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Non-linear spin-density excitations in 1-D organic polymers

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Résumé. — On montre que, lorsque l'état fondamental d'un polymère organique à une dimension correspond à une onde de spin antiferromagnétique, il existe des excitations de type soliton (« kink » et « bag »).

Abstract. — It is shown that kink and bag-like solitons should exist in 1-D organic polymers when the ground state corresponds to an antiferromagnetic spin density wave.

Recently Kivelson and Heim [1] have investigated the role of electron-electron repulsion in one-dimensional organic polymers. The model introduces a Hubbard Hamiltonian on a dimerizable lattice. The problem is then solved within a mean field self-consistent approximation. Analytical formulae lead to a complete discussion of the expected two effects : e-e repulsion and Peierls instability. It is found that, depending on the repulsion parameter U and on α , a parameter introduced by SSH [2] in order to characterize the variation of the transfer term with the distance C-C, three possible ground states exist :

- state *a*) the SSH dimerized state,
- state *b*) a « mixed » state in which coexist a dimerization pattern and a spin density wave,
- state *c*) an antiferromagnetic spin density wave ground state with no dimerization.

The « phase diagram » is best represented in the plane of the two dimensionless parameters :

$$\gamma = \frac{U}{2t_0}, \quad \eta = \frac{8\alpha^2}{Kt_0} \quad (1)$$

where $4t_0$ is the band width, and K the elastic constant of the lattice (see SSH for notations).

The domain of state *b*) is very narrow, and the mixed state can be discarded in a first investigation. Then a two-phase diagram is obtained, the boundary between the two states being given by a curve $\gamma = \gamma_c(\eta)$;

Kivelson and Heim have given the limit values of U so that the ground state be indeed the state *a*) for polyacetylene.

Unaware of the, then unpublished, work of these authors, we had derived the same analytical results, but we arrived at a somewhat different conclusion. We have made a different analysis taking into account the fact that the available values for γ and η , as deduced from the values of U , α , K and t_0 to be found in the literature, are quite different, so that the conclusion about the nature of the ground state appears to be uncertain. Actually, taking into account all the available data, a domain is found in the phase diagram which almost completely falls in the SDW region (Fig. 1). Recent measurements, however, seem to indicate a dimerization pattern in polyacetylene [3], but we remark that, besides the above mentioned uncertainty on the polyacetylene ground state, as deduced from theoretical calculations, other organic polymers exist (e.g. polyparaphenylene) which, while exhibiting analogous properties, cannot be described by the SSH model, since they do not display the doubly degenerate lattice conformation. It is therefore interesting to reexamine the possible excitations in the SDW phase. This appears to be attractive since, in this phase, the double degeneracy is recovered (Fig. 2) for any material and therefore allows for the construction of soliton like excitations as in the beautiful SSH model, but which will now correspond to a modulation of the spin structure.

The easiest way to derive the excitations in the SDW state is to follow the procedure of Brazovskii [4a]

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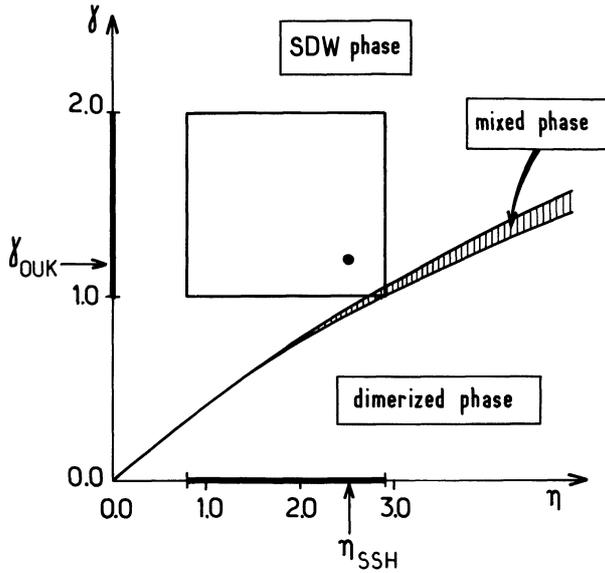


Fig. 1. — Phase diagram in the (γ, η) plane. The rectangle pictures the uncertainty for polyacetylene.

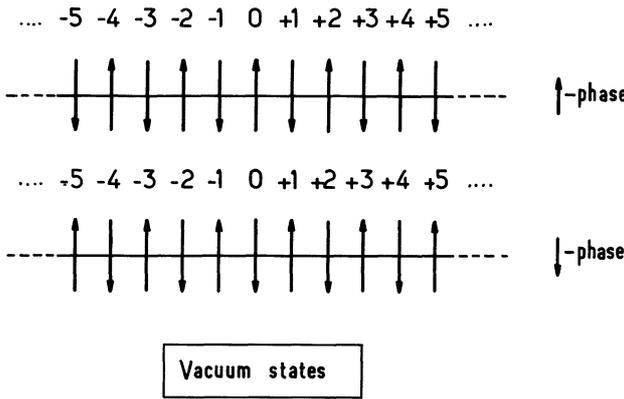


Fig. 2. — Sketch of the doubly degenerate SDW ground state.

and of Takayama *et al.* [4b] (usually referred to as TLM) who introduce a continuous version of the SSH model. Along the same lines one readily obtains a continuous version of the mean-field Hamiltonian, namely :

$$H_{MF} = \sum_s \int dx \psi_s^+(x) \left\{ -i\hbar v_F \sigma_3 \frac{\partial}{\partial x} - 2sU \delta(x) \sigma_1 \right\} \psi_s(x), \quad (2)$$

where we have used the TLM notation. Here $\delta(x)$ is the slowly varying field representing the amplitude of the SDW, and $s = \pm 1/2$.

By comparison with equation (4) of TLM (TLM-4), one can see that $U \delta(x)$ play the same role as TLM's $\Delta(x)$. From equation (2) one easily deduces the BdG equations which are identical with TLM-7, and the

self consistency equation, which is independent of s , and is equivalent to TLM-8 with the identification

$$\frac{aU}{2} = \frac{g^2}{\omega_Q^2}$$

where a is the lattice parameter.

The energy per atom in the SDW manifold is directly computed and reads :

$$E(\delta(x)) = \sum_{k,s}' \varepsilon_{ks} + U \int \frac{dx}{a} \delta^2(x) + \text{Const.} \quad (3)$$

As usual the ε_{ks} 's are the energies corresponding to the BdG eqns, while the second term comes from the expectation value of the repulsion energy. Equation (3) is identical with TLM-9 with the proper identification of the various constants. Note that the role of the elastic term appearing in TLM is here played by the Hubbard mean repulsion.

Following TLM, we first conclude that there exist low energy kink-soliton states involving the spin density field $\delta(x)$ instead of the site displacement one. This is reminiscent of the SSH soliton (see also Rice [4c]).

Taking $U \sim 5$ eV as proposed by Ovchinnikov, Ukrainskii and Kventsel' [5] and $t_0 = 2.5$ eV as usual, we obtain 0.8 eV for the kink-soliton energy, the «kink» with spreading over ~ 8 sites. This is to be compared with the corresponding energy and spreading for the SSH soliton : 0.45 eV and ~ 15 sites (see Fig. 3).

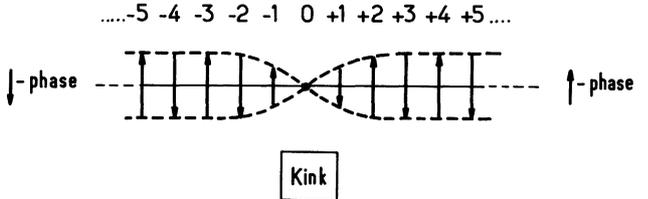


Fig. 3. — Sketch of the kink-like solitonic excitation.

One easily remarks that, except for these numerical differences, the SDW kink soliton has exactly the same properties as the SSH one. Indeed spin charge relations are the same, since mid gap states exist in the two cases. Therefore the usual interpretation scheme for several physical properties will follow along the same way (e.g. spinless conductivity).

Another feature is also present for the SDW state. Campbell and Bishop [6] have shown that the TLM continuous model possesses bag-soliton excitations (polarons). The same conclusion holds for the SDW case (Fig. 4).

Due to topological constraints kink solitons must appear in pairs, so that the bag type excitation should be the lowest excited state available to a single added electron. Note however that the bag-like excitation

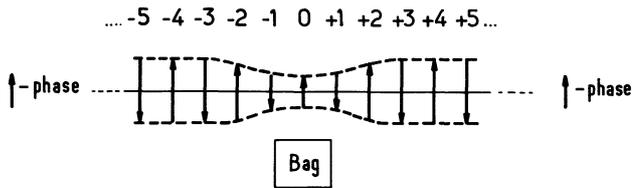


Fig. 4. — Sketch of the bag-like solitonic excitation.

has a finite life time : energetic considerations show that it eventually decays into a free kink anti-kink pair [6].

In conclusion let us say that, within the very simple model used above, we have shown that soliton-like excitations should exist for an organic polymer, the ground state of which being an antiferromagnetic spin density wave. To be sure one can argue that a treatment based on a mean-field (Hartree-Fock) Hamiltonian, supplemented by a continuous reformulation of the TLM type, is disputable for a one-dimensional system. However the possibility of such a ground state is physically not to be excluded, and should not be model dependent (except of course for its domain of existence as a function of the various parameters). When this is recognized, then one remarks that it necessarily exhibits the double degeneracy required to construct a soliton-like excitation,

and as such will apply to various organic polymers even if they cannot display a dimerization pattern of the lattice. In fact, figures 3 and 4 show that the soliton excitations are a quantitative description of a Bloch wall in a one-dimensional antiferromagnet. An analogous conclusion holds for the SSH soliton which describes the Bloch wall equivalent for an antiphase system.

Another interesting point should be the study of soliton-like excitations in the mixed state *b*). To be sure the domain of existence of this state is very narrow, but the question is of interest since it should bring a mixture of SDW and SSH solitons. We are now investigating this point. Other points of interest would be the study of other properties such as magnetic susceptibility at low temperature, neutron diffraction patterns, etc.

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