

Dedicated to Prof. Dorin N. Poenaru's
70th Anniversary

ONE-DIMENSIONAL IONIC HUBBARD MODEL IN THE HIGH IONICITY LIMIT

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(Received February 26, 2007)

Abstract. We consider a Hubbard chain with an energy difference Δ 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 Δ 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]:

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

where $c^\dagger(c)_{j,\sigma}$ 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 Δ 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.

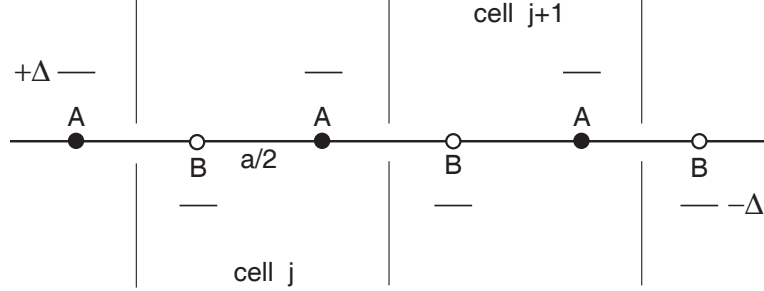


Fig. 1 – Schematic view of the alternating structure corresponding to the one-dimensional ionic Hubbard model.

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 Δ 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 Δ 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

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

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

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

where

$$\begin{cases} A(k) = \frac{1}{\sqrt{2}} \left[1 + \frac{\Delta}{\varepsilon(k)} \right]^{\frac{1}{2}} \\ B(k) = \frac{1}{\sqrt{2}} \left[1 - \frac{\Delta}{\varepsilon(k)} \right]^{\frac{1}{2}} \end{cases} \quad (4)$$

and

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

Eq. (2) becomes then

$$H_0 = \sum_{\alpha;k,\sigma} (-1)^{\alpha-1} \varepsilon(k) c_{k,\sigma}^{(\alpha)\dagger} c_{k,\sigma}^{(\alpha)}, \quad \alpha = 1, 2 \quad (6)$$

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]

$$H_1 = \frac{1}{2N} \sum_{k_{1-4};\sigma} \delta_{k_1+k_2, k_3+k_4} V(k_1, \dots, k_4) c_{k_1,\sigma}^\dagger c_{k_2,-\sigma}^\dagger c_{k_4,-\sigma} c_{k_3,\sigma}, \quad (7)$$

with

$$V = U \left[\prod_{i=1}^4 B(k_i) \pm \prod_{i=1}^4 A(k_i) \right]. \quad (8)$$

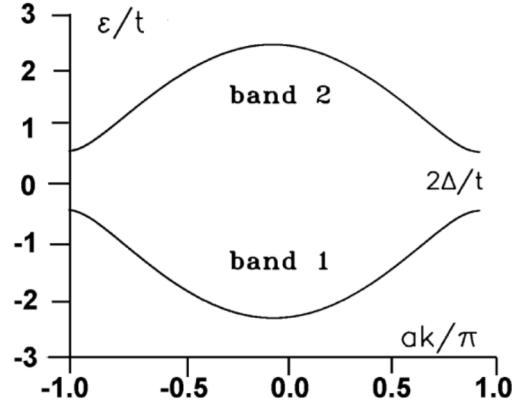


Fig. 2 – The two-band model corresponding to the one-dimensional ionic Hubbard model at $U = 0$.

3. THE HIGH IONICITY REGIME

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

$$|U|/\Delta < 1, \quad t^2/\Delta^2 \ll 1. \quad (9)$$

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/Δ^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)]

$$\varepsilon(k) \approx -2\bar{t} \cos(ak), \quad \bar{t} \equiv \frac{t^2}{2\Delta} \quad (10)$$

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

$$V(k_1, \dots, k_4) \approx \bar{U} + 4\bar{X} [\cos(ak_1) + \cos(ak_3)] \quad (11)$$

with

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

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

$$\begin{aligned}
 H = & -\bar{t} \sum_{j;\sigma} \left(c_{j,\sigma}^\dagger c_{j+1,\sigma} + c_{j+1,\sigma}^\dagger c_{j,\sigma} \right) + \bar{U} \sum_j n_{j,\uparrow} n_{j,\downarrow} \\
 & + \bar{X} \sum_{j,\sigma} \left(c_{j,\sigma}^\dagger c_{j+1,\sigma} + c_{j+1,\sigma}^\dagger c_{j,\sigma} \right) (n_{j,-\sigma} + n_{j+1,-\sigma}) \quad (13)
 \end{aligned}$$

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.

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