



ОБЪЕДИНЕННЫЙ  
ИНСТИТУТ  
ЯДЕРНЫХ  
ИССЛЕДОВАНИЙ

Дубна

E17-97-350

F.D.Buzatu<sup>1</sup>, G.Jackeli<sup>2</sup>

ALTERNATING CHAIN  
WITH HUBBARD-TYPE INTERACTIONS:  
RENORMALIZATION GROUP ANALYSIS

Submitted to «Physics Letters A»

---

<sup>1</sup>Department of Theoretical Physics, Institute for Physics and Nuclear Engineering, P.O.Box Mg-6, Magurele, Bucharest, R-76900, Romania

<sup>2</sup>Permanent address: Department of Solid State Physics, Tbilisi State University, Tbilisi, Georgia

1997

Бузату Ф.Д., Джакели Г.

Альтернирующая цепочка с взаимодействиями типа Хаббарда:  
ренормгрупповой анализ

Используется каноническое преобразование, диагонализирующее одно-частичный гамильтониан в приближении сильной связи для альтернирующей цепочки с двумя неэквивалентными узлами на элементарную ячейку, для введения взаимодействий типа Хаббарда (одноузельное, междуузельное и по одной связи) в соответствующей двухзонной модели. На основе подхода группы перенормировок в терминах эффективных констант взаимодействия исследуется фазовая диаграмма основного состояния системы для произвольного заполнения верхней зоны.

Работа выполнена в Лаборатории теоретической физики им.Н.Н.Боголюбова ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна, 1997

Buzatu F.D., Jackeli G.

Alternating Chain with Hubbard-Type Interactions: Renormalization  
Group Analysis

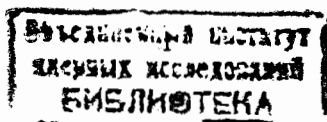
The canonical transformation diagonalizing the one-particle tight binding Hamiltonian for an alternating chain with two non-equivalent sites per unit cell has been used to introduce the Hubbard-like interactions (on-site, inter-site, bond-site and intra-bond) in the corresponding two-band model. For a large enough gap between the two bands, the consideration can be restricted to the partial filled band, as for the undistorted  $3/4$ -filled  $\text{CuO}_3$  chain where the alternating structure comes only from the on-site atomic energies. The renormalization group method has been applied to this model and the corresponding phase diagram has been analyzed in terms of some renormalized (density dependent) Hubbard-type couplings for arbitrary filling of the upper band.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

## I. INTRODUCTION

A large amount of work has been devoted to the study of alternating chains not only due to their interesting structure, but also in connection with a better understanding of the high- $T_c$  superconductivity mechanism. <sup>1</sup> The same phenomenon renewed interest in the Hubbard model and, quite recently, in its one-dimensional extensions. <sup>2</sup> However, the particularities induced by the Hubbard-like couplings in alternating chains are less well known: the charge gap that opens in a one-dimensional dimerized Hubbard model has been estimated in various limits using analytical results and exact diagonalizations of small clusters; <sup>3</sup> a model where the dimerization is induced via alternating on-site repulsions has been studied within a boson representation theory <sup>4</sup> and also by renormalization group (RG) technique. <sup>5</sup> The aim of this paper is to investigate, using the RG method, the effect of the Hubbard-type interactions on the ground-state properties of a chain with alternating on-site atomic energies.

The paper is structured as follows. The one-particle Hamiltonian in the tight binding approximation corresponding to an alternating chain with two nonequivalent sites per unit cell can be diagonalized by a canonical transformation; one gets a two-band model. The Hubbard-type interactions, i.e. interactions which in the site representation couple only electrons belonging to the nearest neighbor sites, give rise to both intra- and inter-band couplings; if the gap between the two bands is large enough, as for the  $CuO_3$  chain occurring in superconductor materials with high critical temperature, the last ones can be neglected. The obtained expressions of the Hubbard-type interactions (upper band), in the particular case of alternating on-site energies and equal hopping amplitudes, close Sec. II. The standard RG analysis (second order), <sup>6</sup> briefly reviewed in Sec III, is done in terms of the  $g$ -constants describing the elementary processes of forward, backward and umklapp scatterings: their expressions are obtained by evaluating the Hubbard-type interactions (upper band) at the Fermi points. Using the scaling to the exact soluble models Tomonaga-Luttinger (TL) <sup>7</sup> and Luther-Emery (LE), <sup>8</sup> we can predict the low energy physics of our system; the ground-state phase diagrams in terms of the model parameters and at arbitrary band filling are presented



in Sec. IV, where we also show that the alternating structure does not favor the occurrence of a possible superconducting state in a system like the undistorted 3/4-filled  $CuO_3$  chain. The last section summarizes the main results of this work.

## II. THE TWO-BAND MODEL

Let us consider the alternating chain from Fig. 1, with two non-equivalent sites per unit cell ( $N$  cells, periodic boundary conditions). Within the *tight binding approximation*, the second quantized form of the one-particle Hamiltonian in the *site representation* of the atomic orbitals reads<sup>9</sup>

$$\mathcal{H}_0 = \epsilon \sum_j (a_j^\dagger a_j - b_j^\dagger b_j) - \sum_j [(t a_j^\dagger + \bar{t} a_{j+1}^\dagger) b_j + H.c.] \quad (1)$$

where  $j = \overline{1, N}$  is the cell index, and the  $a(b)$ -operator corresponds to the annihilation of one electron on a site  $A(B)$ ; we ignore for the moment the spin variable  $\sigma = \uparrow, \downarrow$  of the electron (it can also be considered as included in the cell index). The constants  $\epsilon$  and  $t$  ( $\bar{t}$ ) are positive and denote respectively the site energies and the parameter describing the hopping between  $A$  and  $B$  sites belonging to the same cell (nearest neighbor cells); all of them can be expressed in terms of the atomic quantities.<sup>9</sup> From the site representation we can pass to the *momentum representation* by a usual Fourier transform; Eq. (1) becomes then

$$\mathcal{H}_0 = \epsilon \sum_k (a_k^\dagger a_k - b_k^\dagger b_k) - \sum_k [(t + \bar{t} e^{-iak}) a_k^\dagger b_k + H.c.] \quad (2)$$

where  $k \in (-\pi/a, \pi/a]$  with  $a$  being the lattice constant.

By mixing the  $a$ - and  $b$ -operators, the Hamiltonian  $\mathcal{H}_0$  has not a diagonal form; it can be diagonalized by the canonical transformation<sup>9</sup>

$$\begin{cases} a_k = A(k) e^{-i\phi(k)} c_{1,k} + B(k) c_{2,k} \\ b_k = B(k) c_{1,k} - A(k) e^{i\phi(k)} c_{2,k} \end{cases} \quad (3)$$

with

$$\begin{cases} A(k) = \frac{1}{\sqrt{2}} \left[ 1 - \frac{\epsilon}{\epsilon(k)} \right]^{\frac{1}{2}} \\ B(k) = \frac{1}{\sqrt{2}} \left[ 1 + \frac{\epsilon}{\epsilon(k)} \right]^{\frac{1}{2}} \\ \tan[\phi(k)] = \frac{\bar{t} \sin(ak)}{t + \bar{t} \cos(ak)} \end{cases} \quad (4)$$

$\epsilon(k)$  in Eq. (4) has the form

$$\epsilon(k) = \sqrt{\Delta^2 + 4t\bar{t} \cos^2(ak/2)} \quad (5)$$

where

$$\Delta = \sqrt{\epsilon^2 + (t - \bar{t})^2} \quad (6)$$

In terms of the  $c$  operators, the one-particle Hamiltonian (2) reads as

$$\mathcal{H}_0 = \sum_{k,\sigma} (-1)^\sigma \epsilon(k) c_{k,\sigma}^\dagger c_{k,\sigma}, \quad \alpha = 1, 2 \quad (7)$$

and defines the kinetic part of the two-band model: the dispersion law in the upper (lower) band is given by (minus)  $\epsilon(k)$  with a gap between the two bands equal to  $2\Delta$ ; in the limit  $\Delta \rightarrow 0$ , one recovers the usual dispersion law  $-2t \cos(ak)$  for an ideal (non-alternating) structure.

By analogy with the usual case, the Hubbard-type interactions between the electrons in an alternating chain are introduced in the site representation as follows:

(i) *on-site*

$$\mathcal{H}_1 = \frac{1}{2} \sum_{j,\sigma} (U_A n_{j,\sigma}^A n_{j,-\sigma}^A + U_B n_{j,\sigma}^B n_{j,-\sigma}^B) \quad (8)$$

where  $n_{j,\sigma}^{A(B)} = a_{j,\sigma}^\dagger a_{j,\sigma} (b_{j,\sigma}^\dagger b_{j,\sigma})$ ;

(ii) *inter-site*

$$\mathcal{H}_2 = \sum_{j,\sigma,\sigma'} n_{j,\sigma}^A (V n_{j,\sigma'}^B + \bar{V} n_{j-1,\sigma'}^B) \quad (9)$$

(iii) *bond-site*

$$\begin{aligned} \mathcal{H}_3 = & \sum_{j,\sigma} [a_{j,\sigma}^\dagger (X_A b_{j,\sigma} + \bar{X}_A b_{j-1,\sigma}) + H.c.] n_{j,-\sigma}^A \\ & + \sum_{j,\sigma} [b_{j,\sigma}^\dagger (X_B a_{j,\sigma} + \bar{X}_B a_{j+1,\sigma}) + H.c.] n_{j,-\sigma}^B \end{aligned} \quad (10)$$

(iv) *exchange hopping*

$$\begin{aligned} \mathcal{H}_4 = & -\frac{1}{2} \sum_{j,\sigma,\sigma'} [a_{j,\sigma}^\dagger (W b_{j,\sigma'}^\dagger b_{j,\sigma} \\ & + \bar{W} b_{j-1,\sigma'}^\dagger b_{j-1,\sigma}) a_{j,\sigma'} + H.c.] \end{aligned} \quad (11)$$

(v) *pair hopping*

$$\begin{aligned} \mathcal{H}_5 = & \frac{1}{2} \sum_{j,\sigma} [a_{j,\sigma}^\dagger a_{j,-\sigma}^\dagger (W b_{j,-\sigma} b_{j,\sigma} \\ & + \bar{W} b_{j-1,-\sigma} b_{j-1,\sigma}) + H.c.] \end{aligned} \quad (12)$$

The expressions of the Hubbard-type interactions in the corresponding two-band model are obtained by passing in Eqs. (8)-(12) to the momentum representation and replacing after that the  $a_k$ - and  $b_k$ -operators by the  $c_{\alpha,k}$ -operators, according to Eq. (3). Below we shall restrict our consideration only to the particular case of alternating on-site energies ( $\epsilon \neq 0$ ) and equal hopping amplitudes ( $t = \bar{t}$ ); in this case ( $a_1 = a_2 = a/2$ )

$$\phi = \frac{ak}{2}, \quad \Delta = \epsilon \quad (13)$$

and there will be no distinction between intra-cell interaction constants (without overline) and the inter-cells ones (with overline). Any interaction in terms of the  $a$ - and  $b$ -operators gives rise to both intra- and inter-band couplings. Nevertheless, if the gap between the two bands is large enough, it is reasonable to restrict the consideration only to the partial filled

band. In the case of the  $\text{CuO}_3$  chain, the gap is approximately 1.23 eV, while the total bandwidth (including the gap) is about 6.33 eV;<sup>10</sup> the chain is 3/4-filled, i.e. a half-filled upper band. Consequently, we shall consider only processes from the upper band ( $\alpha = 2$ ); the total Hamiltonian in this case reads as

$$\begin{aligned} \mathcal{H} = & \sum_{k,\sigma} \epsilon(k) c_{k,\sigma}^\dagger c_{k,\sigma} + \frac{1}{2N} \sum_{\beta=1}^5 \sum_{k_1, \dots, k_4; \sigma, \sigma'} \delta_{k_1+k_2, k_3+k_4} \\ & \times V_\beta(k_1, \dots, k_4; \sigma, \sigma') c_{k_1,\sigma}^\dagger c_{k_2,\sigma'}^\dagger c_{k_4,\sigma'} c_{k_3,\sigma} \end{aligned} \quad (14)$$

where  $\epsilon(k)$  is given by Eq. (5);  $V_\beta$  quantities ( $\beta = \overline{1,5}$ ) correspond, respectively, to the five types of the Hubbard interactions defined by Eqs. (8)-(12), and they have the following expressions:

$$V_1 = \left[ U_A \prod_{i=1}^4 B(k_i) \pm (A \leftrightarrow B) \right] \delta_{\sigma, -\sigma'} \quad (15)$$

$$\begin{aligned} V_2 = & 2V \cos[a(k_1 - k_3)/2] \\ & \times [A(k_1)B(k_2)A(k_3)B(k_4) \pm (A \leftrightarrow B)] \end{aligned} \quad (16)$$

$$\begin{aligned} V_3 = & -4 \{ X_A [\cos(ak_1/2)A(k_1)B(k_3) + \cos(ak_3/2) \\ & \times B(k_1)A(k_3)] B(k_2)B(k_4) \pm (A \leftrightarrow B) \} \delta_{\sigma, -\sigma'} \end{aligned} \quad (17)$$

$$\begin{aligned} V_4 = & 2W \cos[a(k_1 - k_4)/2] \\ & \times [A(k_1)B(k_2)B(k_3)A(k_4) \pm (A \leftrightarrow B)] \end{aligned} \quad (18)$$

$$\begin{aligned} V_5 = & 2W \cos[a(k_1 + k_2)/2] \\ & \times [A(k_1)A(k_2)B(k_3)B(k_4) \pm (A \leftrightarrow B)] \delta_{\sigma, -\sigma'} \end{aligned} \quad (19)$$

The  $\delta$ -function in Eq. (14) assures the conservation of the total momentum up to a reciprocal lattice vector, i.e.  $k_1 + k_2 = k_3 + k_4 + Q$  with  $Q = 0$  or  $Q = \pm 2\pi/a$ . In Eqs. (15)-(19), the upper (lower) sign corresponds to the normal (umklapp) scattering, i.e. to  $Q = 0$  ( $\pm 2\pi/a$ ); this fact, characteristic of an alternating structure,<sup>3</sup> comes from the phase factor  $\phi$  of the canonical transformation (3). Let us also note that for the lower band ( $\alpha = 1$ ),  $V_2$ ,  $V_4$  and  $V_5$  have the same expressions while  $V_1 \rightarrow V_1 [U_A \leftrightarrow U_B]$  and  $V_3 \rightarrow -V_3 [X_A \leftrightarrow X_B]$ .

### III. RENORMALIZATION GROUP ANALYSIS

The low energy physics of our model (14) can be described, within the RG method,<sup>6</sup> by assuming: (i) a linear dispersion law

$$\varepsilon(k) \simeq v_F(k_F - |k|), \quad v_F > 0 \quad (20)$$

together with the existence of a momentum cut-off  $k_0$  restricting all possible states of the electrons to those around the Fermi points (or equivalently, a bandwidth cut-off  $E_0 = 2v_F k_0$ ); (ii) all interaction processes can be classified into four different types (see Fig. 3) with the coupling constants  $g_i$  ( $i = \overline{1,4}$ ) obtained by evaluating the bare potentials at the corresponding values  $+$  or  $-k_F$  of the momenta.

In the  $g_1$  process (backward scattering) the momentum transfer is  $2k_F$ ; in the  $g_2$  and  $g_4$  processes (forward scattering), it is zero. The  $g_3$  process (umklapp scattering) is possible only at half-filling when the momentum transfer  $4k_F$  is equal to the reciprocal lattice vector. Each coupling constant has two components as the spins of interacting particles are parallel ( $\parallel$ ) or antiparallel ( $\perp$ ); however, if all momenta are fixed at  $+$  or  $-k_F$ , due to the Pauli principle  $g_{3\parallel}$  and  $g_{4\parallel}$  bring no contribution and thus their spin index can be omitted. The expressions of the  $g$ -constants corresponding to the model (14) and also their form for a non-alternating chain are given Table I where we have introduced the renormalized Hubbard constants

$$\left\{ \begin{array}{l} \mathcal{U} = U_A B^4(k_F) + U_B A^4(k_F) \\ \mathcal{V} = 2V A^2(k_F) B^2(k_F) \\ \mathcal{X} = X_A A(k_F) B^3(k_F) + X_B A^3(k_F) B(k_F) \\ \mathcal{W} = 2W A^2(k_F) B^2(k_F) \end{array} \right. \quad (21)$$

Unlike for a non-alternating chain, they now depend on the band filling  $n$  [ $a k_F = \pi(1 - n)$ ,  $0 \leq n \leq 1$ ]. As can be remarked from Table I, there is an almost complete analogy between

the case of an  $n$ -filled band coming from an alternating chain and an  $(n+1)/2$ -filled band of a non-alternating one; the differences consist in the renormalization of the Hubbard constants and, obviously, in the umklapp process.

All physical results predicted by the RG method (second order) can be discussed in terms of four independent coupling constants:  $g_{1\perp}, g_3$ ,

$$g_\sigma = g_{1\parallel} - g_{2\parallel} + g_{2\perp} \quad (22)$$

and

$$g_\rho = g_{1\parallel} - g_{2\parallel} - g_{2\perp} \quad (23)$$

(the main effect of  $g_4$  can be included in a renormalized Fermi velocity). The coupling constants  $g_\sigma$  and  $g_{1\perp}$  describe the spin sector;  $g_\rho$  and  $g_3$ , the charge sector. The RG equations (in units of  $\pi v_F$ ) read as<sup>6</sup>

$$\left\{ \begin{array}{l} \frac{dg_\sigma}{dx}(x) = g_{1\perp}^2(x) [1 + \frac{1}{2}g_\sigma(x)] \\ \frac{dg_{1\perp}}{dx}(x) = g_\sigma(x)g_{1\perp}(x) [1 + \frac{1}{4}g_\sigma(x)] + \frac{1}{4}g_{1\perp}^3(x) \end{array} \right. \quad (24)$$

$$\left\{ \begin{array}{l} \frac{dg_\rho}{dx}(x) = g_3^2(x) [1 + \frac{1}{2}g_\rho(x)] \\ \frac{dg_3}{dx}(x) = g_\rho(x)g_3(x) [1 + \frac{1}{4}g_\rho(x)] + \frac{1}{4}g_3^3(x) \end{array} \right. \quad (25)$$

where  $x = \ln(E/E_0) \in (-\infty, 0]$ , with  $E$  a smaller cut-off than the original one  $E_0$ . The structure of Eqs. (24) and (25) reflects the spin-charge separation occurring in 1D systems: the evolution of the  $g$ -constants in the spin sector is decoupled from that in the charge sector.

By solving Eqs. (24) and (25), a set of equivalent problems, related by RG transformations, can be found; the low energy physics is essentially the same for all models with the  $g$ -constants along a certain  $g(x)$  curve. The flow diagrams are shown in Fig. (4)

where the arrows indicate the limit  $x \rightarrow -\infty$  ( $E \rightarrow 0$ ) of the fixed points. There are also two important lines in the diagram, related to two exactly soluble models: the vertical axis corresponds to the TL model<sup>7</sup> ( $g_{1\perp} = g_3 = 0$ ) and the horizontal dashed line corresponds to the LE model<sup>8</sup> ( $g_\sigma = g_\rho = -6/5$ ). Two different regimes can be distinguished from the flow diagram drawn in Fig. (4): (i) for  $g_\sigma \geq |g_{1\perp}|$  ( $g_\rho \geq |g_3|$ ) the spin (charge) part of the system scales to the TL model which is also the fixed point (this is the weak coupling regime); (ii) for  $g_\sigma < |g_{1\perp}|$  ( $g_\rho < |g_3|$ ) the spin (charge) part of the system scales to one of the two strong coupling fixed points, but before this it crosses the LE line and thus its behavior can be inferred from the exact solution.

Let us note that for the Hubbard-type interactions, due to the  $SU(2)$ -spin symmetry of the Hamiltonian (14),  $g_\sigma$  is always equal to  $g_{1\perp}$ ; consequently, the scaling in the spin flow diagram is along the first bisectrix  $g_\sigma(x) = g_{1\perp}(x)$  and, therefore, we have four distinct regions

$$I: \begin{cases} g_\sigma \geq 0 \\ g_\rho \geq |g_3| \end{cases} \quad II: \begin{cases} g_\sigma \geq 0 \\ g_\rho < |g_3| \end{cases} \quad (26)$$

$$III: \begin{cases} g_\sigma < 0 \\ g_\rho < |g_3| \end{cases} \quad IV: \begin{cases} g_\sigma < 0 \\ g_\rho \geq |g_3| \end{cases}$$

where, in our case,

$$g_\sigma = \mathcal{U} - 2\mathcal{V} \cos(\pi n) - 8\mathcal{X} \sin(\pi n/2) + 4\mathcal{W} \quad (27)$$

$$g_\rho = -\mathcal{U} - 2\mathcal{V}[2 + \cos(\pi n)] + 8\mathcal{X} \sin(\pi n/2) + 4\mathcal{W} \cos(\pi n) \quad (28)$$

and  $g_3$  can be read from Table I. In terms of the model parameters, the four regions defined by Eq. (26) can be conveniently described in the  $(\mathcal{W}, \mathcal{V})$ -plane as follows:

$$I: \begin{cases} \mathcal{W} \geq F \\ \mathcal{V} \leq G \end{cases} \quad II: \begin{cases} \mathcal{W} \geq F \\ \mathcal{V} > G \end{cases} \quad (29)$$

$$III: \begin{cases} \mathcal{W} < F \\ \mathcal{V} > G \end{cases} \quad IV: \begin{cases} \mathcal{W} < F \\ \mathcal{V} \leq G \end{cases}$$

where

$$F = [-\mathcal{U} + 2\mathcal{V} \cos(\pi n) + 8\mathcal{X} \sin(\pi n/2)]/4 \quad (30)$$

does not depend on  $\mathcal{W}$  and

$$G = \begin{cases} \frac{8\mathcal{X} \sin(\pi n/2) + 4\mathcal{W} \cos(\pi n) - \mathcal{U}}{2[2 + \cos(\pi n)]} & n \neq \frac{1}{2} \\ -\frac{1}{2} \text{Max}\{Y_1, Y_2\} & n = \frac{1}{2} \end{cases} \quad (31)$$

is independent of  $\mathcal{V}$  where

$$Y_1 = U_A B^4 - 4\sqrt{2} X_A A B^3, \quad Y_2 = Y_1[A \leftrightarrow B] \quad (32)$$

$A$  and  $B$  in Eq. (32) stand respectively for  $A(k_F)$  and  $B(k_F)$  [see Eq. (4)] evaluated at half-filling.

The scaling of our system to one of the two exactly soluble models, TL or LE, in each of the four regions, at any density and for both charge and spin sector is summarized in Table I.

#### IV. PHASE DIAGRAMS

Based on the exact results obtained for the TL and LE models and using the scaling arguments, we can now describe the low energy physics of our system: Anytime the system scales to the LE model, there is a gap in the corresponding charge or spin sector; in the TL case, the spectrum is gapless. Following the Sólyom's analysis,<sup>6</sup> we can predict the most

preferred type of instability occurring in the ground-state of the system, corresponding to the most divergent correlation function: charge density wave (*CDW*), spin density wave (*SDW*), singlet superconductivity (*SS*) or triplet superconductivity (*TS*). Before discussing the results, let us remark that the on-site and bond-site interaction constants have always opposite effects; they occur only in the combination

$$Y = U - 8\mathcal{X} \sin(\pi n/2) \quad (33)$$

or, in the half-filled case, through  $Y_1$  or  $Y_2$  with a similar structure. Consequently, a bond-site repulsion acts (in the upper band) as an effective attraction and its effect is enhanced by increasing the electron density  $n$ , a fact already used in the hole superconductivity mechanism.<sup>11</sup> The value of  $Y$  (or  $Y_{1,2}$ ) fixes the position, in the  $(\mathcal{W}, \mathcal{V})$ -plane, of the intersection between the "spin-line" ( $g_s = 0$ ) and the "charge-line" ( $g_p = |g_3|$ ).

Let us first consider the half-filled case ( $n = 1/2$ ). The obtained phase diagram has the structure presented in Fig. 5. The "spin-line" is vertical and the "charge-line" is horizontal; both of them delimit not only different phases, but also the strong coupling regime from the weak coupling one in each corresponding (charge or spin) sector. The critical value  $\mathcal{V}_2 = -\text{Max}\{Y_1, Y_2\}/2$  of the inter-site interaction constant separates a dominant superconductor region ( $\mathcal{V} < \mathcal{V}_2$ ) from a density fluctuation one ( $\mathcal{V} > \mathcal{V}_2$ ). Analogously, by decreasing the intra-bond interaction constant  $\mathcal{W}$  below the critical value  $\mathcal{W}_1 = -Y/4$ , the triplet states (spin-density or superconductor) disappear. Depending on the values of  $U_{A,B}$  and  $X_{A,B}$ , the origin  $\mathcal{W} = \mathcal{V} = 0$  can be found in principle in any of the four regions, but the most probable case for a real system is that considered in the picture ( $Y > 0, Y_{1,2} > 0$ ).

In the non-half-filled case,  $g_3$  is zero and consequently  $g_p$  does not renormalize; thus the charge sector is always in the weak coupling regime and the "charge-line" now separates only different phases. Graphically, two things happen: (i) the intersection between the "charge-line" and the "spin-line" moves in such a way that the origin  $\mathcal{W} = \mathcal{V} = 0$  lies inside either the region II (for  $Y > 0$ ) or the region IV (for  $Y < 0$ ); (ii) by increasing the density  $n$ , the "spin-line" rotates anti-clockwise while the "charge-line" rotates clockwise (by decreasing

$n$ , the effect is reversed). Consequently, on starting from the half-filled case and increasing the electron concentration the regions I and III become smaller while the regions II and IV grow, as it is shown in Fig. 6 for  $Y > 0$ ; the intersection of the "spin-line" with the coordinate axes are given respectively by  $\mathcal{W}_1 = -Y/4$  and  $\mathcal{V}_1 = Y/[2\cos(\pi n)]$  while in the "charge-line" case by  $\mathcal{W}_2 = Y/[4\cos(\pi n)]$  and  $\mathcal{V}_2 = -Y/[4 + 2\cos(\pi n)]$ . The effect of the model parameters on the ground-state phase diagram can easily be inferred from the above discussion.

Let us now discuss if the alternating structure is important in a possible occurrence of superconductivity in the ground-state of the system. In order to do this, we have to compare, as we have mentioned in the previous section, the case of an  $n$ -filled upper band for the alternating chain with the case of an  $(n + 1)/2$ -filled band of a non-alternating one. For simplicity, we shall assume a short range potential between the electrons, i.e. a very effective screening; in this case, the on-site and bond-site interactions are more important than the inter-site and intra-bond ones that can be thus neglected.<sup>12,13</sup> For the undistorted 3/4-filled  $\text{CuO}_3$  chain, the estimations of the band parameters are:<sup>10</sup>  $2\epsilon = 1.23$  eV,  $t = \bar{t} = 1.4$  eV; from Eq. (4) it then follows  $A \simeq 0.6$  and  $B \simeq 0.8$ . According to the phase diagram from Fig. 5, the ground-state is superconducting if  $Y_{1,2} < 0$  or equivalently,  $X_A/U_A > B/(4\sqrt{2}A) \simeq 0.24$  and  $X_B/U_B > A/(4\sqrt{2}B) \simeq 0.13$  [See Eq. (32)]. For a non-alternating chain, the same condition now requires  $Y < 0$ , i.e.  $X_0/U_0 > 1/(4\sqrt{2}) \simeq 0.18$ <sup>14</sup> [See Eq. (33), where we replaced the renormalized coupling constants  $U$  and  $\mathcal{X}$  by respectively  $U_0$  and  $X_0$  of a non-alternating chain]. In order to get a superconductor state, we thus need a bigger ratio of the (*A*) bond- and on-site couplings in the alternating case than in the non-dimerized one; however, in average, the ratio is practically the same. It follows that the alternating structure does not affect the occurrence of superconductivity for a 3/4-filled chain as  $\text{CuO}_3$ ; the renormalization of the coupling constants due to the dimerization seems to be not important in this respect. The same conclusion can be derived for other densities. If a superconductor state exists in such a model, it is due to other factors (as the density, for example, that diminishes the effective repulsion by enhancing



the contribution of the bond-site term) and depends on the effective values of the coupling constants: using a Kronig-Penney model for the potential arising from the ions and for a very screened inter-electronic potential, Campbell et al.<sup>13</sup> estimated  $X_0/U_0$  in the range 0.15 - 0.18; for the  $CuO_3$  chain,  $U_A \approx 3 - 4$  eV,  $U_B \approx 1 - 3$  eV,<sup>10</sup> but the values of  $X_A$  and  $X_B$  are less known.

## V. CONCLUSIONS

The results of this paper can be summarized as follows: the canonical transformation diagonalizing the one-particle Hamiltonian for an alternating chain with two non-equivalent sites per unit cell has been used to find the expressions of the Hubbard-type interactions, initially introduced in the site-representation, in the corresponding two-band model; the consideration has been restricted to the particular case of only alternating on-site energies (and equal hopping amplitudes) and a gap between the two bands large enough to take into account only the processes inside the partial filled band (and we chose the upper band, as for the 3/4-filled  $CuO_3$  chain). A particularity of the alternating structure manifests itself in the dependence of the obtained potentials on the momentum conservation in a given process, i.e. if it is normal or umklapp one. The RG method (second order) has then been applied to this (one-band) model Hamiltonian; all the  $g$ -constants have been obtained by evaluating the corresponding Hubbard-type interactions around the Fermi points. The resulting ground-state phase diagrams have been analyzed in terms of all coupling constants and for an arbitrary band filling. The effect of the bond-site interaction is to renormalize the on-site one. In the chosen coordinates (intra-bond, inter-site) and at half filling, a critical inter-site interaction controls the position of the "charge-line" (separating a dominant superconductor region from a density fluctuation one), and a critical intra-bond-coupling determines the "spin-line" (separating a region of singlet states from one with possible triplet states); the effect of the density is to rotate these two lines and to change the position of their crossing determined by a certain relation between the on-site and bond-site coupling

constants. According to our estimations, the alternating structure does not favor a possible occurrence of a superconducting state in a system like the undistorted 3/4-filled  $CuO_3$  chain.

## ACKNOWLEDGMENTS

The authors are grateful to G. Japaridze for helpful suggestions and stimulating discussions on this subject. One of the authors (G.J.) acknowledges the support from the Russian Foundation for Fundamental Researches (Grant No. 96-02-17527) and from the INTAS-RFBR Program (Grant No. 95-591).

TABLES

TABLE I. The values of the  $g$ -constants for the upper band of a chain with alternating on-site energies and Hubbard-type interactions (last column), compared with the similar quantities for a non-alternating structure (middle column).  $U$ ,  $V$ ,  $X$  and  $W$  are defined in the text by Eq. (21) and they are analogous, for our model, of the Hubbard-like coupling constants  $U_0$ ,  $V_0$ ,  $X_0$  and  $W_0$  from the usual case. By  $n$  we denoted the electron filling of the band, related to the Fermi momentum by  $ak_F = \pi(1 - n)$  for the upper band of the alternating chain, or by  $ak_F = \pi n$  in the non-alternating case ( $0 \leq n \leq 1$ ).

	non-alternating chain	alternating chain
$g_{1\parallel}$	$2V_0 \cos(2\pi n) + 2W_0$	$-2V \cos(\pi n) + 2W$
$g_{1\perp}$	$U_0 + 2V_0 \cos(2\pi n) + 8X_0 \cos(\pi n) + 4W_0$	$U - 2V \cos(\pi n) - 8X \sin(\pi n/2) + 4W$
$g_{2\parallel}$	$2V_0 + 2W_0 \cos(2\pi n)$	$2V - 2W \cos(\pi n)$
$g_{2\perp}$	$U_0 + 2V_0 + 8X_0 \cos(\pi n) + 2W_0 \{1 + \cos(2\pi n)\}$	$U + 2V - 8X \sin(\pi n/2) + 2W \{1 - \cos(\pi n)\}$
$g_3$	$(U_0 - 2V_0 - 4W_0)\delta_{n,1/2}$	$\{(U_A B^4 - 4\sqrt{2}X_A A B^3) - (A \leftrightarrow B)\}\delta_{n,1/2}$
$g_4$	$U_0 + 2V_0 + 8X_0 \cos(\pi n) + 2W_0 \{1 + \cos(2\pi n)\}$	$U + 2V - 8X \sin(\pi n/2) + 2W \{1 - \cos(\pi n)\}$

TABLE II. The scaling of the considered model (14) to one of the two exactly soluble models - Tomonaga-Luttinger (TL) or Luther-Emery (LE), in each of the four regions defined by Eq. (27) in both the charge (c) and spin (s) sector.

	half filling ( $n = 1/2$ )		not half filling ( $n \neq 1/2$ )	
	c	s	c	s
I	TL	TL	TL	TL
II	LE	TL	TL	TL
III	LE	LE	TL	LE
IV	TL	LE	TL	LE

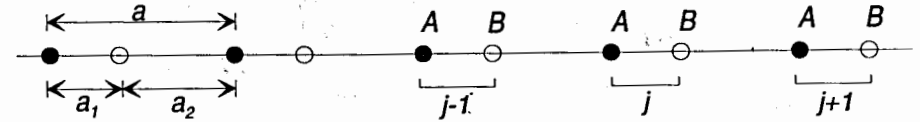


FIG. 1. Alternating chain with two non-equivalent sites per unit cell.

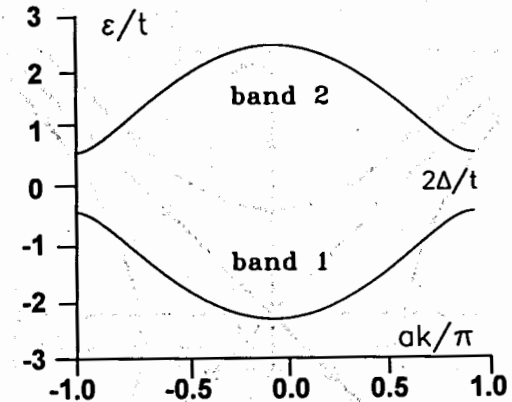


FIG. 2. The two bands corresponding to the one-particle tight binding Hamiltonian for an alternating chain with two non-equivalent sites per unit cell.

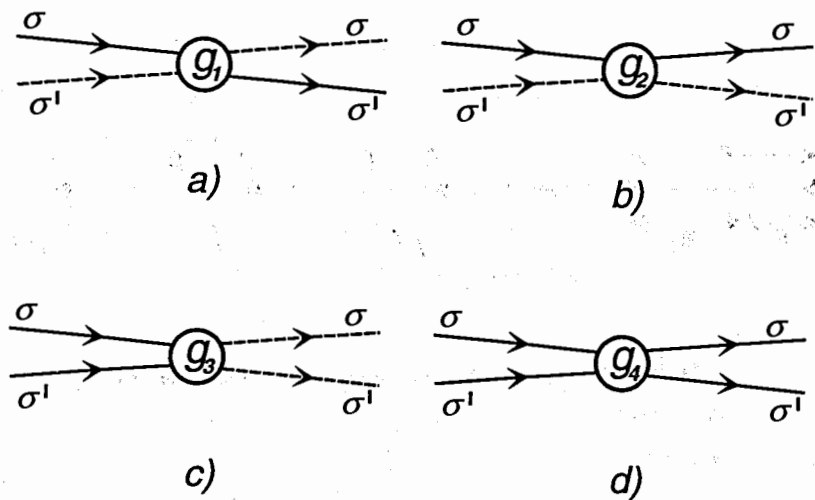


FIG. 3. The  $g$ -processes of the backward (a), forward (b,d) and umklapp (c) scattering.

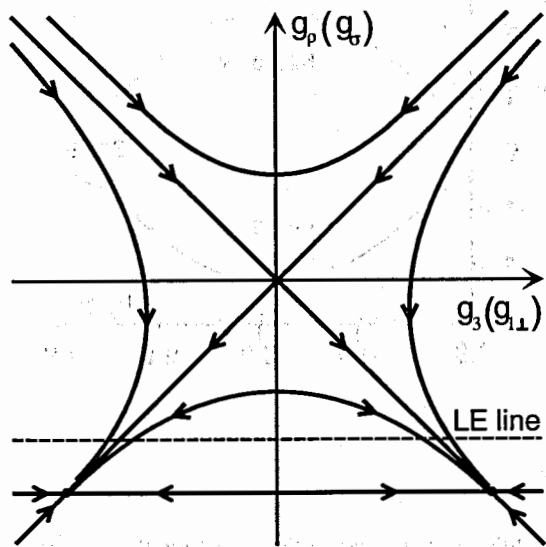


FIG. 4. The flow diagram in the charge (spin) sector. The vertical axis corresponds to the Tomonaga-Luttinger model and the horizontal dashed line to the Luther-Emery model.

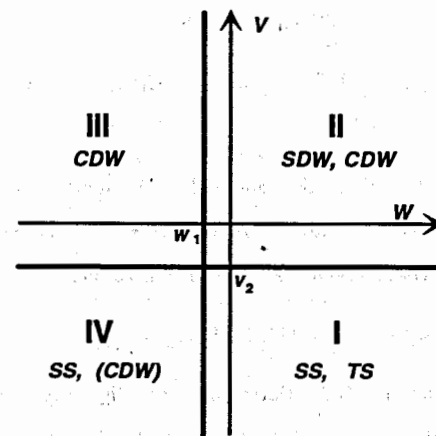


FIG. 5. The phase diagram corresponding to a chain with alternating on-site atomic energies and Hubbard-type interactions for a half-filled upper band.  $\mathcal{W}_1 = -Y/4$  and  $\mathcal{V}_2 = -\text{Max}\{Y_1, Y_2\}/2$  [see Eqs. (32) and (33) in the text]. The response functions corresponding to the phases shown in the parentheses have a lower degree of divergence than the others.

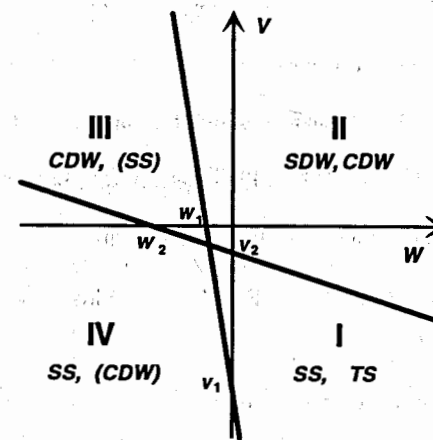


FIG. 6. The phase diagram of the considered model away from half filling.  $\mathcal{W}_1 = -Y/4$  and  $\mathcal{V}_1 = Y/[2\cos(\pi n)]$  determine the "spin-line", while the "charge-line" is determined by  $\mathcal{W}_2 = Y/[4\cos(\pi n)]$  and  $\mathcal{V}_2 = -Y/[4 + 2\cos(\pi n)]$  (here  $Y > 0$  and the band filling  $n > 1/2$ ).

## REFERENCES

- <sup>1</sup> See, for example, S.-L. Drechsler, J. Malek and H. Eschrig, Phys. Rev. B **55**, 606 (1997) and references therein.
- <sup>2</sup> See, for example: L. Arrachea, E. R. Gagliano and A. A. Aligia, Phys. Rev. B **55**, 1173 (1997); D. M. Luz and R. R. dos Santos, Phys. Rev. B **54**, 1302 (1996); A. Belkasri and F. D. Buzatu, Phys. Rev. B **53**, 7171 (1996) and references therein.
- <sup>3</sup> K. Penc and F. Mila, Phys. Rev. B **50**, 11429 (1994).
- <sup>4</sup> G. Japaridze, D. Komsii and E. Müller-Hartmann, Ann. Phys. (Leipzig) **2**, 38 (1993); G. Japaridze and E. Müller-Hartmann, *ibid*, **3**, 163 (1994); **3**, 421 (1994).
- <sup>5</sup> G. Jackeli and G. Japaridze, Int. J. Mod. Phys. B **11**, 1925 (1997).
- <sup>6</sup> J. Sólyom, Adv. Phys. **28**, 201 (1979).
- <sup>7</sup> S. Tomonaga, Prog. Theor. Phys. **5**, 349 (1950); J. M. Luttinger, J. Math. Phys. **4**, 1154 (1963).
- <sup>8</sup> A. Luther and V. J. Emery, Phys. Rev. Lett. **33**, 589 (1974).
- <sup>9</sup> F. D. Buzatu and E. Pieleanu (unpublished).
- <sup>10</sup> S.-L. Drechsler, J. Malek, M. Yu. Lavrentiev and H. Köppel, Phys. Rev. B **49**, 233 (1994).
- <sup>11</sup> J. E. Hirsch, Physica C **158**, 326 (1989); Phys. Lett. A **138**, 83 (1989).
- <sup>12</sup> A. Painelli and A. Girlando, Phys. Rev. B **39**, 2830 (1989).
- <sup>13</sup> D. K. Campbell, J. Tinka Gammel and E.Y. Loh, Jr., Phys. Rev. B **38**, 12043 (1988); Phys. Rev. B **42**, 475 (1990).
- <sup>14</sup> Practically the same value of the ratio  $X_0/U_0$  required for the occurrence of a superconductor state follows from the phase diagram of the  $(t, U, X)$ -model (with 3/4-filled band) in a mean-field-type approximation: F. D. Buzatu, Phys. Rev. B **49**, 10176 (1994).

Received by Publishing Department  
on November 14, 1997.