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HUBBARD-TYPE INTERACTIONS
IN ALTERNATING CHAINS

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1   Introduction

The properties of alternating chains have been intensively investigated in the last time [1, 2, 3] not only due to their interesting structure, but also in connection with a better understanding of the high-T_c superconductivity mechanism. The same phenomenon renewed the interest for the Hubbard model [4], a large number of papers being devoted to its one-dimensional (1D) extensions [5, 6, 7, 8, 9]. However, the particularities of the Hubbard-like couplings in alternating chains are less well known. It is the aim of this paper to derive the corresponding expressions of the Hubbard-type interactions in the equivalent two-band model and to discuss a possible occurence of a superconductor state in such structures.

The one-particle hamiltonian in the tight binding approximation for an alternating chain with two non-equivalent sites per unit cell is defined, in terms of the atomic quantities, in Sec. 1. This hamiltonian can be diagonalized by a canonical transformation, as it is shown in Sec. 2; one gets a two-band (free) hamiltonian in the Bloch representation. The Hubbard-type interactions, initially introduced in the site representation, give rise to both intra- and inter-band couplings; if the gap between the two bands is large enough, as for CuO_3 chain, the last ones can be neglected. The intra-band interactions are described by some k-dependent potentials with rather complicate expressions; they are presented in Sec. 4. An evaluation of the coupling constants $g_1, .., g_4$ around the Fermi points is discussed for the case of CuO_3 chain in the same section; the effect of the Hubbard-type interactions in the upper half-filled band is similar, excepting an Umklapp term, to the case of a 3/4-filled ideal chain. The bond-site interaction acts as an effective attraction and it can determine in some circumstances the occurence of a superconductor instability. The last section contains some remarks about possible extensions and further developments of the present work.

2   The one-particle hamiltonian

Let us consider the alternating chain from Fig. 1, with two non-equivalent sites per unit cell (N cells, periodic boundary conditions); the one-particle hamiltonian corresponding to this structure can be written as

$$\mathcal{H} = \mathcal{H}_{j,s} + V - V_{j,s} \ , \quad j = 1, N \ , \ s = A, B \tag{1}$$

where j is the cell index and s specifies the site in the cell. $\mathcal{H}_{j,s}$ denotes the atomic hamiltonian defined by its action on the orbital $\phi_{j,s}$ corresponding to

the atomic energy level E_s :

$$(\mathcal{H}_{j,s}\phi_{j,s})(x) = -\frac{1}{2m}\frac{d^2\phi_{j,s}}{dx^2} + V_{j,s}(x)\phi_{j,s}(x) \qquad (2)$$

$$\mathcal{H}_{j,s}\phi_{j,s} = E_s\phi_{j,s} \qquad (3)$$

where $V_{j,s}$ and m in Eq. (2) are respectively the ionic potential of the site (j,s) and the electron mass. V in Eq. (1) is the periodical potential of the lattice:

$$V(x+a) = V(x) \quad , \quad a = a_1 + a_2 \qquad (4)$$

Within the *tight binding approximation*, we assume that: (i) the atomic orbitals $\phi_{j,s}$ form an orthogonal and normalized set

$$< \phi_{j,s} \mid \phi_{j',s'} > = \delta_{j,j'}\delta_{s,s'} \qquad (5)$$

which generates the one-particle Hilbert space corresponding to the motion of one electron in the chain (this condition can be in fact relaxed by allowing a small overlap between the atomic orbitals and then orthogonalizing them [7]); (ii) the matrix elements of the hamiltonian (1) are of the following form:

$$< \phi_{j,s} \mid \mathcal{H}\phi_{j',s'} > = \epsilon_s\delta_{j,j'}\delta_{s,s'} - t\left(\delta_{s,A}\delta_{s',B} + \delta_{s,B}\delta_{s',A}\right)\delta_{j,j'} - \bar{t}\left(\delta_{s,A}\delta_{s',B}\delta_{j,j'+1} + \delta_{s,B}\delta_{s',A}\delta_{j,j'-1}\right) \qquad (6)$$

which account for the jump of electrons only between the nearest neighbour sites. $\epsilon_{A(B)}$ and $t(\bar{t})$ can be easily expressed in terms of the atomic quantities as

$$\epsilon_s = E_s + < \phi_{j,s} \mid (V - V_{j,s})\phi_{j,s} > \quad , \quad s = A, B$$

$$t = < \phi_{j,B} \mid (V_{j,A} - V)\phi_{j,A} > = < \phi_{j,A} \mid (V_{j,B} - V)\phi_{j,B} > \qquad (7)$$

$$\bar{t} = < \phi_{j+1,A} \mid (V_{j,B} - V)\phi_{j,B} > = < \phi_{j-1,B} \mid (V_{j,A} - V)\phi_{j,A} >$$

where we used also the hermiticity of the hamiltonian (1). Without loss of generality, we can choose the zero of energy such that

$$\epsilon_A = -\epsilon_B \equiv \epsilon > 0 \qquad (8)$$

The second quantized form of the tight binding hamiltonian in the (j,s)-representation of the atomic orbitals is

$$\mathcal{H} = \epsilon\sum_j\left(a_j^\dagger a_j - b_j^\dagger b_j\right) - t\sum_j\left(a_j^\dagger b_j + b_j^\dagger a_j\right) - \bar{t}\sum_j\left(a_{j+1}^\dagger b_j + b_j^\dagger a_{j+1}\right) \qquad (9)$$

where $a(b)$ operators correspond to the annihilation of electrons on $A(B)$ sites. For simplicity we neglect for the moment (until Sec. 4) the spin variable of electrons. From the (j,s)-representation we can pass to the (k,s)-representation by a usual Fourier transform

$$a_j^\dagger = \frac{1}{\sqrt{N}}\sum_k e^{-iajk}a_k^\dagger \quad , \quad a_j = \frac{1}{\sqrt{N}}\sum_k e^{iajk}a_k \quad , \quad k \in BZ = \left(-\frac{\pi}{a}, \frac{\pi}{a}\right] \qquad (10)$$

and the same for the b operators. Eq. (9) becomes then

$$\mathcal{H} = \epsilon\sum_k\left(a_k^\dagger a_k - b_k^\dagger b_k\right) - \sum_k\left[\left(t + \bar{t}e^{-iak}\right)a_k^\dagger b_k + H.c.\right] \qquad (11)$$

The a and b operators satisfy the usual anticommutation relations:

$$\left\{a_k^\dagger, a_{k'}\right\} = \left\{b_k^\dagger, b_{k'}\right\} = \delta_{k,k'} \quad , \quad \left\{a_k^\dagger, b_{k'}\right\} = 0 \qquad (12)$$

$$\left\{a_k^\dagger, a_{k'}^\dagger\right\} = \left\{a_k, a_{k'}\right\} = \left\{b_k^\dagger, b_{k'}^\dagger\right\} = \left\{b_k, b_{k'}\right\} = 0$$

3 The canonical transformation

By mixing the a and b operators, the hamiltonian (9) or equivalently (11) has not a diagonal form; it can be diagonalized by a canonical transformation

$$\begin{cases} a_k = \alpha(k)c_{1,k} + \beta(k)c_{2,k} \\ b_k = \gamma(k)c_{1,k} + \theta(k)c_{2,k} \end{cases} \qquad (13)$$

where the c operators obey the same anticommutation relations as a and b operators:

$$\left\{c_{n,k}^\dagger, c_{n'k'}\right\} = \delta_{n,n'}\delta_{k,k'} \quad , \quad \left\{c_{n,k}^\dagger, c_{n',k'}^\dagger\right\} = \left\{c_{n,k}, c_{n',k'}\right\} = 0 \qquad (14)$$

From Eqs. (12)-(14) it follows

$$\begin{cases} |\alpha(k)|^2 + |\beta(k)|^2 = 1 \\ |\gamma(k)| = |\beta(k)| \\ |\theta(k)| = |\alpha(k)| \\ arg[\alpha(k)] - arg[\beta(k)] - arg[\gamma(k)] + arg[\theta(k)] = \pi \end{cases} \qquad (15)$$

and from the requirement the hamiltonian to be diagonal we get an additional complex equation:

$$\varepsilon\left[\alpha^*(k)\beta(k) - \gamma^*(k)\theta(k)\right] - \left(t + \bar{t}e^{-iak}\right)\alpha^*(k)\theta(k) - \left(t + \bar{t}e^{iak}\right)\beta(k)\gamma^*(k) \quad (16)$$

Eqs. (15) and (16) form a system of six real equations with eight unknowns; we can make a particular choice for two of the phase factors, for instance

$$arg[\beta(k)] = arg[\gamma(k)] = 0 \quad (17)$$

The canonical transformation takes then the form

$$\begin{cases} a_k = A(k)e^{-i\phi(k)}c_{1,k} + B(k)c_{2,k} \\ b_k = B(k)c_{1,k} + A(k)e^{i\phi(k)}c_{2,k} \end{cases} \quad A, B > 0 \quad (18)$$

with the conditions

$$\begin{cases} A^2 + B^2 = 1 \\ \dfrac{2\varepsilon AB}{B^2 - A^2} = t\cos(\phi) + \bar{t}\cos(ak - \phi) \\ t\sin(\phi) = \bar{t}\sin(ak - \phi) \end{cases} \quad (19)$$

where the k-dependence has been omitted. The system (19) has the solution

$$\begin{cases} A = \dfrac{1}{\sqrt{2}}\left[1 - \dfrac{\varepsilon}{\sqrt{\Delta^2 + 4t\bar{t}\cos^2(ak/2)}}\right]^{\frac{1}{2}} \\ B = \dfrac{1}{\sqrt{2}}\left[1 + \dfrac{\varepsilon}{\sqrt{\Delta^2 + 4t\bar{t}\cos^2(ak/2)}}\right]^{\frac{1}{2}} \\ \tan(\phi) = \dfrac{\bar{t}}{t + \bar{t}\cos(ak)} \end{cases} \quad (20)$$

with the notation

$$\Delta = \sqrt{\varepsilon^2 + (t - \bar{t})^2} \quad (21)$$

In terms of the c operators, the one-particle hamiltonian for the alternating chain becomes

$$\mathcal{H} = \sum_k \left[\varepsilon_1(k)c_{1,k}^\dagger c_{1,k} + \varepsilon_2(k)c_{2,k}^\dagger c_{2,k}\right] \quad (22)$$

and we will call it the *Bloch representation*; the energies in Eq. (22) have the expresions

$$\varepsilon_2(k) = -\varepsilon_1(k) = \sqrt{\Delta^2 + 4t\bar{t}\cos^2(ak/2)} \quad (23)$$

and are graphically represented in Fig. 2 for the parameters corresponding to the CuO_3 chain: $2\varepsilon = 1.23\ eV$, $t = \bar{t} = 1.4\ eV$ [3]. The gap between the two bands is 2Δ and each bandwidth is $\sqrt{\Delta^2 + 4t\bar{t}} - \Delta$; in the limit $\Delta \to 0$, one recovers the usual dispersion law for the ideal chain $\varepsilon(k) = -2t\cos(ak)$, as it is shown in Fig. 3.

4 Hubbard-type interactions

By *Hubbard-type interactions* we understand interactions which in the site representation couple only electrons belonging to the nearest neighbour sites. There are five types of such elementary processes, schematically represented in Fig. 4: a) on-site; b) inter-site (diagonal interactions); c) bond-site; d) intra-bond – exchange hopping; e) intra-bond – pair hopping (off-diagonal interactions). By analogy with the case of the ideal chain, the hamiltonians corresponding to the Hubbard-type interactions in an alternating chain are introduced in the site representation as follows:

$$\mathcal{H}_{on-site} = \frac{1}{2}\sum_{j,\sigma}\left(U_A n_{j,\sigma}^A n_{j,-\sigma}^A + U_B n_{j,\sigma}^B n_{j,-\sigma}^B\right) \quad (24)$$

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

$$U_{A(B)} = \int\int dx\, dy\, \phi_{j,A(B)}^2(x)V_{ee}(|x - y|)\phi_{j,A(B)}^2(y) \quad (25)$$

with V_{ee} the interaction potential between the electrons (we used also the fact that in 1D the atomic orbitals can be chosen real functions);

$$\mathcal{H}_{inter-site} = \sum_{j,\sigma,\sigma'} n_{j,\sigma}^A\left(V n_{j,\sigma'}^B + \overline{V} n_{j-1,\sigma'}^B\right) \quad (26)$$

with

$$\begin{cases} V = \int\int dx\, dy\, \phi_{j,A}^2(x)V_{ee}(|x - y|)\phi_{j,B}^2(y) \\ \overline{V} = \int\int dx\, dy\, \phi_{j,A}^2(x)V_{ee}(|x - y|)\phi_{j-1,B}^2(y) \end{cases} \quad (27)$$

$$\mathcal{H}_{bond-site} = \sum_{j,\sigma} \left[a_{j,\sigma}^\dagger \left(X_A b_{j,\sigma} + \overline{X}_B b_{j-1,\sigma} \right) + H.c. \right] n_{j,-\sigma}^A +$$

$$\sum_{j,\sigma} \left[b_{j,\sigma}^\dagger \left(X_B a_{j,\sigma} + \overline{X}_A a_{j+1,\sigma} \right) + H.c. \right] n_{j,-\sigma}^B \tag{28}$$

with

$$\begin{cases} X_{A(B)} = \int \int dx\, dy\, \phi_{j,A(B)}(x) \phi_{j,B(A)}(x) V_{ee}(|x-y|) \phi_{j,A(B)}^2(y) \\ \\ \overline{X}_{A(B)} = \int \int dx\, dy\, \phi_{j-1(j+1),B(A)}(x) \phi_{j,A(B)}(x) V_{ee}(|x-y|) \phi_{j,A(B)}^2(y) \end{cases} \tag{29}$$

$$\mathcal{H}_{intra-bond}^{exch.} = -\frac{1}{2} \sum_{j,\sigma,\sigma'} \left[a_{j,\sigma}^\dagger \left(W b_{j,\sigma'}^\dagger b_{j,\sigma} + \overline{W} b_{j-1,\sigma'}^\dagger b_{j-1,\sigma} \right) a_{j,\sigma'} + H.c. \right] \tag{30}$$

$$\mathcal{H}_{intra-bond}^{pair} = \frac{1}{2} \sum_{j,\sigma} \left[a_{j,\sigma}^\dagger a_{j,-\sigma} \left(W b_{j,-\sigma} b_{j,\sigma} + \overline{W} b_{j-1,-\sigma} b_{j-1,\sigma} \right) + H.c. \right] \tag{31}$$

with

$$\begin{cases} W = \int \int dx\, dy\, \phi_{j,A}(x) \phi_{j,B}(x) V_{ee}(|x-y|) \phi_{j,A}(y) \phi_{j,B}(y) \\ \\ \overline{W} = \int \int dx\, dy\, \phi_{j,A}(x) \phi_{j-1,B}(x) V_{ee}(|x-y|) \phi_{j,A}(y) \phi_{j-1,B}(y) \end{cases} \tag{32}$$

Let us remark that for the inter-site and intra-bond interaction constants the site index (A or B) does not occur; they are invariant under the transformation $(j,A) \leftrightarrow (j,B)$ (for intra-cell quantities, without overline) or $(j,A) \leftrightarrow (j-1,B)$ (for inter-cell quantities, with overline).

Replacing now the a and b operators by the corresponding c operators according to Eq. (18), we get the form of the Hubbard-type interactions in the two-band model (Bloch representation). For simplicity, we consider the particular case $a_1 = a_2 = a/2$ when $t = \bar{t}$ and

$$\phi = \frac{ak}{2} \ , \quad \Delta = \epsilon \tag{33}$$

In this case will be no distinction between intra-cell interaction constants and the inter-cell ones.

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 (comparable with the bandwidth), the inter-band interactions can be neglected and we may restrict the considerations only to one of the bands (depending on the Fermi level). For CuO_3 the gap is about half of the bandwidth and the filling factor is 3/4, that means a half-filled upper band.

The intra-band interactions in the Bloch representation have the following general form

$$\frac{1}{2N} \sum_{k_1,...,k_4;\sigma,\sigma'} V_{\sigma,\sigma'}(k_1,..,k_4) \delta_{k_1+k_2,k_3+k_4} c_{k_1,\sigma}^\dagger c_{k_2,\sigma'}^\dagger c_{k_4,\sigma'} c_{k_3,\sigma} \tag{34}$$

where the δ-function assures the conservation of the total momentum up to a reciprocal lattice vector. We give below the obtained expressions for V in each band corresponding to the different kinds of interactions:

$$\begin{cases} V_{on-site;1} = [U_A A(k_1) A(k_2) A(k_3) A(k_4) + (A \to B)] \delta_{\sigma,-\sigma'} \\ \\ V_{on-site;2} = [U_B A(k_1) A(k_2) A(k_3) A(k_4) + (A \leftrightarrow B)] \delta_{\sigma,-\sigma'} \end{cases} \tag{35}$$

$$\begin{cases} V_{inter-site;1} = 4V A(k_1) B(k_2) A(k_3) B(k_4) \\ \\ V_{inter-site;2} = V_{inter-site;1}(A \leftrightarrow B) \end{cases} \tag{36}$$

$$\begin{cases} V_{bond-site;1} = 4 \{ X_A [\cos(ak_1/2) B(k_1) A(k_3) + \\ \qquad \cos(ak_3/2) A(k_1) B(k_3)] A(k_2) A(k_4) + (A \leftrightarrow B) \} \delta_{\sigma,-\sigma'} \\ V_{bond-site;2} = -4 \{ X_A [\cos(ak_1/2) A(k_1) B(k_3) + \\ \qquad \cos(ak_3/2) B(k_1) A(k_3)] B(k_2) B(k_4) + (A \leftrightarrow B) \} \delta_{\sigma,-\sigma'} \end{cases} \tag{37}$$

$$\begin{cases} V_{intra-bond;1}^{exch.} = 4W \cos[a(k_1-k_4)/2] A(k_1) B(k_2) B(k_3) A(k_4) \\ \\ V_{intra-bond;2}^{exch.} = V_{intra-bond;1}^{exch.}(A \leftrightarrow B) \end{cases} \tag{38}$$

$$\begin{cases} V_{intra-bond;1}^{pair} = 2W \cos[a(k_1+k_2)/2] [A(k_1) A(k_2) B(k_3) B(k_4) + \\ \qquad\qquad\qquad\qquad\qquad\qquad (A \leftrightarrow B)] \delta_{\sigma,-\sigma'} \\ V_{intra-bond;2}^{pair} = V_{intra-bond;1}^{pair} \end{cases} \tag{39}$$

All the obtained potentials have a complicated k-dependence; however, they are separable functions of the k-variables. A first step in analyzing the possible efect of these interactions is to evaluate them around the Fermi points $\pm k_F$; we do this in terms of the g-constants which describe the elementary processes of backward, forward and Umklapp scatterings, characteristic to the 1D *Fermi gaz model* [10, 11]:

$$backward \quad g_1 \; : \; k_1 = k_4 = \pm k_F \; , \; k_2 = k_3 = \mp k_F$$

$$forward \quad g_2 \; : \; k_1 = k_3 = \pm k_F \; , \; k_2 = k_4 = \mp k_F$$
$$g_4 \; : \; k_1 = k_2 = k_3 = k_4 = \pm k_F \qquad (40)$$

$$Umklapp \quad g_3 \; : \; k_1 = k_2 = \pm k_F \; , \; k_3 = k_4 = \mp k_F \; (ak_F = \pi/2)$$

In the backward scattering process, the momentum transfer is $2k_F$; in the forward one, it is zero (g_2 couples electrons from different branches, g_4 from the same branch); g_3 process is possible only at half-filling, when $4k_F$ is equal to the reciprocal lattice vector. Each coupling constant has two components, as the spins are parallel (∥) or antiparallel ($\perp$), but from the expression of the hamiltonian it is clear that $g_{3,\parallel}$ and $g_{4,\parallel}$ bring no contribution and thus the spin index can be omitted. For the Hubbard-type models it can be shown that always $g_{2,\perp} = g_4$ and therefore only five constants are independent. The values of these constants for the Hubbard-like interactions in an ideal chain (with 1/2- and 3/4- filled band) and in an alternating one (with parameters as in CuO_3 chain) are presented in Table 1.

As can be observed from Table 1, the g-constants for a band coming from an ideal chain differ considerably from one corresponding to an alternating chain, both of them at half-filling; maybe the most important difference consists in the occurence of the bond-site interaction term, which in an ideal chain brings no contribution at half-filling [6]. There is an almost complete analogy between a half-filled band of an alternating chain and a 3/4-filled band of an ideal chain; the differences consist in an appearence of an Umklapp term in the first case and of course in the values of the constants which are given by

$$\mathcal{U} = 0.41 U_A + 0.13 U_B \; , \; \mathcal{V} = 0.46 V \; , \; \mathcal{X} = 0.31 X_A + 0.18 X_B \; , \; \mathcal{W} = 0.46 W \quad (41)$$

If we assume the same interaction constants for A and B sites, it follows a decreasing of their values (in comparison with the ideal chain) with a factor around two. The on-site effective constants for the CuO_3 chain have been estimated at the values $U_A \approx 3-4$ eV , $U_B \approx 1-3$ eV [3]; the other effective constants are less well known. It is reasonable to consider them as positive and to assume an ordering $U > V \gg X > W$ ($U > X \gg V \simeq W$) for a long

(short) range inter-electronic potential V_{ee}, as it has been shown in the case of the ideal chain [6, 7, 12].

Table 1

A comparison between the g-constants (at the Fermi level) for an ideal chain (1/2- and 3/4-filled band) and the alternating CuO_3 chain ($2\epsilon = 1.23$ eV, $t = 1.4$ eV, half-filled upper band [3]); the interaction constants from the last column are defined in Eq. (41).

	Ideal chain		Alternating chain
	$n = 1$	$n = 3/2$	*half-filled upper band*
$g_{1,\parallel}$	$-2V + 2W$	$2W$	$2\mathcal{W}$
$g_{1,\perp}$	$U - 2V + 4W$	$U - 4\sqrt{2}X + 4W$	$\mathcal{U} - 4\sqrt{2}\mathcal{X} + 4\mathcal{W}$
$g_{2,\parallel}$	$2V - 2W$	$2V$	$2\mathcal{V}$
$g_{2,\perp}$	$U + 2V$	$U + 2V - 4\sqrt{2}X + 2W$	$\mathcal{U} + 2\mathcal{V} - 4\sqrt{2}\mathcal{X} + 2\mathcal{W}$
g_3	$U - 2V - 4W$	–	$\mathcal{U} - 4\sqrt{2}\mathcal{X}$
g_4	$U + 2V$	$U + 2V - 4\sqrt{2}X + 2W$	$\mathcal{U} + 2\mathcal{V} - 4\sqrt{2}\mathcal{X} + 2\mathcal{W}$

In terms of the g-constants, a superconductor state is expected in the region [10, 11]

$$g_{1,\parallel} - g_{2,\parallel} - g_{2,\perp} \geq |g_3| \qquad (42)$$

at exactly half-filling, or

$$g_{1,\parallel} - g_{2,\parallel} - g_{2,\perp} \geq 0 \qquad (43)$$

if the Umklapp process does not occur. For the upper band of an alternating chain, the condition (42) becomes

$$\theta\left(\mathcal{U} - 4\sqrt{2}\mathcal{X}\right)\left|\mathcal{U} - 4\sqrt{2}\mathcal{X}\right| \le -2\mathcal{V} \qquad (44)$$

with θ the step function; from Eq. (43) we get

$$\mathcal{U} - 4\sqrt{2}\mathcal{X} + 4\mathcal{V} \le 0 \qquad (45)$$

The condition (44) cannot be fulfiled for any positive $\mathcal{V}$; the dominant phase will be a charge density wave (CDW) if the quantity $g_{1,\parallel} - g_{2,\parallel} + g_{2,\perp} - |g_{1,\perp}|$ (i.e., $\mathcal{U} - 4\sqrt{2}\mathcal{X} + 4\mathcal{W}$) is less than zero or a spin density wave (SDW) otherwise. Nevertheless, let us notice that for a very small inter-site attraction and $\mathcal{U} \le 4\sqrt{2}\mathcal{X}$, the occurence of a superconductor state becomes possible.

If the Umklapp term is neglected, accordingly to Eq. (45) the superconductor phase can appear for a strong enough bond-site repulsion. For short range inter-electronic potentials (when both the inter-site and intra-bond interactions can be neglected), this happens when $\mathcal{X}/\mathcal{U} \ge 0.18$; in the case of an ideal chain and for a very effective screening, the ratio $X/\mathcal{U}$ has been estimated in the range $0.15 - 0.18$ [12]. Such a value may be consequently considered as realistic for un alternating chain too, but this question depends of course on a proper evaluation of the model parameters.

5 Conclusions

The results obtained in 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 was explicitly derived; it has been used after that to find the expressions of the Hubbard-type interactions, initially introduced in the site-representation, in the corresponding two-band model. A qualitative discussion in terms of the g-ology constants, using renormalization group results, indicate the range of the parameters where different kind of instabilities can occur. For the half-filled upper band of the CuO_3 chain, the dominant phases are SDW or CDW as for the Hubbard model with an effective constant $\mathcal{U} - 4\sqrt{2}\mathcal{X} + 4\mathcal{W}$; if the band is not exactly half-filled, a superconductor state can appear for $\mathcal{U} - 4\sqrt{2}\mathcal{X} + 4\mathcal{V} \le 0$.

The alternating chain considered in this paper does not account for an already dimerized system due to other degrees of freedom, as the interaction with the lattice. A more realistic model for the CuO_3 chain should start with a distorted alternating structure (a CDW ground state) [3]; in this case the

number of the non-equivalent sites per unit cell will be four, leading to a four-band model where the first three bands are filled and the highest one is empty. The form of the Hubbard-like interactions in such a model can be a subject of future investigations.

The evaluation of the inter-electronic potentials around the Fermi level, as it was discussed above, provides only a qualitative information about the role played by the Hubbard-type interactions in alternating chains. A deeper analysis requires a complete accounting for the k-dependence of both the energy and the two-particle interactions in the given band. A ground-state phase diagram in a mean-field-type approximation can be found by similar calculations as it was done for the 1D Hubbard model with a bond-site interaction [13]. In spite of the complicate form of the determined potentials, such a method can be in principle applied; due to their separability in the k-variables, the approximate Bethe-Salpeter equation can be solved analytically.
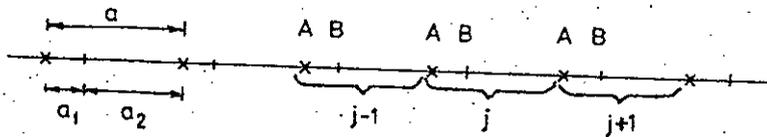
Figure 1. Alternating chain with two non-equivalent sites per unit cell.
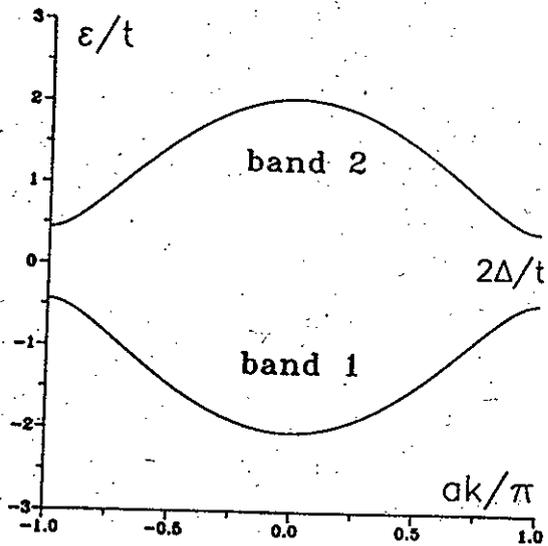
Figure 2. The two-band model corresponding to the one-particle hamiltonian in the tight binding approximation for an alternating chain with two non-equivalent sites per unit cell.
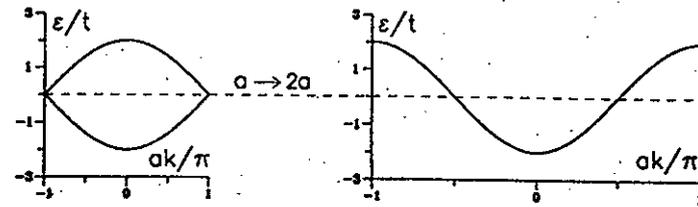
Figure 3. In the limiting case $\Delta \to 0$, the usual dispersion law for an ideal chain $\varepsilon(k) = -2t\cos(ak)$ is recovered.

Figure 4. Hubbard-type interactions: a) on-site; b) inter-site; c) bond-site; d) intra-bond – exchange hopping; e) intra-bond – pair hopping.

References

[1] J.Tinka Gammel, A.Saxena, I.Batistić, A.R.Bishop and S.R.Phillpot, Phys.Rev. B **45**, 6408 (1992).

[2] S.M.Weber-Milbrodt, J.Tinka Gammel, A.R.Bishop and E.Y.Loh, Jr., Phys.Rev. B **45**, 6435 (1992).

[3] S.-L.Drechsler, J.Malek, M.Yu.Lavrentiev and H.Köppel, Phys.Rev. B **49**, 233 (1994).

[4] J.Hubbard, Proc.Roy.Soc.(London) A **276**, 238 (1963).

[5] J.Hubbard, Phys.Rev. B **17**, 494 (1978).

[6] S.Kivelson, W.-P.Su, J.R.Schrieffer and A.J.Heeger, Phys.Rev.Lett. **58**, 1899 (1987).

[7] A.Painelli and A.Girlando, Phys.Rev. B **39**, 2830 (1989).

[8] S.Tang and J.E.Hirsh, Phys.Rev. B **42**, 771 (1990).

[9] A.Hui and S.Doniach, Phys.Rev. B **48**, 2063 (1993).

[10] V.N.Prigodin and Yu.A.Firsov, Zh.Eksp.Teor.Fiz. **71**, 2252 (1976) [Sov.Phys. JETP **44**, 1187 (1976)].

[11] J.Sólyom, Adv.Phys. **28**, 201 (1979).

[12] D.K.Campbell, J.Tinka Gammel and E.Y.Loh, Jr., Phys.Rev. B **38**, 12043 (1988).

[13] F.D.Buzatu, Phys.Rev. B **49**, 10176 (1994); Int.J.Mod.Phys. B **9**, 1503 (1995).