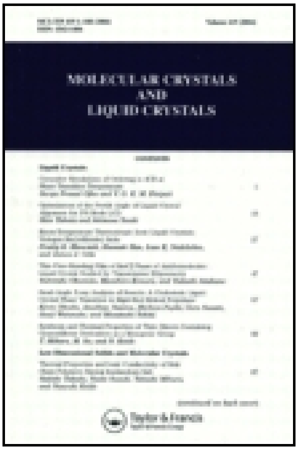

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The Moving Modified KdV Solitons In Polyacetylene

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THE MOVING MODIFIED KdV SOLITONS IN POLYACETYLENE

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Abstract The fact is explored that the continuum model of polyacetylene is isomorphic to the well-known Zakharov-Shabat problem of 1-d scattering. It is shown that the gap parameter $\Delta(x,t)$ may be viewed as some solution to the modified Korteweg-de Vries equation.

INTRODUCTION

The competition between the "solitonization"[1] and "polaronization"[2] of the excitations resulting in the course of electron-phonon interactions in *trans*-polyacetylene seems to be winned[9] by the former, mainly due to the specific polymer structure and degeneracy of ground state. However, the existence of kinks is strongly connected with dynamics[3]. I argue that the continuum model of polyacetylene allows for discussing "bumps" /whatever they are named/ in terms of KdV waves.

BASIC EQUATIONS

The Takayama, Lin-Liu and Maki[4] /TLM/ continuum model of polyacetylene yields for the mean-field gap parameter Δ and components of the spinor $\Psi(x) = \{u(x),\ v(x)\}$ the following set of equations which are obtained from a variational principle

$$\epsilon_n u^n = -iv_F u_x^n + \Delta v^n \qquad (1)$$

$$\epsilon_n v^n = iv_F v_x^n + \Delta u^n \qquad (2)$$

$$\Delta(x) = -\frac{2g^2}{\omega^2}\sum_n \left[\overset{*}{u}{}^n(x)\,v^n(x) + u^n(x)\,\overset{*}{v}{}^n(x)\right] \qquad (3)$$

where ϵ_n play the role of Lagrange multipliers. After the linear transformation $f = u + iv$, $g = u - iv$, equations (1) and (2) can be set in the form

$$f_{xx} + \left\{E^2 - U^+(x)\right\} f = 0 \qquad (4)$$

$$g_{xx} + \left\{E^2 - U^-(x)\right\} g = 0 \qquad (5)$$

where $U^{\pm} = \Delta^2 \pm \Delta_x$, $E = \epsilon/v_F$, $\Delta = \Delta/v_F$ and the subscripts n are omitted. A similar eigenvalue problem has been discussed long ago for U being a Lamé function[5]. For periodic eigenfunctions the continuous /or quasi-continuous/ spectrum reveals the gap. In fact, in our case there are two gaps connected with two potentials $U^{\pm}$. As the problem issues in considering the stability of soliton solutions to other non-linear field theories, Horovitz[6] concluded that the sine-Gordon physics can be introduced for solitons in polyacetylene.

For the Sturm-Liouville problem as given by equations (4) and (5) it appears that there is also discrete /infinite/ spectrum of eigenvalues with eigenstates being square-integrable[7]. The important feature of the discrete part of the spectrum reveals the significant property that if we allow for $U^{\pm}$ to be time-dependent, the eigenvalues E are constants of motion. And then $U^{\pm}$ should satisfy the Korteweg-de Vries equation

$$U^{\pm}_{t} + 6U^{\pm}U^{\pm}_{x} + U^{\pm}_{xxx} = 0 \,. \tag{6}$$

In fact, in polyacetylene we seek for excitations with a time-independent spectrum. It is not so obvious that electronic energies are time-independent since the starting problem is non-linear and solutions to the non-linear equations of motion depend usually explicitly on time and space /Fourier components are mixed locally/.

It is worth to notice that $U^{\pm}$ resembles the transformation introduced by Miura[7] which connects the KdV and modified KdV equations. Substitution both of the potentials $U^{\pm}$ into equation (6) shows that they can be satisfied simultaneously only if $\Delta(x,t)$ satisfies the modified KdV equation

$$\Delta_t - 6\Delta^2\Delta_x + \Delta_{xxx} = 0 \,. \tag{7}$$

This is the exact equation for the time and space evolution of the gap parameter.

Time dependence of wave functions

Assuming the equations for space and time evolution for u and v are of the same shape and putting $u_t = Au + Bv$, $v_t = Cv + Du$, we obtain

$$u_t = E(\Delta^2 + 2E^2)u - \left\{2\Delta(\Delta^2 + 2E^2) + -2i\Delta_x E + \Delta_{xx}\right\}v \tag{8}$$

$$v_t = -E(\Delta^2 + 2E^2)v + \left\{2\Delta(\Delta^2 + 2E^2) + + 2i\Delta_x E - \Delta_{xx}\right\}u \tag{9}$$

under the additional assumption that the coefficients

A,...,D are polynomials in E of a degree not higher than three.

Taking time derivative of both sides of eq. (3) and using equations (1), (2), (8), (9) it can be shown that

$$\Delta_t = \Delta_x E(|u|^2 + |v|^2) + iE(\Delta^2 + 2E^2)(u^* v - v^* u) =$$
$$= 6\Delta^2 \Delta_x - \Delta_{xxx} \qquad (10)$$

thus the modified KdV equation is compatible with the self-consistency condition (3).

Simple solutions

The moving SSH domain-wall $\Delta = \Delta_0 \tanh \xi/\xi_0$, where $\xi = x - ct$, satisfies equation (7) in the dimensional form

$$1/c\Delta_t - \Delta_0^{-2} \Delta^2 \Delta_x + \xi_0^2/2\Delta_{xxx} = 0 \qquad (11)$$

as well as KdV equation for U. The velocity c can be obtained from energy considerations. Also the polaron solution of Onodera and Okuno[8] admits this point of view. Unfortunately no soliton lattice that would satisfy all above conditions does exist although the multi-soliton as well as breathers can be found.

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