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

ONE-DIMENSIONAL IONIC HUBBARD MODEL IN THE HIGH IONICITY LIMIT

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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]:

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

where $c^{\dagger}(c)_{j,\sigma}$ are the usual Fermi creation (annihilation) operators in the Wannier representation and $n_{j,\sigma} = c^{\dagger}_{j,\sigma} c_{j,\sigma}$. 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.

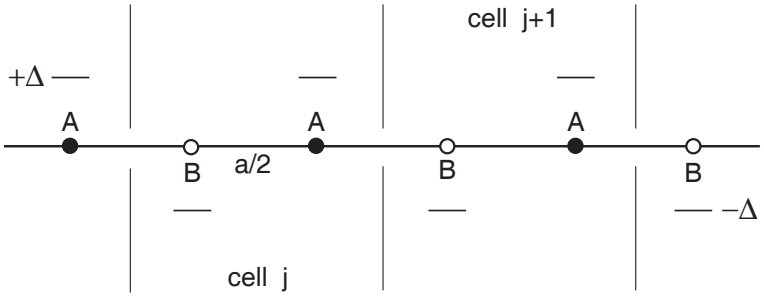

Fig. 1 – Schematic view of the alternating structure corresponding to the one-dimensional ionic Hubbard model.

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

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

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

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

where

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

and

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

Eq. (2) becomes then

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

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]

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

with

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

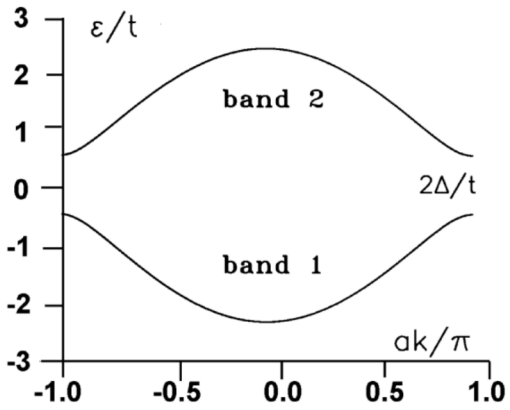

Fig. 2 – The two-band model corresponding to the one-dimensional ionic Hubbard model at $U = 0$.

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.,

$$|U|/\Delta < 1, \quad t^2/\Delta^2 \ll 1. \tag{9}$$

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)]

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

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

$$V(k_1, \ldots, k_4) \approx \overline{U} + 4\overline{X}\left[\cos\left(ak_1\right) + \cos\left(ak_3\right)\right] \tag{11}$$

with

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

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

$$H = -\overline{t}\sum_{j;\sigma}\left(c^{\dagger}_{j,\sigma}c_{j+1,\sigma} + c^{\dagger}_{j+1,\sigma}c_{j,\sigma}\right) + \overline{U}\sum_{j} n_{j,\uparrow}n_{j,\downarrow} + \overline{X}\sum_{j,\sigma}\left(c^{\dagger}_{j,\sigma}c_{j+1,\sigma} + c^{\dagger}_{j+1,\sigma}c_{j,\sigma}\right)\left(n_{j,-\sigma} + n_{j+1,-\sigma}\right) \tag{13}$$

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.

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REFERENCES

1. J.B. Torrance, J.E. Vazquez, J.J. Mayerle, and V.Y. Lee, Phys. Rev. Lett., **46**, 253 (1981); **47**, 1747 (1981).
2. DM.J. Rice and E.J. Mele, Phys. Rev. Lett., **49**, 1455 (1982).
3. N. Nagaosa and J. Takimoto, J. Phys. Soc. Jpn., **55**, 2735 (1986); **55**, 2745 (1986); *ibid.*, **55**, 2754 (1986).
4. A. Girlando and A. Painelli, Phys. Rev., B **34**, 2131 (1986); A. Painelli and A. Girlando, *ibid.*, **37**, 5748 (1988); **39**, 9663 (1989).
5. T. Egami, S. Ishihara, and M. Tachiki, Science, **261**, 1307 (1993); S. Ishihara, T. Egami, and M. Tachiki, Phys. Rev., B **49**, 8944 (1994).
6. R. Resta and S. Sorella, Phys. Rev. Lett., **74**, 4738 (1995); **82**, 370 (1999).
7. J. Hubbard and J. B Torrance, Phys. Rev. Lett., **47**, 1750 (1981).
8. M. Fabrizio, A.O. Gogolin, and A.A. Nersesyan, Phys. Rev. Lett., **83**, 2014 (1999).
9. M. Nakamura, J. Phys. Soc. Jpn., **68**, 3123 (1999); Phys. Rev., B **61**, 16377 (2000).
10. F.D. Buzatu and E. Pieleanu, Rom. J. Phys., **42**, 185 (1997).
11. F.D. Buzatu and G. Jackeli, Phys. Lett., A **246**, 163 (1998).

12. A. Painelli and A. Girlando, Phys. Rev., B **39**, 2830 (1989).
13. J.E. Hirsch, Phys. Lett., A **134**, 452 (1989); Physica, C **158**, 326 (1989).
14. F.D. Buzatu, Phys. Rev., B **49**, 10176 (1994).
15. A. Painelli and A. Girlando, in *Interacting Electrons in Reduced Dimensions*, eds. D. Baeriswyl and D.K. Campbell, NATO ASI B 213, Plenum Press, New York, 1988, p. 165.