FIELD THEORY APPLIED TO POLYMERS*,**

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We describe how the formalism of Field Theory can be applied in the study of linear polymers. Fractional fermion number due to topological backgrounds is used to probe for fermion bound states associated to deformations of the linear lattice. A transition is exhibited and its phenomenological consequences are explored.

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1. Introduction

The formalism of Field Theory has encountered widespread application in Physics. Particle physicists rely on it to describe phenomena that occur from Mev's to (10^2) Gev's and to speculate as high as 10^5 Gev, or more. Yet, its deep connections with Statistical Mechanics make it a useful tool even at energies of a few electronvolts, in the realm of Condensed Matter Physics.

In this talk I shall describe one such application which enjoys the property of being, at the same time, very simple and very rich. It consists of the investigation of the continuum limit of a class of models for linear polymers. The resulting Field Theory exhibits topologically nontrivial configurations in its bosonic sector which induce fractional number in its fermionic sector. The analysis of the topological properties of the Field Theory finds an illuminating realization in the phenomenology of such polymers.

The outline of the talk is as follows: (*i*) in Sect. 2 we briefly review some essential facts about the Physics of polymers; (*ii*) in Sect. 3 we describe the Field Theory approach to a class of models for linearly conjugated polymers; (*iii*) Sect. 4 makes a brief digression on the relationship between fermion number and topology; (*iv*) Sect. 5 applies these ideas to polymers and discusses a transition with well defined phenomenological consequences; (*v*) Sect. 6 presents conclusions.

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2. *The physics of polymers*

We shall briefly review some of the essential properties of linear polymers. The prototype we shall adopt in the discussion is polyacetylene, a long chain made up of carbon and hydrogen atoms (C—H).

Carbon has a ground state where 1*s* and 2*s* levels are filled and, furthermore, there are two unpaired electrons in two of the 2p orbitals. One of its first excited states, however, has four unpaired electrons, one in each of the 2s, $2p_x$, $2p_y$ and $2p_z$ orbitals. When carbon atoms bind to form compounds they hybridize, that is, they form linear combinations of the orbitals in level 2 which determine the directions along which bonds are formed. One such example is shown in Fig. 1a. It corresponds to sp^3 hybridization which is a linear combination of the four orbitals of level 2. Fig. 1b shows yet another type of hybrid, called sp^2 since it only involves two of the p-orbitals. The third p-orbital (p_z) will give rise to a different type of bond. Finally, Fig. 1c exhibits an sp-hybrid. It is this latter form which

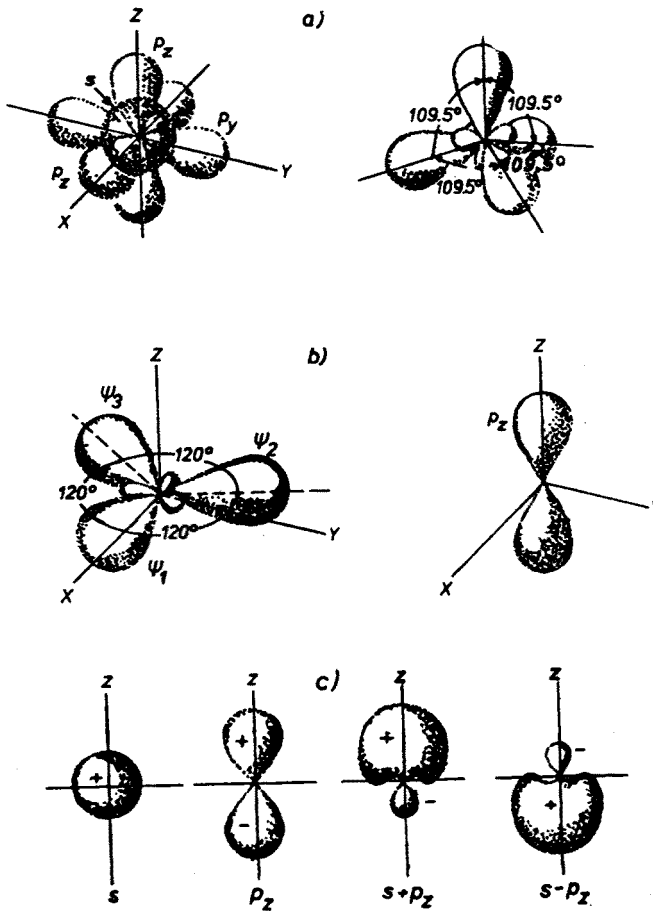

Fig. 1. Hybrids of carbon: a) — sp^3; b) — sp^2, p_z; c) — sp, p_x, p_y

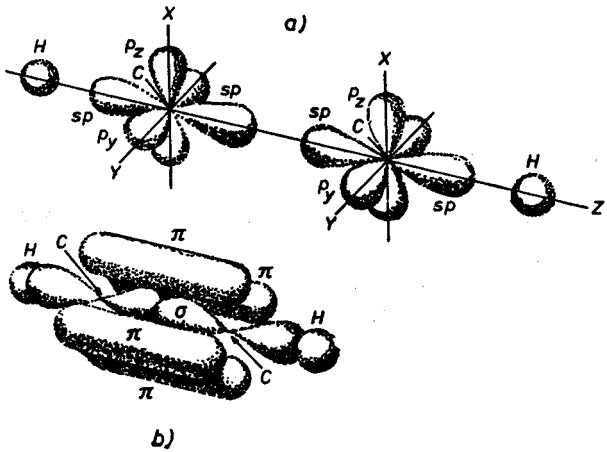

Fig. 2. Acetylene orbitals

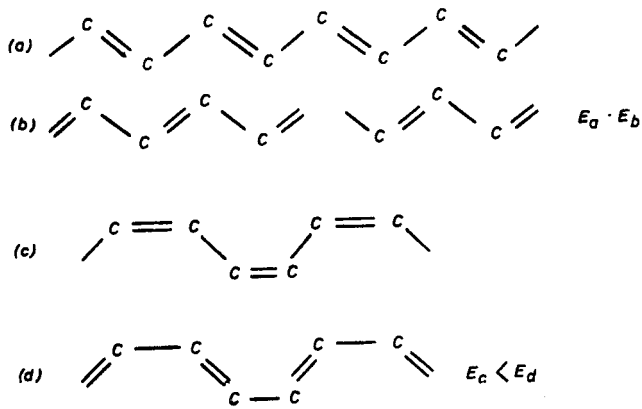

Fig. 3a)–b) — degenerate ground states of transpolyacetylene; c)–d) — nondegenerate ($E_c < E_d$) lowest energy states of cispolyacetylene

determines the bond structure of acetylene (H—C ≡ C—H) shown in Fig. 2. The bond between the two carbons coming from the sp-hybrid is called a σ-bond, whereas the two bonds coming from the remaining p orbitals are called π-bonds, in analogy to the terminology used for diatomic molecules.

Polyacetylene is formed by chemically breaking one of the π-bonds of acetylene so that a bond to a new carbon can be created. More and more carbon atoms are attached in the process, forming a long polymer whose basic structure is the monomer (C—H). The bonds between carbon atoms are of either the σ- or the π-type. Electrons will be more localized in σ-bonds; π-electrons are less localized along the chain. However, as a consequence of the interaction of these π-electrons with lattice phonons they are not uniformly distributed. π-bonds end up restricted to certain pairs of atoms, forming a structure which

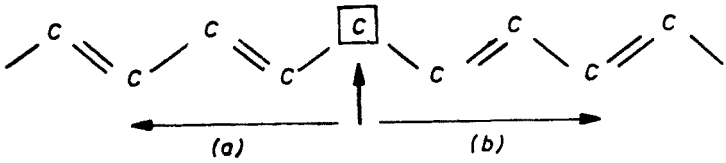

Fig. 4. Schematic representation of a soliton defect

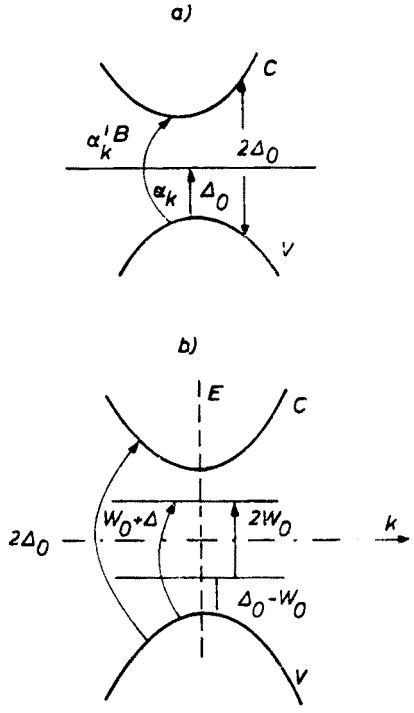

Fig. 5a) — midgap state in the soliton case; b) — midgap states in the polaron case

alternates single (σ-type) and double (σ and π-type) bonds. This process is called *dimerization* of the chain; it is a direct consequence of the compromise between vibrational and electronic energy (Peierls transition mechanism). It yields a chain with bonds of alternating lengths and splits an ideal lattice of spacing a into two sublattices of spacing $2a$.

Dimerization leads to a number of properties: (*i*) the alternating structure of single and double bonds gives rise to two types of polyacetylene, depending on whether the two carbon atoms singly bound to those in a double bond are on the same side (cis-polyacetylene) or on opposite sides (trans-polyacetylene) of the bond (see Fig. 3). The figure also shows the *doubly degenerate* ground state of trans-polyacetylene. The cis-polyacetylene chain, however, does not have a degenerate ground state. The two states shown have different energies due to the presence of hydrogen atoms whose interactions distinguish them;

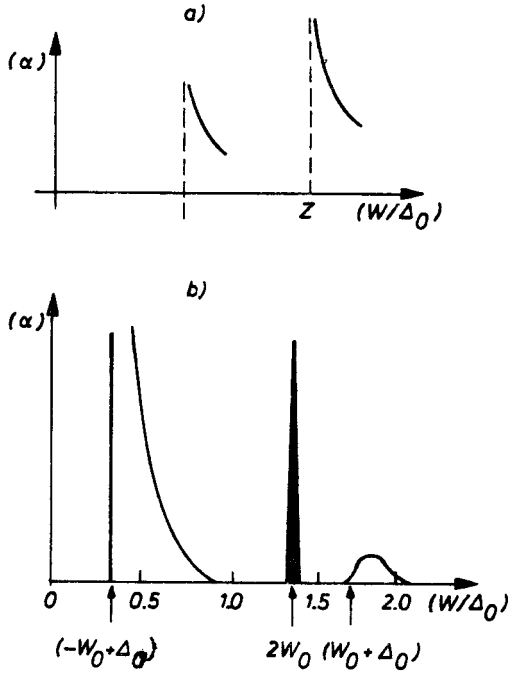

Fig. 6a) — optical absorption coefficient in the soliton case (without solitons the line at $\omega_0 = \Delta_0$ is absent); b) — same in the polaron case (only $2\Delta_0$ line appears if no polarons are present)

(*ii*) another consequence of dimerization is the appearance of an energy gap at $k = \pi/2a$; (*iii*) furthermore, the degeneracy of the ground state of transpolyacetylene allows for the appearance of configurational defects of the *soliton* (kink) type (see Fig. 4) as we either dope or heat up the polymer. Cispolyacetylene does not admit solitons as its ground state is non-degenerate. Nevertheless, it does allow for configurational defects of another type, the so-called *polarons*, which are essentially soliton-antisoliton pairs. Polarons can, obviously, also appear in transpolyacetylene.

The occurrence of solitons and polarons is always accompanied by one or two bound states in the π-electron spectra, respectively. These states appear in the middle of the gap between valence and conduction band. They play a role in the peculiar semiconducting behavior and can be detected in magnetic resonance and/or optical absorption properties of the electronic spectrum. Fig. 5 illustrates the presence of these states whereas Fig. 6 compares optical absorption coefficients in situations with and without solitons in transpolyacetylene.

As we shall see in the sequel, the existence of solitons and polarons and their respective fermionic bound states finds a natural description if one resorts to the language of Field Theory. Fermion number and its relationship to Topology are, then, instrumental concepts in the analysis.

3. *The field theory approach*

There exists a class of models for linearly conjugated polymers which are natural generalizations of the original Su-Schrieffer-Heeger (SSH) Hamiltonian [1]. In particular, the one introduced by Mele and Rice [2] applies to polymers made up of diatomic monomers. Its Hamiltonian is:

$$H_{\mathrm{TOT}} = \sum_j \frac{p_j^2}{2M_A} + \sum_l \frac{p_l^2}{2M_B} + \sum_n V(y_n - y_{n+1}) + \delta \sum_j a_j^+ a_j - \delta \sum_l b_l^+ b_l$$
$$- \sum_j t_{j+1,j}(a_j^+ b_{j+1} + b_{j+1}^+ a_j) - \sum_l t_{l+1,l}(b_l^+ a_{l+1} + a_{l+1}^+ b_l). \tag{1}$$

It describes atoms of type $A(B)$, of mass $M_A(M_B)$, on the odd (even) sites of a linear lattice. The $\{y_n\}$ characterize the displacement of the position of the n^{th} atom from an ideal lattice of spacing s and $\{p_n\}$ are their canonically conjugated momenta, V is the potential associated with lattice vibrations; $\{a_j^+\}$ and $\{a_j\}$ ($\{b_l^+\}$ and $\{b_l\}$) denote creation and annihilation operators for π-electrons at site $j(l)$, 2δ is the difference in valence energy of the π-electrons at sites of types A and B and $t_{n+1,n}$ is the hopping parameter from site n to $n+1$. We shall take it to be:

$$t_{n+1,n} \equiv t_0 + (-1)^{n+1} 2\mu - \gamma(y_{n+1} - y_n). \tag{2}$$

If $\mu = 0$ we recover the case treated in Ref. [3]. Nonvanishing μ amounts to $t_{j+1,j} = t_1 - \gamma(y_{j+1} - y_j)$ and $t_{l+1,l} = t_2 - \gamma(y_{l+1} - y_l)$, where $t_1 = t_0 + 2\mu$ and $t_2 = t_0 - 2\mu$. It is this form that contains, for $\gamma \neq 0$, the electron-phonon interaction responsible for the Peierls mechanism.

The Field Theory approach consists of taking the continuum limit of the model and dealing with the resulting field theory model in $1+1$ dimensions. We can obtain the continuum limit by introducing $a_j \equiv (-1)^{j/2}(2s)^{1/2}\, U(js)$, $b_l \equiv (-1)^{l/2}(2s)^{1/2} V(ls)$ and $y_n \equiv (-1)^n \varphi(ns)$. U's(V's) can be extended to even (odd) points by taking the average of their values on either side. The limit corresponds to taking $s \to 0$ ($ns \to x$) and, at the same time, identifying finite sums ($s\sum_n$) with integrals ($\int dx$) and finite differences with derivatives. If we group the U's and V's into a doublet, $\psi(x) \equiv (1 + i\sigma_3)/\sqrt{2} \begin{pmatrix} U(x) \\ V(x) \end{pmatrix}$, ($\sigma_3$ is the Pauli matrix) and redefine constants, we obtain for the electron-dependent part of H_{TOT}

$$H(\varepsilon) = \int dx \psi^+(x) \{\alpha p + \beta[\varphi(x) - \mu]\} \psi(x) + \varepsilon \int dx \psi^+(x) \sigma_3 \psi(x), \tag{3}$$

where $\alpha(\equiv \sigma_3)$ and $\beta(\equiv \sigma_1)$ are the Dirac (Pauli) matrices in $1+1$ dimensions. The paremeter ε is proportional to δ. As we are interested in $A = B$ (for polyacetylene $M_A = M_B = M_{CH}$), then, $\varepsilon = \delta = 0$. The Hamiltonian H is invariant under a charge conjugation operation which takes positive energy into negative energy states and vice-versa, since $\{H, \sigma_3\} = 0$. The ε-term would spoil this. This continuum (field theory)

approximation is certainly justified for phenomena which take place over distances much larger than the separation between adjacent carbons.

Although we have not written it explicitly, the phonon Hamiltonian is just that of a scalar field with a self-interacting potential $V(\varphi)$. The system of coupled equations of motion for this fermion-boson model, for the case of STATIC configurations of the scalar field is then:

$$-\frac{d^2\varphi}{dx^2}+V'(\varphi)=\bar{\chi}\chi, \tag{4a}$$

$$(i\partial\!\!\!/-\varphi)\chi=\omega\chi, \tag{4b}$$

where we have used $\varphi(x,t)=e^{-i\omega t}\chi(x)$. These equations constitute the basis of a semiclassical approximation to the problem. They can be shown to be derivable from a Gross-Neveu (GN) model treated in a static semiclassical approximation. The scalar field is related to the auxiliary field commonly introduced in the GN model to transform the quartic fermionic coupling into a Yukawa-type coupling.

The important point is that the coupled equations of motion possess solutions which will correspond to the three types of ground states of polyacetylene. For the scalar field they are:

$$\varphi(x)=\varphi_0, \quad \text{dimerized} \tag{5a}$$

$$\varphi(x)=\pm\varphi_0\tanh(k\varphi_0|x-x_0|), \quad \text{soliton (antisoliton)} \tag{5b}$$

$$\varphi(x)=\Phi_0\pm\Phi_1\tanh[K\Phi_1(x-X_0)]\mp\Phi_1\tanh[K\Phi_1(x+X_0)], \quad \text{polaron (antipolaron)} \tag{5c}$$

In the case of solitons and polarons, the spectra of the fermionic equations of motion possess bound states: one zero energy state in the soliton case and two charge-conjugate states in the polaron case. This comes out of the analysis of Eqs (3), (4b), with $\varphi(x)$ given by one of the scalar solutions just mentioned.

The Eqs (4a) and (4b), which led to solitons, polarons and their corresponding bound states, can also be obtained from a phenomenological scalar potential of the form $V(\varphi)=\frac{\lambda}{4}(\varphi^2-\varphi_0^2)^2$. There exists an interesting relation [4] between those equations and nontrivial solutions of a purely scalar theory in the presence of an external (constant) current j (a term $j\varphi$ in the Lagrangian). This connection allows one to solve the coupled system without resorting to inverse-scattering methods [4, 5].

4. Fermion number and topology

We shall just outline the connection between fermion number and topology. For a more complete treatment we refer the reader to the review article by Niemi and Semenoff

[6]. The definition of fermion number is obtained from the normal ordered operator:

$$:\hat{N}: \equiv \int_{-\infty}^{\infty} dx :\hat{\bar{\psi}}\gamma^0\hat{\psi}: = \int_{-\infty}^{\infty} dx[\hat{\psi}^+\hat{\psi} - \langle\Omega|\hat{\psi}^+\hat{\psi}|\Omega\rangle], \tag{6}$$

$|\Omega\rangle$ is taken to be the vacuum state for the unperturbed system. However, in the presence of a topologically nontrivial external background the vacuum state is modified to $|\tilde{\Omega}\rangle$. Thus, if we maintain the normal ordering instruction with respect to the unperturbed vacuum, we may obtain a nonvanishing (perturbed) vacuum expectation value of the number operator:

$$N = \langle\tilde{\Omega}|:\hat{N}:|\tilde{\Omega}\rangle - \langle\Omega|:\hat{N}:|\Omega\rangle \neq 0. \tag{7}$$

In fact, it may be shown that any type of real value may be obtained for the fermion number of states generated from the vacuum by the action of local operators, as long as we have our fermionic system under the action of a global (topological) external field. In the particular case of charge-conjugation ($\hat{C}$) invariant Hamiltonians, the values of fermion number thus obtained are either integer or half-integer. This is easily seen if we use local operators $\hat{L}$ such that: (*i*) $[:\hat{N}:, \hat{L}] = z\hat{L}$, z an integer; and (*ii*) $\{:\hat{N}:, \hat{C}\} = 0$. Taking two of these operators acting on the vacuum to create states that are charge-conjugate, we immediately see that twice the fermion number of any of them has to be integer. Therefore, they can have either integer or half-integer values.

The charge-conjugate invariant case corresponds to $\varepsilon = 0$ in equation (3) and amounts to treating polyacetylene-type Hamiltonians. We shall now show that, in a topologically nontrivial background, the vacuum value for fermion number may indeed be half-integer. We shall compare two Hamiltonians, $\tilde{H}$ and H, corresponding to a fermionic system with and without an external topological background, respectively. We assume that both have a complete set of states which are orthogonal eigenfunctions $|\tilde{\psi}(\tilde{E})\rangle$ and $|\psi(E)\rangle$, respectively, with eigenenergies $\{\tilde{E}\}$ and $\{E\}$ (both discrete andcon tinuum spectra are included). Charge conjugation takes $|\psi(E)\rangle \to |\psi(-E)\rangle$, $|\tilde{\psi}(\tilde{E})\rangle \to |\tilde{\psi}-(\tilde{E})\rangle$. Our definition for fermion number yields:

$$N = \int_{-\infty}^{\infty} dx\{\sum_{\tilde{E}<0} \tilde{\psi}^+(\tilde{E}, x)\tilde{\psi}(\tilde{E}, x) - \sum_{E<0} \psi^+(E, x)\psi(E, x)\}. \tag{8}$$

We have assumed that only negative energy states are occupied in the vacuum state. This is quite natural for H, however, in the case of $\tilde{H}$ special care must be taken. The reason is that topological backgrounds induce the appearance of zero-energy bound (normalizable) states, as established by the Atiyah-Singer theorem [7]. The vacuum is, then, *degenerate*; we have chosen to consider the zero-energy state unoccupied. The sequence:

$$\begin{aligned}\sum_{E>0} |\psi(E)\rangle\langle\psi(E)| &= \sum_{E<0} |\psi(E)\rangle\langle\psi(E)| \\ &= \tfrac{1}{2}\sum_{E} |\psi(E)\rangle\langle\psi(E)| = \tfrac{1}{2}\sum_{\tilde{E}} |\tilde{\psi}(\tilde{E})\rangle\langle\tilde{\psi}(\tilde{E})|,\end{aligned} \tag{9}$$

where the two last sums extend over the whole spectra and charge-conjugation and completeness were used, leads to:

$$N = \int_{-\infty}^{\infty} dx\{\sum_{\tilde{E}<0} \tilde{\psi}^+(\tilde{E}, x)\tilde{\psi}(\tilde{E}, x) - \tfrac{1}{2}[\sum_{\tilde{E}>0} \tilde{\psi}^+(\tilde{E}, x)\tilde{\psi}(\tilde{E}, x) + \sum_{\tilde{E}<0} \tilde{\psi}^+(\tilde{E}, x)\tilde{\psi}(\tilde{E}, x) + \tilde{\psi}^+(0, x)\tilde{\psi}(0, x)]\}. \tag{10}$$

Using charge-conjugation once more, we obtain:

$$N = -\tfrac{1}{2} \int_{-\infty}^{\infty} dx \psi^+(0, x)\psi(0, x) = -\tfrac{1}{2}, \tag{11}$$

where the zero energy (normalized) bound state was the only one to contribute.

Clearly, this result may be generalized to a statement that the fermion number of the vacuum (one of the degenerate ones) is given by one-half the number of occupied zero modes minus one-half the number of unoccupied ones. Thus, topology leads to zero energy bound states which, in turn, may yield fractional fermion number.

5. *A curious transition* [8]

We shall consider the Hamiltonian in Eq. (3) in the presence of a soliton background, $\varphi(x) = \varphi_0 \tanh(k\varphi_0 x)$. The form we have chosen for the hopping parameter generalizes the work of Ref. [3], however the spectrum can still be obtained *exactly*. The eigenvalue problem is equivalent to:

$$\begin{pmatrix} 0 & D(\mu) \\ D^+(\mu) & 0 \end{pmatrix} \begin{pmatrix} u_+ \\ u_- \end{pmatrix} = E \begin{pmatrix} u_+ \\ u_- \end{pmatrix} \tag{12}$$

with $D(\mu) \equiv -\dfrac{d}{dx} + \varphi(x) - \mu$, $\varphi(x)$ the kink field. As the square of H is diagonal, the system in (12) can be show to correspond to

$$[D(\mu)D^+(\mu)]u_+ = E^2 u_+, \tag{13a}$$

$$[D^+(\mu)D(\mu)]u_- = E^2 u_-. \tag{13b}$$

For $E^2 \neq 0$, every solution u_+ of (13a) or u_- of (13b) yields two solutions of (12) since Du_- and D^+u_+ satisfy (13a) and (13b), respectively. Whenever $E = 0$, the unique zero mode of (12) will be mapped into one only of the equations (13).

Equations (13a) and (13b) lead, both, to Schrödinger problems:

$$\left[-\frac{d^2}{dz^2} + V(z)\right] u_\pm = \varepsilon u_\pm \tag{14a}$$

$$V(z) \equiv \beta \tanh z - \gamma_\pm \operatorname{sech}^2 z \tag{14b}$$

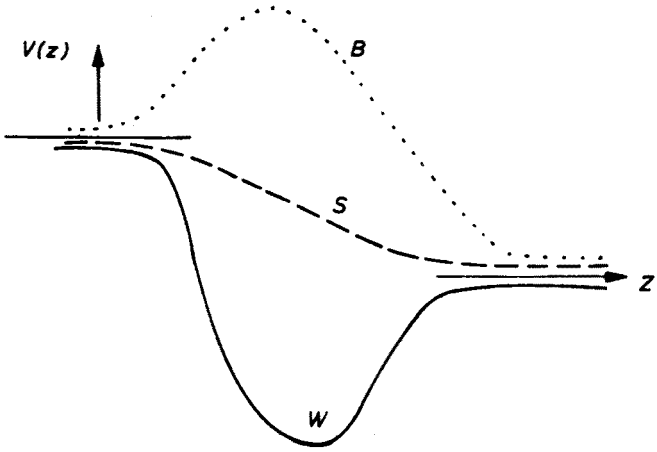

Fig. 7. The three types of potentials that occur — a well (W), a step (S) or a barrier (B)

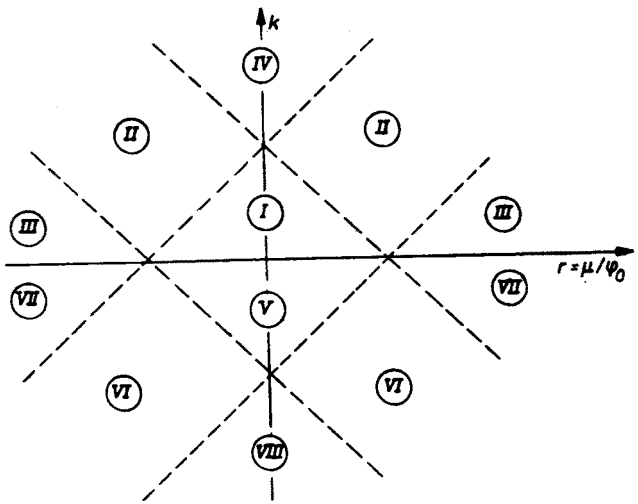

Fig. 8. Regions in the $(r\text{-}k)$ plane corresponding to the various situations allowed for Eqs (13a) and (14b). In the convention of Fig. 7 we have: I → W(a), W(b); II → W(a), S(b); III → S(a), S(b); IV → W(a), B(b); V → W(a), W(b); VI → S(a), W(b); VII → S(a); S(b); VIII → B(a), W(b). The indices (a) and (b) refer to Eq. (13)

with $\beta \equiv 2\mu/k^2\varphi_0$, $\gamma_\pm \equiv (1 \pm k)/k^2$ and $\varepsilon \equiv (E^2 - \varphi_0^2 - \mu^2)/k^2\varepsilon_0^2$. Depending on the values of $r \equiv \mu/\varphi_0$ and k we may have different types of potential for the two equations of interest. The possibilities are shown in Fig. 7 and correspond to a well (W), a step (S) and a barrier (B). Fig. 8 shows the combinations that occur as we move on the $(r-k)$ plane. The labels $(+)$ and $(-)$ refer to Eqs (13a) and (13b). We note that the $k < 0$ portion of the plane describes the solution for an antisoliton and may be obtained from the $k > 0$ case quite easily.

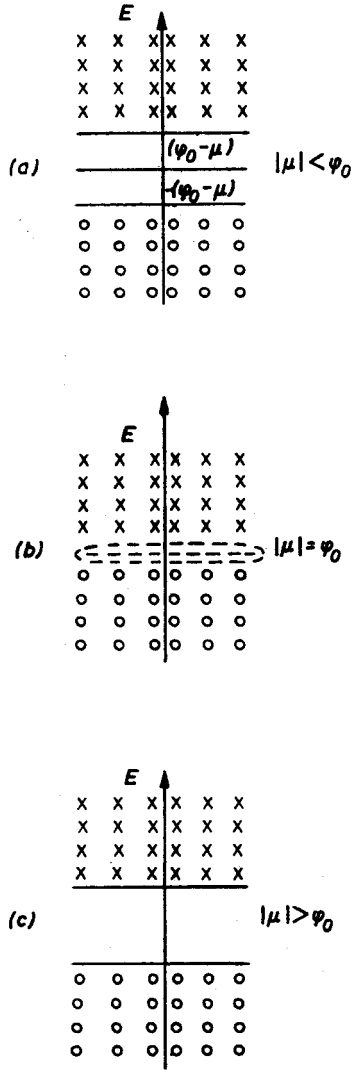

Fig. 9. The spectrum of H corresponding to different values of $|\mu|/\phi_0$. In a) there is a zero bound state, in b) this state is squeezed by the continua; in c) it has disappeared

Let us analyze what happens for $0 \leqslant k \leqslant 1$ as we change the value of r. We start from a situation $|r| \leqslant |1-k|$ (region I), where both equations are potential wells. Depending on r, these wells may have several bound states and a continuum. The spectrum of eigenvalues of the two equations is *identical* (a consequence of C-invariance) except for a zero eigenvalue which *only* occurs for the (+) Eq. (13a). As we change r, we gradually transform the well of (13b) into a step with *no* bound states (region II). This happens for $|r| = |1-k|$ and although (13a) remains a well, it does not contain any bound states other than the zero eigenmode, as all nonzero modes are identical between the two equations. Furthermore,

the value of the continuum threshold also changes with r, as $(E)_{\text{th}} = \varphi_0^2(1-|r|)^2$. Still inside region II we reach $|r| = 1$, where this threshold vanishes. The continuum then starts from zero and, for (13a), it overlaps with the zero bound state. As $|r|$ continues to increase the potential well of (13a) ceases to have a bound state and $(E)_{\text{th}}$ becomes nonvanishing again. Finally, a $|r|$ reaches $|1+k|$, the well of (13a) also turns into a step.

We can use this information to extract the spectrum of the Hamiltonian. The eigenvalues are simply $E_\pm = \pm\sqrt{E^2}$ and are obviously related by $\hat{C}$. The zero eigenvalue of (13a) is just the *normalizable* zero mode of D^+, whereas D has no such mode, i.e., (13b) has no zero bound state. The variation of $|r|$ corresponds to a process whereby the continua of positive and negative energy states close their gap around the zero bound state. As we reach $|r| = 1(\mu = \pm\varphi_0)$ the gap has shrunk to zero and we have a continuum from minus to plus infinity. For $|r| > 1$, the gap reopens but, now, without any bound state. The situation is illustrated in Fig. 9.

We can now draw some interesting consequences on the behavior of fermion number from the mechanism just described. Its overall effect is to do away with a zero energy bound state which existed in the middle of the gap. The results of the previous Section lead us to conclude that for $|r| < 1$ we shall have $N = \pm 1/2$, whereas for $|r| > 1$ no bound state at zero will appear, meaning $N = 0$. Therefore

$$N(r) = \pm \tfrac{1}{2}\,\theta(1-|r|), \tag{15}$$

with $\theta(x)$ the Heaviside function. A couple of comments are in order: (*i*) if we look at the zero mode of D^+ we find

$$\psi_0(x) = \psi_0(0)e^{\mu x}\,\operatorname{sech}^{1/k}(k\varphi_0 x). \tag{16}$$

The point $|r| = 1$ corresponds to the point where the norm of (11), $\int_{-\infty}^{\infty} dx|\psi_0(x)|^2$, *diverges*. The zero energy state becomes non-normalizable and disappears from the spectrum; (*ii*) the transition in fermion number could also be derived by looking at trace identities [6, 9] which relate it to topological (asymptotic) properties of the external (scalar) field. The inclusion of a mass term replaces the soliton with an effective field, $\varphi_{\text{eff}} = \varphi(x) - \mu$. Since fermion number is proportional to $\Delta = \operatorname{sign}\varphi_{\text{eff}}(+\infty) - \operatorname{sign}\varphi_{\text{eff}}(-\infty)$, it will vanish for $|\mu| > \varphi_0$. The topological nature of the soliton, which connects negative and positive values of the scalar field, is washed out by the mass term if $|\mu| \geqslant \varphi_0$.

We may go back to the model for polyacetylene and identify the positive and negative energy continua of the field theory (continuum) limit with the conduction and valence bands for π-electrons. The zero energy bound state corresponds to an introband localized level. As the conductivity along the polymer chain is enhanced by the propagation of these soliton solutions, the presence of intraband states as well as the narrowing of the gap will certainly affect it. Thus, the transition in fermion number we have just described would amount to a variation in the conductivity of the semiconducting polymer.

It remains to decide under what circumstances hopping parameters of the type exhibited in (2) will occur. In fact, they appear quite naturally in polymers of the cis-type such as cis-

-polyacetylene. The alternating phonon independent part of the hopping is due to the presence of the hydrogens which couple to carbon atoms. However, as was already mentioned, cis-type polymers do not have degenerate ground-states. As a consequence, they do *not* admit *soliton* deformations. Yet, they do allow *polaron* configurations. We will now show that the problem was have just solved is quite useful in focusing a case of real physical interest, i.e. polarons in cis-type polymers such as cis-polyacetylene.

The polaron solution can be written as:

$$\varphi(x) = \Phi_0 - \Phi_1 \tanh\left[K\Phi_1(x+X_0)\right] + \Phi_1 \tanh\left[K\Phi_1(x-X_0)\right], \tag{17}$$

where Φ_0 and Φ_1 are slightly different mass scales, K is a pure number and X_0 an arbitrary distance. If $x_0 \gg (K\Phi_1)^{-1}$ this reduces to a widely separated kink-antikink pair. It should be clear that the topological properties of such a solution are no different than those of a dimerized phase with $\varphi = \Phi_0$. Yet, the limit of wide separation allows us to construct the set of eigenstates of the Dirac Hamiltonian in a polaron background in terms of those in a soliton (antisoliton) background. The curious behavior of the latter as we vary μ allows us to infer that, in the polaron case, a similar phenomenon will take place: as $|\mu|$ approaches Φ_0, the gap will close squeezing the (now) two localized (bound) states in between. As the gap reopens for $|\mu| > \Phi_0$ we shall have no more localized states with a corresponding change in the conductivity properties of the system.

We may illustrate this effect by showing that the spacing between the two bound states of the fermionic spectrum in the polaron field goes to zero as $|\mu|$ approaches Φ_0 from below. For simplicity, we shall examine the case of very large separation. It is, then, convenient to write the fermion Hamiltonian as

$$H = H_S + H_{\bar{S}} + H_I, \tag{18}$$

with H_S and $H_{\bar{S}}$ the asymptotic forms of H at (x_0) and $(-x_0)$. Each term in H has the same form of the matrix appearing in (7) where:

$$D_S(\mu) = -\tfrac{1}{2}\frac{\partial}{\partial(x-X_0)} - \mu + (\Phi_0 - \Phi_1) + \Phi_1 \tanh\left[K\Phi_1(x-X_0)\right], \tag{19a}$$

$$D_{\bar{S}}(\mu) = -\tfrac{1}{2}\frac{\partial}{\partial(x+X_0)} - \mu + (\Phi_0 - \Phi_1) - \Phi_1 \tanh\left[K\Phi_1(x+X_0)\right], \tag{19b}$$

$$D_I(\mu) = -\left[(\Phi_0 - \mu) + (\Phi_0 - \Phi_1)\right]. \tag{19c}$$

We know the spectra of H_S and $H_{\bar{S}}$ exactly. Furthermore, the full Hamiltonian, H, is invariant under the change $(X_0, K) \to (-X_0, -K)$, which amounts to exchanging soliton and antisoliton. Also, the property

$$\psi_{S,E}(x+X_0) = \psi_{\bar{S},E}(x, -X_0) \tag{20}$$

holds for $\psi_S(\psi_{\bar{S}})$ eigenfunction of $H_S(H_{\bar{S}})$ of eigenenergy E. Thus, for wide separations, we expect that any eigenfunction of H will be approximated by a superposition

$$\psi(x) = \sum_E \left\{a_S(E)\psi_{S,E}(x-X_0) + a_{\bar{S}}(E)\psi_{\bar{S},E}(x+X_0)\right\}. \tag{21}$$

Since H is invariant under the change $(X_0, K) \to (-X_0, -K)$ the transformed wave function ψ' will be related to ψ by just an overall phase factor

$$\psi'(x) = e^{i\theta}\psi(x). \tag{22}$$

Making use of the orthogonality properties of the kink (antikink), spectrum we obtain

$$a_S(E) = e^{i\theta}a_{\bar{S}}(E) \tag{23a}$$

$$a_S(E) = e^{-i\theta}a_{\bar{S}}(E). \tag{23b}$$

Thus, θ has to be either 0 or π, i.e., $a_S(E) = \pm a_{\bar{S}}(E)$. Then

$$\psi_\pm(x) = \sum_E a_S(E)\,[\psi_{S,E}(x-X_0) \pm \psi_{\bar{S},E}(x+X_0)]. \tag{24}$$

As we are interested in the bound state spectrum only, we confine our attention to the bound states of the kink and antikink spectra (both are zero eigenstates). Denoting the fermion (polaron) bound states by $|\pm\rangle$

$$|\pm\rangle = [\psi_{S,0}(x-X_0) \pm \psi_{\bar{S},0}(x+X_0)]. \tag{25}$$

We, then, compute the matrix elements of H in the basis $\{|+\rangle, |-\rangle\}$. Using $X_0 \gg (K\Phi_0)^{-1}$ and $\Phi_0 - \Phi_1 \sim \ln(K\Phi_1 x_0) \equiv j$, we obtain, to lowest order in j, for $\mu > 0$:

$$H \cong \begin{bmatrix} -(\Phi_0-\mu)f(j) & 0 \\ 0 & +(\Phi_0-\mu)f(j) \end{bmatrix}. \tag{26}$$

The splitting between the levels, $2(\Phi_0-\mu)f(j)$, does indeed vanish as $\mu \to \Phi_0$.

6. *Conclusions*

The physical consequences of our calculations seem quite interesting. Different polymers in the cis-configuration may exhibit different ratios $|\mu|/\Phi_0$ (for a given polymer the ratio may be varied by stretching). This ratio is a comparison between the difference of extrinsic hoppings and the energy gap between valence and conduction bound. Our prediction is that, as this ratio approaches unity, the polymer will undergo a change in its conductivity and optical absorption properties, as a consequence of the disappearance of the intraband states. Furthermore, one can show that, even in the case of *trans*-polyacetylene, alternating hoppings may be achieved if we use an external stationary electromagnetic field along the polymer axis with wavelength twice the period of the lattice. Although such fields cannot be produced experimentally (we would need x-ray frequencies), they play a role very much similar to the staggered fields which are commonly invoked to describe the physics of anti-ferromagnets. This would, then, be the setting for the problem with the soliton background.

Finally, it remains to present a more complete treatment of the fermion spectrum in the polaron background. This work is already under way and will be presented shortly [10].

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