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A Luttinger model for 1-d organic polymers

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Résumé. — Nous montrons que pour une interaction de Luttinger entre électrons quelconque, il n'y a pas de dimérisation du réseau pour un polymère organique à une dimension.

Abstract. — We demonstrate that for a Luttinger type interaction between electrons, no dimerization is found in a 1-d organic polymer whatever the interaction strength.

1. Introduction.

In a preceding paper [1] (hereafter referred to as I), we have shown that a model for 1-d organic polymers in the presence of lattice distortion and electron correlation can be obtained by taking the continuum limit of a Hamiltonian built up by the combination of the SSH Hamiltonian and a Hubbard-type repulsion term. Our starting point was thus the Hamiltonian [2, 3] of I, namely (see I for notations) :

$$H = \sum_s \int dx \left\{ \psi_s^\dagger \left(-i\hbar v_F \tau_3 \frac{\partial}{\partial x} + m\tau_1 \right) \psi_s + a \frac{U}{2} [(\psi_s^\dagger \psi_s)(\psi_{-s}^\dagger \psi_{-s}) + (\psi_s^\dagger \tau_2 \psi_s)(\psi_{-s}^\dagger \tau_2 \psi_{-s})] \right\} + \frac{1}{2} \int \frac{dx}{a} K \left(\frac{m}{2\alpha} \right)^2. \quad (1.1)$$

In reference [1] we remarked that in the present state of the art no exact diagonalization of this Hamiltonian is known. The temptation is great to resort to a simpler description of the electron interaction for which the diagonalization is known, namely the so-called massive Thirring model, the Hamiltonian of which being :

$$H_1 = \sum_s \int dx \left\{ \psi_s^\dagger \left(-i\hbar v_F \tau_3 \frac{\partial}{\partial x} + m\tau_1 \right) \psi_s + a \frac{U}{2} \psi_{1s}^\dagger \psi_{2s}^\dagger \psi_{2s} \psi_{1s} \right\}. \quad (1.2)$$

As is well known (2), the Hamiltonian (1.2) is the continuum version of the so-called Luttinger model for which the interaction is between electrons, disregarding the spin, located on neighbouring sites, namely of the form :

$$c_{n+1}^\dagger c_n^\dagger c_{n+1} c_n.$$

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We postpone to the end of this paper the discussion of the physical meaning of such a description for the case of 1-d polymers and we rewrite Hamiltonian (1.2), supplemented with the elastic term, in a convenient form for further use of the results of Thacker's paper (3) :

$$(2 at_0)^{-1} H_l = \sum_s \int dx \left[\psi_s^+ \left(-i\tau_3 \frac{\partial}{\partial x} + m\tau_1 \right) \psi_s + g_0 \psi_{1s}^+ \psi_{2s}^+ \psi_{2s} \psi_{1s} \right] + \frac{2}{\eta} \int m_0^2 dx \quad (1.3)$$

with the identification

$$\hbar v_F = 2 at_0; \quad m_0 = \frac{m}{2 at_0}; \quad \eta = \frac{8 \alpha^2}{K t_0}; \quad g_0 = \frac{U}{4 t_0}. \quad (1.4)$$

Note that m_0 and $\psi^+ \psi$ have the dimension L^{-1} , whereas η and g_0 are dimensionless quantities. α , K and t_0 are the standard parameters introduced by SSH [4].

2. Energy of the ground state.

We start from Hamiltonian (1.3) and we use the results of Thacker [3] (hereafter referred to as T) in order to diagonalize it. Thacker has shown that the energy is given by (T. Eq. 2-56) :

$$E_T = m_0 \sum_{i=1}^n \cosh \xi_i \quad (2.1)$$

where ξ_i is the so-called rapidity. For the ground state Thacker shows that :

$$\xi_i = i\pi - \alpha_i \quad (2.2)$$

where α_i is a real number. The moment k_i of each state i is related to α_i by :

$$k_i = m_0 \sinh \alpha_i. \quad (2.2a)$$

In order to compute (2.1), one introduces the density of states which according to T (2.77) is the solution of

$$2 \pi \rho_1(\alpha) = m_0 \cosh \alpha - \int_{-A}^A d\alpha' K(\alpha - \alpha') \rho(\alpha') \quad (2.3)$$

where

$$K(\alpha) = \frac{\sin 2\mu}{\cosh \alpha - \cos 2\mu} \quad (2.3a)$$

$$\mu = -\cotan^{-1} \left(\frac{g_0}{2} \right) \quad \mu > \pi/2 \quad (2.3b)$$

and A is a cut-off introduced in order to avoid undesirable ultra-violet divergencies. For $A \gg 1$ the solution of (2.3) can be obtained by a Fourier transform, and is found to be :

$$\rho(\alpha) = \frac{1}{2\pi} \frac{m_0 \gamma e^{A(1-\gamma)}}{\pi(\gamma-1)} \tan \pi\gamma \cosh \gamma\alpha \quad (2.4)$$

where

$$\gamma = \frac{\pi}{2\mu}. \quad (2.4a)$$

The energy of the ground state then reads

$$E_{GS} = \frac{m_0^2 \gamma e^{A(1-\gamma)}}{2\pi^2(\gamma-1)} \int_{-A}^A \cosh \alpha \cosh \gamma\alpha d\alpha \quad (2.5)$$

so that the total energy density in $\hbar v_F$ units is given by

$$(L\hbar v_F)^{-1} = \frac{m_0^2 \gamma e^{A(1-\gamma)}}{\pi \pi(\gamma-1)} \tan \pi\gamma \left[\frac{\sinh(\gamma+1)A}{\gamma+1} + \frac{\sinh(\gamma-1)A}{\gamma-1} \right] + \frac{2}{\eta} m_0^2. \quad (2.6)$$

Note an extra factor of 2 in the first term of the r.h.s. which takes spin degeneracy into account. L is the length of the system.

3. Results.

Equation (2.6) depends on the cut-off Λ . This is a particularity of the Thirring model, and as such the « exact » solution (2.6) is of no practical use if no prescription is given in order to determine Λ . Such a prescription must rely on physical grounds.

Let us first investigate the case $g_0 = 0$, i.e. no correlation between the electrons. Hamiltonian (1.3), or (1.2), reduces to the form of Takayama, Lin-liu and Maki's [5] (hereafter referred to as TLM); (2.6) gives the ground state in this case by setting

$$\gamma = \lim_{\epsilon \rightarrow 0^+} (1 - \epsilon)$$

and reduces to (see Eq. (3.5) of paper I with $U = 0$)

$$(L\hbar v_F)^{-1} E_{GS}^0 = -\frac{m_0^2}{\pi} [\sinh \Lambda \cosh \Lambda + \Lambda] + \frac{2}{\eta} m_0^2. \tag{3.1}$$

Introducing a cut-off in the momentum space by (cf. Eq. (2.2a)) :

$$\sinh \Lambda = \frac{k_c}{m_0} \tag{3.2}$$

E_{GS}^0 takes the form

$$(L\hbar v_F)^{-1} E_{GS}^0 = -\frac{m_0^2}{\pi} \left\{ \frac{k_c}{m_0} \left(1 + \left(\frac{k_c}{m_0} \right)^2 \right)^{1/2} + \log \left[\frac{k_c}{m_0} + \left(1 + \left(\frac{k_c}{m_0} \right)^2 \right)^{1/2} \right] \right\} + \frac{2}{\eta} m_0^2 \tag{3.3}$$

which is TLM result.

The desired energy is obtained by fixing m_0 through the relation

$$\frac{dE}{dm_0} = 0$$

which after a slight algebra yields :

$$\Lambda = \Lambda_0 = \frac{2\pi}{\eta}. \tag{3.4}$$

Equations (3.4) and (3.2) determine m_0 when k_c is known and E_{GS}^0 takes the very simple form

$$(L\hbar v_F)^{-1} E_{GS}^0 = -\frac{k_c^2}{\pi} \coth \frac{2\pi}{\eta} \tag{3.5}$$

in agreement with equation (3.5a) of paper I.

In order to be complete, one has to determine k_c . This is best achieved by comparing the results of TLM with those of SSH. According to SSH the displacement m_0 is given by

$$K(1 - a^2 m_0^2) - E(1 - am_0^2) = \frac{2\pi}{\eta} am_0 \tag{3.6}$$

where K and E are elliptic functions of the first and second kinds. In the limit of small m_0 , i.e. $am_0 \ll 1$ this reduces to :

$$am_0 \sim 4 \exp \left[- \left(1 + \frac{2\pi}{\eta} \right) \right]. \tag{3.7}$$

Comparing this result with m_0 obtained from the above treatment, namely :

$$am_0 = \frac{ak_c}{\sinh \frac{2\pi}{\eta}} \simeq 2 ak_c e^{-2\pi/\eta} \tag{3.8}$$

k_c turns out to be a universal constant :

$$k_c = \frac{2}{e}. \tag{3.9}$$

Let us now return to the expression (2.6) for the energy in the presence of electron correlation. At this point one could make the assumption that k_c is a constant, possibly $2/e$. However when minimizing E_{GS} with respect to m_0 , it is found that Λ decreases and tends toward zero when γ decreases from 1 to $1/2$. In physical words this means that the more effective, the repulsion is the more the system tends to dimerize, since, according to equation (3.2), m_0 , i.e. the displacement, increases when Λ decreases. An unphysical result indeed. We therefore conclude that k_c must be a function of γ .

This dependency will be obtained by using a physical prescription. Thacker has demonstrated the energy of the lowest unbound fermion-antifermion pair in the massive Thirring model is given by (T Eq. (2.118)) :

$$E_1 = 2 m_F = 2 m_0 \frac{\tan \pi \gamma}{\pi(\gamma - 1)} e^{\Lambda(1-\gamma)}. \quad (3.10)$$

If one identifies this energy with the optical gap Λ_{opt} one is led to minimize E_{GS} with the restriction $E_1 = \Lambda_{opt}$ a given value, i.e.

$$m_0 e^{\Lambda(1-\gamma)} = m_{opt} \frac{\pi(\gamma - 1)}{\tan \pi \gamma} \quad (3.11)$$

where m_{opt} is a constant. Note that this equation determines k_c , through equation (3.2) as a function of γ and m_0 .

The ground state energy now reads

$$(L\hbar v_F)^{-1} E_{GS} = -\frac{1}{\pi} \frac{\pi(\gamma - 1)}{\tan \pi \gamma} m_{opt}^2 \left\{ e^{-\Lambda(1-\gamma)} \left(\frac{\sinh(\gamma + 1)\Lambda}{\gamma + 1} + \frac{\sinh(\gamma - 1)\Lambda}{\gamma - 1} \right) - \frac{2\pi}{\eta} \frac{e^{-2\Lambda(1-\gamma)} \pi(\gamma - 1)}{\tan \pi \gamma} \right\} \quad (3.12)$$

E_{GS} is now a function of Λ and one should determine m_0 by setting

$$\frac{dE_{GS}}{dm_0} = 0 \quad \text{i.e.} \quad \frac{dE_{GS}}{d\Lambda} = 0.$$

It is easily found that this condition will lead to $\Lambda \rightarrow \infty$, i.e. $m_0 \rightarrow 0$. In other terms the system, in the presence of repulsion, even small, will not be dimerized. Note that $\Lambda \rightarrow \infty$ does not impose $k_c \rightarrow \infty$ since $m_0 \rightarrow 0$ and that, therefore, no undesirable divergencies have been introduced into the computation.

4. Conclusions.

We have now to precise the physical content of the above model. As quoted in the introduction, the chosen interaction is of the Luttinger type. It is plausible that this interaction is in fact equivalent to an extended Hubbard Hamiltonian with an on site repulsion U_0 and a next neighbour interaction U_1 , in the limit $U_0/2 t_0 \gg 1$. Indeed, in this model the presence of two electrons on the same site is prohibited by the Pauli exclusion principle, since the effect of spin (except for a trivial factor of 2 in the energies) has been discarded. This is pictured by the anticommutation relations. In other terms, the presence of two electrons of opposite spins on the same site is also forbidden.

In the language of Hubbard Hamiltonian this means that $U_0/2 t_0 \gg 1$, while the remaining Luttinger like term may be interpreted as the interaction between two electrons on adjacent sites.

It is therefore not surprising to find that dimerization does not occur in this situation. In a way it confirms the result of the self-consistent field calculation as presented in paper I which finds that dimerization decreases when on-site interaction increases.

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References

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| [1] ASLANGUL, C., SAINT-JAMES, D., <i>J. Physique</i> 45 (1984).
Preceding paper. | [4] SU, W. P., SCHRIEFFER, J. R. and HEEGER, A. J., <i>Phys. Rev. B</i> 22 (1980) 2099. |
| [2] GAUDIN, M., <i>La fonction d'onde de Bethe</i> (Masson, Paris) 1983. | [5] TAKAYAMA, H., LIN-LIU, Y. R. and MAKI, K., <i>Phys. Rev. B</i> 21 (1980) 2388. |
| [3] THACKER, H. B., <i>Rev. Mod. Phys.</i> 53 (1981) 253. | |