta N_c}{2\det Z}\right)^2 + N_s^\pm \ . \tag{B3}$$

$\Delta N_{c,s}, D_{c,s}, N_{c,s}^\pm$ are the quantum numbers characterizing the low energy excitations. ΔN_c and ΔN_s are integers denoting the number of electrons and down spins with respect to the groundstate and are fixed by the correlator under consideration. The summation runs over all integers or half integers $D_{c,s}$ (depending on the parity of ΔN_c, ΔN_s) and on positive integers $N_c^\pm$, $N_s^\pm$.

By analysing the leading contributions to the fermion two-point correlator, one can write down, after some algebra, the bosonized fermion operator:

$$\begin{aligned}
\psi_\downarrow = \ & e^{-ik_{F\downarrow}x} \ e^{i\sqrt{4\pi}\phi_{R\downarrow}(x)} \ (r_1 + r_2 \ e^{-i2k_{F\uparrow}x} \ e^{i\sqrt{4\pi}\phi_\uparrow} + r_3 \ e^{i2k_{F\uparrow}x} \ e^{-i\sqrt{4\pi}\phi_\uparrow} \\
& \qquad\qquad +r_4 \ e^{-i2k_{F\downarrow}x} \ e^{i\sqrt{4\pi}\phi_\downarrow} + r_5 \ e^{-i2k_+x} \ e^{i\sqrt{4\pi}(\phi_\uparrow + \phi_\downarrow)} + \ldots) \\
& + e^{ik_{F\downarrow}x} \ e^{-i\sqrt{4\pi}\phi_{L\downarrow}(x)}(l_1 + l_2 \ e^{i2k_{F\uparrow}x} \ e^{-i\sqrt{4\pi}\phi_\uparrow} + l_3 \ e^{-i2k_{F\uparrow}x} \ e^{i\sqrt{4\pi}\phi_\uparrow} \\
& \qquad\qquad +l_4 \ e^{i2k_{F\downarrow}x} \ e^{-i\sqrt{4\pi}\phi_\downarrow} + l_5 \ e^{i2k_+x} \ e^{-i\sqrt{4\pi}(\phi_\uparrow + \phi_\downarrow)} + \ldots)
\end{aligned} \tag{B4}$$

where r_i, l_i are unknown numerical constants. Notice that at $U = 0$, $h = 0$ all these constants vanish except $r_1 = l_1 = 1/\sqrt{2\pi a}$. At $h = 0$, the scaling dimensions of the different contributions in eq. (B4) are known from BA for arbitrary repulsion U and density $n \neq 1$. It follows that it is sufficient to retain only the following terms

$$\begin{aligned}
\psi_\downarrow = \ & e^{-ik_{F\downarrow}x} \ e^{i\sqrt{4\pi}\phi_{R\downarrow}(x)}(r_1 + r_2 \ e^{-i2k_{F\uparrow}x} \ e^{i\sqrt{4\pi}\phi_\uparrow} + r_3 \ e^{i2k_{F\uparrow}x} \ e^{-i\sqrt{4\pi}\phi_\uparrow} + \ldots) \\
& + e^{ik_{F\downarrow}x} \ e^{-i\sqrt{4\pi}\phi_{L\downarrow}(x)}(l_1 + l_2 \ e^{i2k_{F\uparrow}x} \ e^{-i\sqrt{4\pi}\phi_\uparrow} + l_3 \ e^{-i2k_{F\uparrow}x} \ e^{i\sqrt{4\pi}\phi_\uparrow} + \ldots)
\end{aligned} \tag{B5}$$

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The expression for $\psi_\uparrow$ can be easily obtained by exchanging $\downarrow$ and $\uparrow$, with the numerical constants generically different.

Using this expression for $\psi_\downarrow$ and $\psi_\uparrow$, one obtains:

$$\psi_\downarrow^\dagger \psi_\downarrow = const\ \partial_x \phi_{R\downarrow} + const\ \partial_x \phi_{L\downarrow} + 2r_1 l_1\ \sin(2k_{F\downarrow}x - \sqrt{4\pi}\phi_\downarrow)$$
$$+2(r_1 l_2 + r_2 l_1)\ \sin[2k_+ x - \sqrt{4\pi}(\phi_\uparrow + \phi_\downarrow)]$$
$$-2(r_1 l_3 + r_3 l_1)\ \sin[2k_- x - \sqrt{4\pi}(\phi_\uparrow - \phi_\downarrow)] + \ldots \tag{B6}$$

and

$$\psi_\uparrow^\dagger \psi_\uparrow = const\ \partial_x \phi_{R\uparrow} + const\ \partial_x \phi_{L\uparrow} + 2r_1' l_1'\ \sin(2k_{F\uparrow}x - \sqrt{4\pi}\phi_\uparrow)$$
$$+2(r_1' l_2' + r_2' l_1')\ \sin[2k_+ x - \sqrt{4\pi}(\phi_\uparrow + \phi_\downarrow)]$$
$$+2(r_1' l_3' + r_3' l_1')\ \sin[2k_- x - \sqrt{4\pi}(\phi_\uparrow - \phi_\downarrow)] + \ldots \tag{B7}$$

where we assumed the constants r, l to be real. Otherwise, the only modification would consist in shifts of the arguments of the sines or cosines by unknown constant phases.

Now, assuming the constants to be equal for up and down fields, and adding eqs. (B6) and (B7) we obtain for the bosonized density operator

$$\rho = \psi_\uparrow^\dagger \psi_\uparrow + \psi_\downarrow^\dagger \psi_\downarrow = const\ \partial_x(\phi_\uparrow + \phi_\downarrow) + 4r_1 l_1\ \sin[k_+ x - \sqrt{\pi}(\phi_\uparrow + \phi_\downarrow)]$$
$$\times \cos[k_- x - \sqrt{\pi}(\phi_\uparrow - \phi_\downarrow)] + 4(r_1 l_2 + r_2 l_1)\ \sin[2k_+ x - \sqrt{4\pi}(\phi_\uparrow + \phi_\downarrow)] + \ldots \tag{B8}$$

Substituting finally (2.9), one obtains (2.14).

Similarly, the difference of eqs. (B6) and (B7) yields the S^z operator:

$$2S^z = \psi_\uparrow^\dagger \psi_\uparrow - \psi_\downarrow^\dagger \psi_\downarrow = const\ \partial_x(\phi_\uparrow - \phi_\downarrow) + 4r_1 l_1\ \cos[k_+ x - \sqrt{\pi}(\phi_\uparrow + \phi_\downarrow)]$$
$$\times \sin[k_- x - \sqrt{\pi}(\phi_\uparrow - \phi_\downarrow)] - 4(r_1 l_3 + r_3 l_1)\ \sin[2k_- x - \sqrt{4\pi}(\phi_\uparrow - \phi_\downarrow)] + \ldots \tag{B9}$$

Notice the last term in the S^z operator. In the usual treatments, (see for example [26]), this term does not appear. As it is obvious from eq. (B9), this term would be absent if we retain only the first two terms in eq. (B5) or if $r_1 = l_1$ and $r_3 = -l_3$.

The assumptions on the constants r_i, l_i, r_i', l_i' to be real and equal for up and down fields are supported by operator product expansion computations of the original free fermion operator with the perturbing Umklapp operator of the Hubbard Hamiltonian,

$$\cos[2k_+ x - \sqrt{4\pi}(\phi_\uparrow + \phi_\downarrow)]\ . \tag{B10}$$

These computations also show that, at lowest order, the constants r_2, r_3, l_2, l_3 are linear in U.

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