Abstract. We consider a Hubbard chain with an energy difference $\Delta$ between the odd and even sites. The model, known as the one-dimensional ionic Hubbard model, is used to describe the neutral-ionic transition in mixed-stack charge-transfer organic crystals and the displacive-type ferroelectric transition in perovskite oxide compounds. We show that for sufficiently large $\Delta$ and electron densities less than half-filling the system reduces to the one-band Hubbard model with a bond-site interaction, model known as relevant to quasi-one-dimensional materials with a large conduction bandwidth.

Key words: Hubbard model, alternating chain, bond-site interaction.

1. THE MODEL

The one-dimensional (1D) ionic Hubbard model (IHM) was introduced as a minimal model to describe the neutral-ionic transition that takes place in mixed-stack charge-transfer organic crystals [1, 2, 3, 4]; later, it has been used to explain the displacive-type ferroelectric transition in perovskite oxide compounds [5, 6]. The Hamiltonian of the model is [7]:

$$H_{\text{IHM}} = -t \sum_{j, \sigma} \left( c_{j, \sigma}^{\dagger} c_{j+1, \sigma} + H.c. \right) + \Delta \sum_{j, \sigma} \left( -1 \right)^j n_{j, \sigma} + U \sum_j n_{j, \uparrow} n_{j, \downarrow},$$

where $c_{j, \sigma}^{\dagger}$ are the usual Fermi creation (annihilation) operators in the Wannier representation and $n_{j, \sigma} = c_{j, \sigma}^{\dagger} c_{j, \sigma}$. Let us remark, in addition to the band term $t$ and to the on-site interaction $U$ (Hubbard model), the existence...
of the one-particle alternating potential $\Delta$ that changes the periodicity of the chain: the lattice constant $a$ is equal to the double distance between two consecutive and equidistant sites, as it is shown in Fig. 1.

![Schematic view of the alternating structure corresponding to the one-dimensional ionic Hubbard model.](image)

Fig. 1 – Schematic view of the alternating structure corresponding to the one-dimensional ionic Hubbard model.

The model has been intensively investigated only at half filling where it exhibits remarkable properties. At $U = 0$ the system is an usual band insulator (BI) because the $\Delta$ term determines the occurrence of a gap in the single-particle excitations and the lower band is completely filled. When $U \ll \Delta$ the system is still a BI and a charge density wave (CDW) occurs in the ground-state (alternating double-occupied and empty sites). For $U \gg \Delta$ (negligible gap) the system behaves like the 1D Hubbard model which is a Mott insulator (MI – occurrence of a gap in the charge excitation spectrum) with a spin density wave (SDW) in the ground-state. Consequently, a transition between the two regimes is expected at $U \approx \Delta$. The interest for the model renewed once with the work of Fabrizio et al. [8] that proved the existence of a spontaneously dimerized insulating (SDI) phase between BI and MI phases at half-filling. The SDI phase is essentially identical with the bond charge density wave (BCDW) state that seems to occur also in the 1D half-filled extended Hubbard Model [9].

In the present work we start from the $U = 0$ case when the Hamiltonian given by Eq. (1) can be easily diagonalized by a canonical transformation; we get a two-band model of non-interacting electrons. The on-site interaction from Eq. (1) induces both intra- and inter-band two-particle interactions [10, 11]. However, in the high ionicity regime when $\Delta$ is larger than $U$ and much larger than $t$, and for electron concentrations less than half-filling, one can restrict the considerations to the lower band. The resulting model exhibits only on-site and bond-charge interactions, model known also as the 1D ($t,U,X$)-model and used to describe electronic properties of conducting polymers [12]. The 2D version of the ($t,U,X$)-model was proposed to describe the hole superconductivity mechanism [13].
2. THE CANONICAL TRANSFORMATION

In order to put in evidence the alternating structure of the system, let us denote, as in Fig. 1, the even sites by A and the odd sites by B; the Fermi operators \( c_{2j,\sigma} \) from Eq. (1) will be consequently denoted by \( a_{j,\sigma} \) and the \( c_{2j+1,\sigma} \) operators by \( b_{j,\sigma} \).

The Hamiltonian corresponding to the first two terms from Eq. (1) can be easily diagonalized. At first we pass from the Wannier representation to the Bloch representation

\[
H_0 = -2t \sum_{k,\sigma} \cos \frac{ak}{2} \left( e^{-iak/2} a_{k,\sigma}^\dagger b_{k,\sigma} + H.c. \right) + \Delta \sum_{k,\sigma} \left( a_{k,\sigma}^\dagger a_{k,\sigma} - b_{k,\sigma}^\dagger b_{k,\sigma} \right) \tag{2}
\]

and then we apply the following canonical transformation [10, 11]

\[
\begin{align*}
\begin{cases}
  a_k = A(k)e^{-iak/2}c_{k,\sigma}^{(1)} + B(k)c_{k,\sigma}^{(2)} \\
  b_k = B(k)c_{k,\sigma}^{(1)} - A(k)e^{iak/2}c_{k,\sigma}^{(2)}
\end{cases}
\end{align*}
\tag{3}
\]

where

\[
\begin{align*}
A(k) &= \frac{1}{\sqrt{2}} \left[ 1 + \frac{\Delta}{\varepsilon(k)} \right]^{\frac{1}{2}} \\
B(k) &= \frac{1}{\sqrt{2}} \left[ 1 - \frac{\Delta}{\varepsilon(k)} \right]^{\frac{1}{2}}
\end{align*}
\tag{4}
\]

and

\[
\varepsilon(k) = -\sqrt{\Delta^2 + 4t^2 \cos^2(ak/2)}. \tag{5}
\]

Eq. (2) becomes then

\[
H_0 = \sum_{\alpha,k,\sigma} (-1)^{\alpha-1} \varepsilon(k)^{(\alpha)} c_{k,\sigma}^{(\alpha)} c_{k,\sigma}^{(\alpha)}, \quad \alpha = 1, 2 \tag{6}
\]

and we get thus the two-band model represented in Fig. 2.

The last term in Eq. (2) introduces in the above representation both intra- and inter-band two-particle interactions. For example, the interaction induced by \( U \) in the lower band is [10, 11]

\[
H_1 = \frac{1}{2N} \sum_{k_1,\ldots,k_4} \delta_{k_1+k_2+k_3+k_4} V(k_1, \ldots, k_4) c_{k_1,\sigma}^{(\dagger)} c_{k_2,\sigma}^{(\dagger)} c_{k_2,\sigma} c_{k_4,\sigma}, \tag{7}
\]

with

\[
V = U \left[ \prod_{i=1}^{4} B(k_i) \pm \prod_{i=1}^{4} A(k_i) \right]. \tag{8}
\]
3. THE HIGH IONICITY REGIME

We consider now the case when the gap parameter $\Delta$ is larger than the Hubbard constant $U$ and much larger than the bandwidth parameter $t$, i.e.,

$$\frac{|U|}{\Delta} < 1, \quad \frac{t^2}{\Delta^2} \ll 1.$$  \hspace{1cm} (9)

For electron concentrations less than half-filling ($ak_F < \pi$), the first condition from Eq. (9) allows us to restrict the considerations to the lower band. The second condition from Eq. (9) is a simplifying assumption that defines a small parameter; all the terms of order greater than $t^2/\Delta^2$ will be neglected. In these conditions we get a one-band model with the same dispersion law as for free electrons in an usual non-alternating chain [see Eq. (5)]

$$\varepsilon(k) \approx -2t \cos(ak), \quad \mathcal{T} \equiv \frac{t^2}{2\Delta}$$  \hspace{1cm} (10)

and the following two-particle interaction [see Eq. (8)]

$$V(k_1, \ldots, k_4) \approx \mathcal{U} + 4\mathcal{X} [\cos (ak_1) + \cos (ak_3)]$$  \hspace{1cm} (11)

with

$$\mathcal{U} \equiv \left(1 - \frac{t^2}{\Delta^2}\right) U, \quad \mathcal{X} \equiv -\frac{t^2}{8\Delta^2} U.$$  \hspace{1cm} (12)

The expression obtained for $V$ coincides with the interaction potential of the 1D $(t, U, X)$-model in the Bloch representation (with renormalized parameters), as can be seen by comparing the Eq. (11) from above with the Eq. (5).
from Ref. [14]. In the Wannier representation, the Hamiltonian corresponding to the Eqs. (10) and (11) writes

\[ H = -t \sum_{j, \sigma} \left( c_{j, \sigma}^\dagger c_{j+1, \sigma} + c_{j+1, \sigma}^\dagger c_{j, \sigma} \right) + U \sum_j n_{j, \uparrow} n_{j, \downarrow} \]

\[ + X \sum_{j, \sigma} \left( c_{j, \sigma}^\dagger c_{j+1, \sigma} + c_{j+1, \sigma}^\dagger c_{j, \sigma} \right) \left( n_{j, -\sigma} + n_{j+1, -\sigma} \right) \]  

(13)

and it is the standard form of the 1D \((t, U, X)\)-model, describing electrons with on-site \((U)\) and bond-site \((X)\) interactions. For quasi-1D materials with large bandwidth like conducting polymers, it has been shown that the \(X\) term is the next important term after the on-site repulsion \(U\) [12] and it takes negative values [15], in agreement with the Eq. (12) from above. The ground-state instabilities (charge and spin density waves, singlet superconductivity) of the 1D \((t, U, X)\)-model have been analyzed in a mean-field-like approach in the Ref. [14].

In conclusion, in the high ionicity regime and below half-filling, the 1D IHM can be approximated by a one-band model with a narrower bandwidth, a reduced on-site interaction, and a small bond-site coupling term proportional to the on-site interaction and with opposite sign. Our result can be regarded as another derivation of the 1D \((t, U, X)\)-model: the \(X\) term can appear from the on-site repulsion in the presence of a large site-alternating potential.

Acknowledgement. This work was supported by the research project CERES C4-163.

REFERENCES