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Doping-dependent magnetization plateaux in p -merized Hubbard chains*

D.C. Cabra¹, A. De Martino², A. Honecker^{3†‡}, P. Pujol² and P. Simon⁴

¹*Departamento de Física, Universidad Nacional de la Plata, C.C. 67, (1900) La Plata, Argentina.
Facultad de Ingeniería, Universidad Nacional de Lomas de Zamora, Cno. de Cintura y Juan
XXIII, (1832) Lomas de Zamora, Argentina.*

²*Laboratoire de Physique[§] Groupe de Physique Théorique ENS Lyon, 46 Allée d'Italie, 69364
Lyon Cédex 07, France.*

³*Institut für Theoretische Physik, ETH-Hönggerberg, 8093 Zürich, Switzerland.*

⁴*International School for Advanced Studies, Via Beirut 2-4, 34014 Trieste, Italy.
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Abstract

We study zero-temperature Hubbard chains with periodically modulated hopping at arbitrary filling n and magnetization m . We show that the magnetization curves have plateaux at certain values of m which depend on the periodicity p and the filling. At commensurate filling n a charge gap opens and then magnetization plateaux correspond to fully gapped situations. However, plateaux also arise in the magnetization curves at fixed n between the commensurate values and then the plateau-value of m depends continuously on n and can thus also become irrational. In particular for the case of dimerized hopping ($p = 2$) and fixed doping we find that a plateau appears at $m = 1 - n$. In this case, there is still a gapless mode on the plateau leading to thermodynamic behavior which is different from a completely gapped situation.

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†A Feodor-Lynen fellow of the Alexander von Humboldt-foundation.

‡Present address: Institut für Theoretische Physik, TU Braunschweig, 38106 Braunschweig, Germany.

§URA 1325 du CNRS associée à l'Ecole Normale Supérieure de Lyon.

I. INTRODUCTION AND SUMMARY OF RESULTS

Macroscopic quantum phenomena in strongly correlated electron systems in low dimensions are presently the subject of intense research. In particular, plateaux in magnetization curves of quantum magnets have recently received much attention, a central observation being that the plateaux occur at (typically simple) *rational* fractions of the saturation magnetization. In one dimension, this is by now rather well theoretically understood in terms of a quantization condition that involves the volume of a translationally invariant unit cell (see e.g. [1–4]). Various materials exhibiting plateaux have also been studied during the past few years, including e.g. a new candidate for a frustrated trimerized chain material [5]. One of the clearest examples is given by the low-temperature magnetization process of NH_4CuCl_3 [6] where one observes plateaux with $1/4$ and $3/4$ of the saturation magnetization thus demonstrating rationality even if it is theoretically still unclear why precisely those two numbers are observed in NH_4CuCl_3 .

The purpose of the present letter is to start a systematic investigation of the effect of doping on the quantization condition for the appearance of magnetization plateaux. We will show with examples that plateaux can appear in doped systems at magnetization values which depend continuously on the doping and are thus in general *irrational*. This observation itself is not entirely new, but we believe our physical interpretation in terms of one class of excitations (say the up electrons) being pinned at commensurate filling while the filling of a different class of excitations (the down electrons) remains adjustable to be new. This interpretation also suggests that doping-dependent magnetization plateaux are probably a generic phenomenon. One of the known cases is the one-dimensional Kondo lattice model [7] where unpaired spins behave ferromagnetically thus giving rise to a spontaneous magnetization of a value controlled by doping. The other example is an integrable spin- S generalization of the $t - J$ chain doped with $(S - 1/2)$ carriers [8] where, however, the appearance of plateaux is restricted to large magnetization values.

As a first step towards a general understanding we study the effect of both a magnetic field and a periodic modulation of the hopping amplitude (p -merization) on a *doped* one-band Hubbard chain. One simple motivation is that for pure spin systems (corresponding to a half-filled Hubbard model) in a magnetic field, p -merized Heisenberg chains have turned out to be among the simplest examples [4]. In addition, structural modulations can give rise to dimerized coupling constants e.g. in chains and ladders [9], the organic (super)conductors [10] (some of which come naturally at quarter filling) and the ferroelectric perovskites [11].

The one-band Hubbard model is not only used to describe realistic situations, but at least in one dimension it is also a useful model for technical reasons. For example, the Hubbard chain is exactly solvable by means of the Bethe Ansatz (BA) [12]. This can be used as an input to a bosonization analysis [13–15] in order to study generalizations of this model (see e.g. [16]).

In this letter we show that there are several different phases in the μ - h plane (see Fig. 1 for a schematic illustration of the cases $p = 2$ and $p = 3$; abbreviations refer to the corresponding regions of this figure):

i) If both quantization conditions¹

$$\frac{p}{2}(n \pm m) \in \mathbb{Z} \quad (1)$$

are satisfied, both spin and charge excitations are gapful and hence all correlators decay exponentially at large distances (regions labeled by fixed n and m in Fig. 1). In this case, we find plateaux in the magnetization curves since the presence of a spin gap is equivalent to the appearance of a plateau.

ii) A charge gap ('CG') can open if the combination $pn \in \mathbb{Z}$ of the conditions (1) is satisfied. This includes the well-known charge gap at half filling ($n = 1$) and also the charge gap in the quarter-filled ($n = 1/2$) dimerized Hubbard chain ($p = 2$) [17].

iii) If only one of the conditions (1) is fulfilled (solutions are indicated in the corresponding regions of Fig. 1) and in addition doping n is kept fixed, a magnetization plateau opens, *but one mode remains gapless* (similar observations have been made in other systems [3,8,18,19]). In contrast to the gapful magnetic behavior, charge transport remains metallic in this phase.

The existence of these plateau phases is the main result of the present letter. A particularly appealing aspect of the plateaux predicted here is that they can appear at low magnetization (and thus at small magnetic fields) if the doping is chosen suitably.

In the remaining cases, both spin and charge sectors are massless, leading to a Luttinger liquid ('LL').

II. HAMILTONIAN AND STRONG-COUPPLING LIMIT

To be concrete, we study the following model Hamiltonian

$$\begin{aligned} H = & - \sum_{x=1}^L t(x) \sum_{\sigma} \left(c_{x+1,\sigma}^{\dagger} c_{x,\sigma} + c_{x,\sigma}^{\dagger} c_{x+1,\sigma} \right) \\ & + U \sum_{x=1}^L n_{x,\uparrow} n_{x,\downarrow} + \mu \sum_{x=1}^L (n_{x,\uparrow} + n_{x,\downarrow}) \\ & - \frac{h}{2} \sum_{x=1}^L (n_{x,\uparrow} - n_{x,\downarrow}) \end{aligned} \quad (2)$$

where $t(x) = t$ if $x \neq mp$ and $t(mp) = t' = t + \delta$. Here, $c^{\dagger}$ and c are electron creation and annihilation operators, $n_{x,\sigma} = c_{x,\sigma}^{\dagger} c_{x,\sigma}$ the number operator and $\sigma = \uparrow, \downarrow$. μ is the chemical potential and h is a magnetic field.

First we consider the limit $t' = 0$. Then the chain (2) decouples into clusters of p sites and one can use simple arguments in the spirit of [3,4]: The number of up and down electrons

¹ n and m are normalized such that $0 \leq n \leq 2$ and $|m| \leq 1$.

on a p -site cluster must both be integer which is equivalent to imposing both conditions (1). All these states are clearly fully gapped at $t' = 0$. Thus, they will remain fully gapped if one switches on a small perturbation $t' > 0$, only the transitions between these fully gapped states will soften. In fact, we will argue soon that these fully gapped states survive even until $t' = t$.

III. BOSONIZATION

Now we turn to a bosonization analysis starting with $h = 0$ (for a related recent study of a dimerized Hubbard chain see [20]). For $t' = t$ ($\delta = 0$) and $n \neq 1$, the Hubbard chain (2) can be represented by two bosonic fields with Hamiltonian [13]

$$\sum_{i=c,s} \frac{v_i}{2} \int dx \left[(\partial_x \phi_i)^2 + (\partial_x \theta_i)^2 \right], \quad (3)$$

where $\phi = \phi_R + \phi_L$ and $\theta = \phi_R - \phi_L$. The spin and charge fields are given by $\phi_s = \frac{1}{\sqrt{2}}(\phi_{\uparrow} - \phi_{\downarrow})$ and $\phi_c = \frac{1}{\xi}(\phi_{\uparrow} + \phi_{\downarrow})$, where $\phi_{\uparrow,\downarrow}$ are compactified with periodicity $\phi_{\uparrow,\downarrow} \rightarrow \phi_{\uparrow,\downarrow} + \sqrt{\pi} \mathbb{Z}$. The parameter ξ and the Fermi velocities v_i can be obtained exactly from the BA solution of the model in terms of U and μ .

If we now turn on a non-zero but small δ , one can show using the continuum representation of creation and annihilation operators in terms of the bosonic fields that the most relevant perturbations to the free Hamiltonian are given by

$$O_{pert} = \lambda \sin[k_+/2 + pk_+x - \sqrt{\pi}\xi\phi_c] \times \cos[\sqrt{2\pi}\phi_s] + \lambda' \cos(k_+ + 2pk_+x - \sqrt{4\pi}\xi\phi_c), \quad (4)$$

where λ and λ' are proportional to δ and $k_+ = k_{F,\uparrow} + k_{F,\downarrow} = \pi n$. We can now study the values of n for which these operators are commensurate. In this way, if $pn \in \mathbb{Z}$ the λ' term appears as a relevant perturbation, opening a charge gap. If we restrict further to $pn/2 \in \mathbb{Z}$ the λ term is present as well and opens also a spin gap.

We consider now the more complicated case of non-zero magnetization. The Hubbard chain in the presence of a magnetic field is also integrable [13,14]. The large-scale behavior of the system is given by a two-field Hamiltonian like (3), but now the effective charge and spin fields are given by [15]

$$\begin{pmatrix} \phi_c \\ \phi_s \end{pmatrix} = \frac{1}{\det Z} \begin{pmatrix} Z_{ss} & Z_{ss} - Z_{cs} \\ Z_{sc} & Z_{sc} - Z_{cc} \end{pmatrix} \begin{pmatrix} \phi_{\uparrow} \\ \phi_{\downarrow} \end{pmatrix}, \quad (5)$$

where Z is the so-called charge matrix given in [13], whose entries can be obtained exactly from the BA solution in terms of U , μ and h . These quantities determine the scaling dimensions of the vertex operators.

For small δ the perturbing operators read

$$\begin{aligned} O_{pert} = & \lambda \sin[k_+/2 + pk_+x - \sqrt{\pi}(Z_{cc}\phi_c - Z_{cs}\phi_s)] \\ & \times \cos[k_-/2 + pk_-x \\ & \quad - \sqrt{\pi}((Z_{cc} - 2Z_{sc})\phi_c - (Z_{cs} - 2Z_{ss})\phi_s)] \\ & + \lambda' \cos(k_+ + 2pk_+x - \sqrt{4\pi}(Z_{cc}\phi_c - Z_{cs}\phi_s)), \end{aligned} \quad (6)$$

where now $k_- = k_{F,\uparrow} - k_{F,\downarrow} = \pi m$. If all the operators are commensurate both degrees of freedom are massive since the perturbing operators are relevant. We thus have a magnetization plateau with a charge gap. This is achieved when the two conditions (1) are simultaneously satisfied, which generalizes the result for p -merized spin chains [4] to $n \neq 1$.

When only one of these conditions is satisfied, say $p(n+m)/2 \in \mathbb{Z}$, the Hamiltonian can be written as

$$H = \int dx \frac{v_{\uparrow}}{2} [(\partial_x \phi_{\uparrow})^2 + (\partial_x \theta_{\uparrow})^2] + \frac{v_{\downarrow}}{2} [(\partial_x \phi_{\downarrow})^2 + (\partial_x \theta_{\downarrow})^2] + \lambda \sin 2\sqrt{\pi} \phi_{\uparrow}. \quad (7)$$

Terms mixing derivatives of the up and down fields, which come from the U interaction, can be shown to be irrelevant using a treatment similar to Ref. [16]. One can integrate out the massive field $\phi_{\uparrow}$ and obtain an effective large scale Hamiltonian for $\phi_{\downarrow}$, with an effective Fermi velocity and Luttinger parameter K . This field is apparently massless but constrained to be in a particular topological sector if one imposes fixed filling (which seems to be natural from the experimental point of view). In a system of finite size L , this constraint takes the form $Ln = \frac{1}{\sqrt{\pi}}(\phi_{\uparrow} + \phi_{\downarrow})|_0^L$ and allowing only small energy fluctuations locks the quantity $Q = \frac{1}{\sqrt{\pi}}\phi_{\downarrow}|_0^L$ to be also constant (see [21] for more details).

If this constraint were not imposed, Q would vary and the susceptibility would then have the standard form $\chi = K/(2\pi v)$. On the other hand, if we impose $Q_0 = L(n-m)/2$, we obtain $\chi = \frac{1}{\beta L} (\langle Q^2 \rangle - \langle Q \rangle^2) = 0$, indicating the presence of a magnetization plateau. Since the local part of the down sector in (7) remains massless, local correlation functions of the spin-down field decay algebraically and one can also show that the low-temperature specific heat is linear in the temperature. This situation is interesting since it combines a massless behavior with a magnetization plateau at $p(n+m)/2 \in \mathbb{Z}$ for arbitrary values of n .

IV. SMALL ON-SITE REPULSION

A complementary derivation of these doping-dependent magnetization plateaux (at fixed n) is given by the following discussion of the limit of small interaction U .

For the non-interacting case $U = 0$, the Hamiltonian (2) can be diagonalized easily and is found to have p bands $\varepsilon^{\lambda}(k)$. This is illustrated in Fig. 2 for the case $p = 3$ (the band structure for $p = 2$ is shown e.g. in Fig. 2 of [17]). In the presence of a magnetic field $h \neq 0$, the up and down electrons are subject to different chemical potentials ($\mu - h/2$ and $\mu + h/2$, respectively). A doping-dependent magnetization plateau then corresponds to a situation where 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. Imposing the constraint of fixed filling n then requires a finite change in magnetic field in order to move the chemical potential for the up electrons into one of the bands next to the gap, leading to a plateau in the magnetization curve. However, the filling of the down electrons remains adjustable and one obtains a doping-dependent value of the magnetization on the plateau.

A finite on-site repulsion $U > 0$ leads to corrections to this non-interacting picture which can be treated to first order in U using standard quantum mechanical perturbation theory. We are interested in a situation where one band for say the up electrons is either

completely filled or empty. It is therefore sufficient to look at diagonal matrix elements of $H_I = U \sum_{x=1}^L n_{x,\uparrow} n_{x,\downarrow}$ in the basis diagonalizing (2) with $U = 0$, *i.e.* scattering processes (as would be present for half-filled bands) are absent in the present situation. This then leads to a simple shift of the critical fields $h_{\pm}$ for a doping dependent magnetization plateau. In particular, the plateau is non-vanishing also in the presence of interaction at least if U is small enough.

For $p = 2$ this computation can be carried out explicitly (details will be presented in [21]). One finds that the matrix elements of H_I are of a mean-field type, *i.e.* simple products of the filling of up and down electrons. The final result for the lower and upper boundaries of the $m = 1 - n$ plateau for $p = 2$ is given by

$$h_{\pm} = \pm|t - t'| - \sqrt{t^2 + t'^2 + 2tt' \cos((2n - 1)\pi)} + (n - 1)U + \mathcal{O}(U^2). \quad (8)$$

This leads to a plateau width $h_+ - h_- = 2|t - t'| + \mathcal{O}(U^2)$ which is independent of U at first order in U . The latter is a direct consequence of the mean-field form of the matrix elements of H_I and is specific to $p = 2$.

We have also performed Lanczos diagonalizations of the Hamiltonian (2) for $p = 2$ and $p = 3$ at $U = 3t$, $t' = 0.7t$ to confirm the overall picture. Here we just mention that the schematic Figs. 1 are in fact based on these numerical results, but otherwise postpone a detailed presentation to [21].

V. CONCLUSION

To conclude, we have shown that there are two types of situations with plateaux in the magnetization curve of a p -merized Hubbard chain at arbitrary filling n : One where both pn and pm are integers and the complete excitation spectrum is gapful and a second one where only one of the conditions (1) is satisfied and part of the excitations remain gapless. If one works at fixed filling n , the latter leads to doping-dependent magnetization plateaux.

Although we have studied p -merized Hubbard chains, doping-dependent magnetization plateaux should exist in more general situations and indeed, similar phenomena have been theoretically observed in other systems [7,8].

From the experimental point of view, the most direct check would be a magnetization experiment on a p -merized chain with controlled doping. As we have mentioned earlier, materials realizing dimerized and trimerized chains do exist (also at non-trivial fillings). However, doping can be controlled better in a different class of quasi one-dimensional materials, namely the high- T_c related realizations of N -leg ladders [9]. In these materials, a doping dependence could be particularly intriguing since it could be used to push magnetization plateaux into experimentally accessible field regions despite the large coupling constants. We therefore regard the magnetization process of doped N -leg Hubbard ladders as an interesting field for further research.

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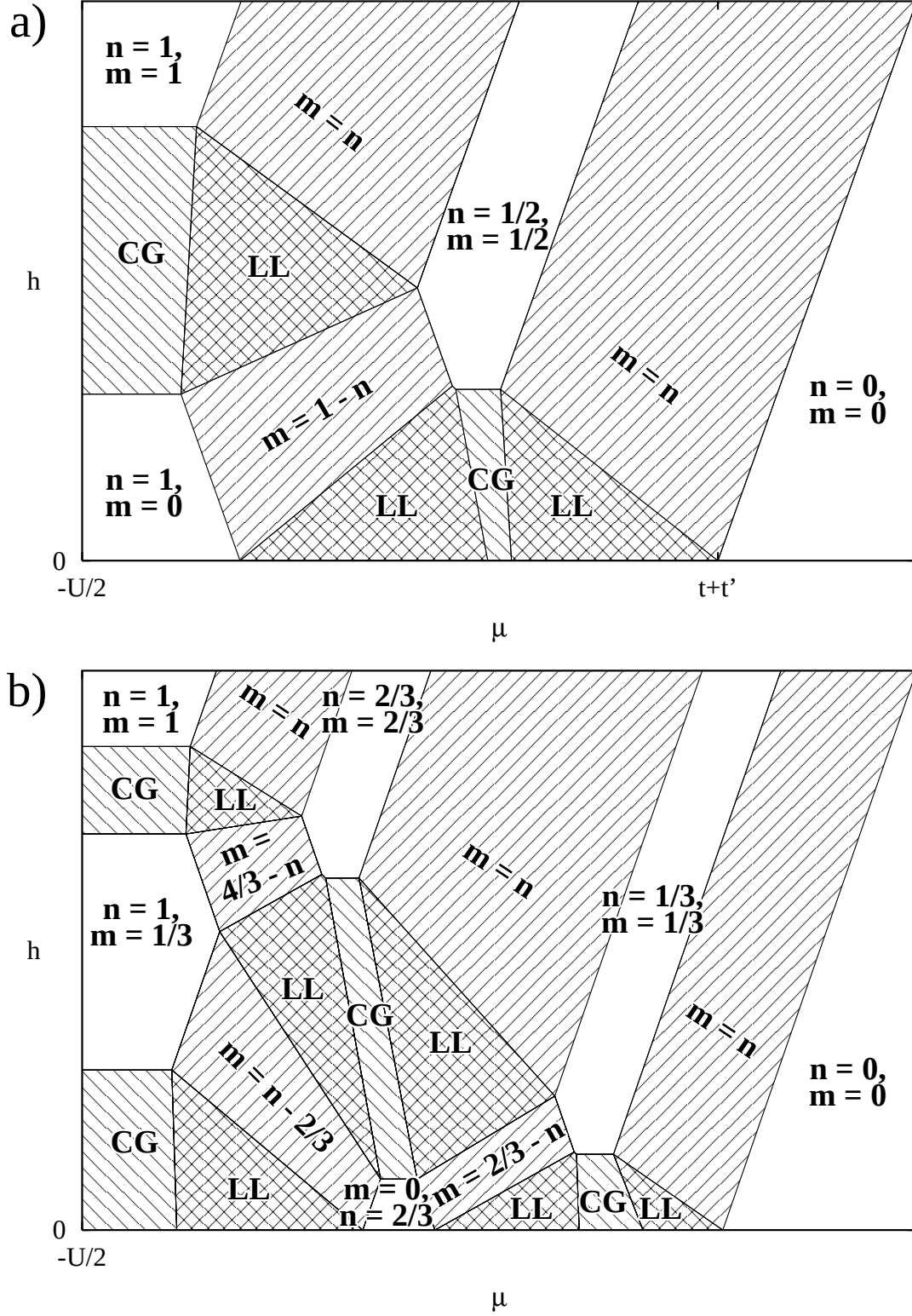


FIG. 1. Schematic groundstate phase diagram of a) the dimerized Hubbard chain ($p = 2$) and b) the trimerized chain ($p = 3$). For explanations compare the text.

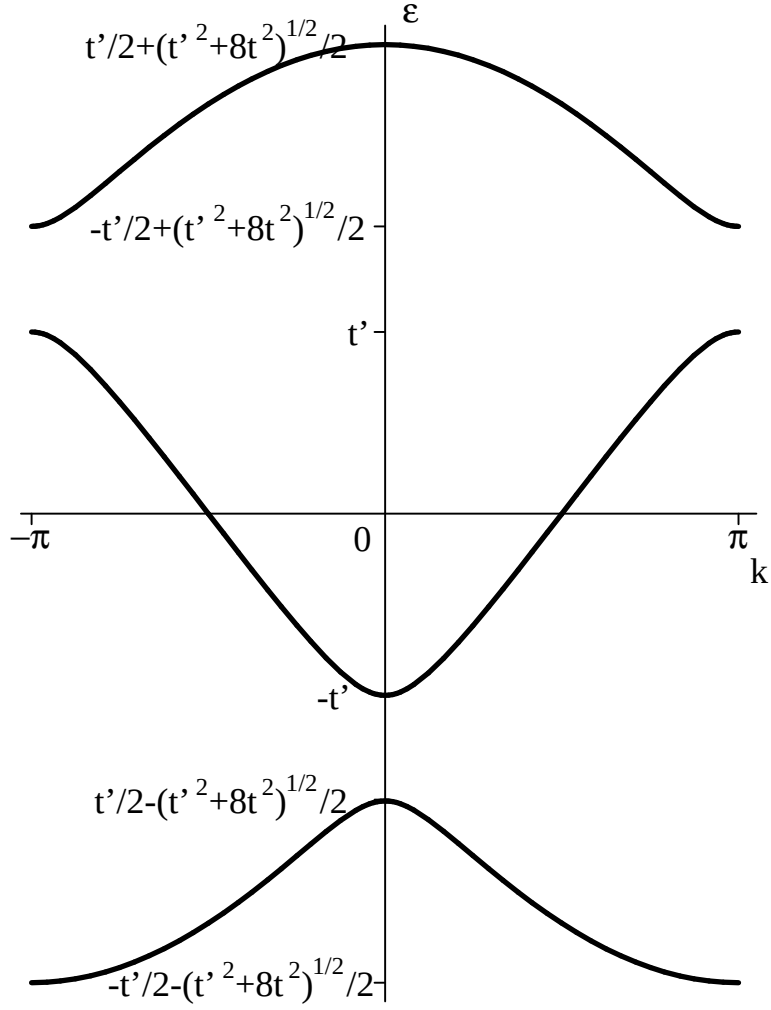


FIG. 2. Band structure of the trimerized chain ($p = 3$) at $U = 0$ for $t' < t$.