

This article was downloaded by: [Tomsk State University of Control Systems and Radio]

On: 20 February 2013, At: 12:44

Publisher: Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954

Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:

<http://www.tandfonline.com/loi/gmcl16>

The Moving Modified KdV Solitons In Polyacetylene

Karol Pesz^a

^a Institute of Organic and Physical Chemistry
Technical University, 50-370, Wroclaw, Poland

Version of record first published: 17 Oct 2011.

To cite this article: Karol Pesz (1985): The Moving Modified KdV Solitons In Polyacetylene, *Molecular Crystals and Liquid Crystals*, 118:1, 81-84

To link to this article: <http://dx.doi.org/10.1080/00268948508076192>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.tandfonline.com/page/terms-and-conditions>

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae, and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand, or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

THE MOVING MODIFIED KdV SOLITONS IN POLYACETYLENE

KAROL PESZ

Institute of Organic and Physical Chemistry
 Technical University, 50-370 Wrocław, Poland

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 won⁹ by the former, mainly due to the specific polymer structure and degeneracy of ground state. However, the existence of kinks is strongly connected with dynamics³. 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 Maki⁴ /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

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

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

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

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

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

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

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 function⁵. 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, Horowitz⁶ 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-integrable⁷. 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

$$U_t^\pm + 6U^\pm U_x^\pm + U_{xxx}^\pm = 0. \quad (6)$$

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 Miura⁷ 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

$$\Delta_t - 6\Delta^2 \Delta_x + \Delta_{xxx} = 0. \quad (7)$$

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

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

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

under the additional assumption that the coefficients

A, \dots, 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

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

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

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

as well as KdV equation for U . The velocity c can be obtained from energy considerations. Also the polaron solution of Onodera and Okuno⁸ 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.

REFERENCES

1. W. P. Su, J. R. Schrieffer and A. J. Heeger, Phys. Rev. B **22**, 2099 (1980).
2. D. K. Campbell, A. R. Bishop and K. Fesser, Phys. Rev. B **26**, 6862 (1982).
3. J. C. Kimball, Phys. Rev. B **21**, 2104 (1980).
4. H. Takayama, Y. R. Lin-Liu and K. Maki, Phys. Rev. B **21**, 2388 (1980).
5. B. Sutherland, Phys. Rev. A **8**, 2514 (1973).
6. B. Horowitz, Phys. Rev. Lett. **46**, 742 (1981).
7. R. M. Miura, J. Math. Phys. **9**, 1202 (1968).
8. Y. Onodera and S. Okuno, J. Phys. Soc. Japan **52**, 2478 (1983).
9. S. Stafström and K. A. Chao, Phys. Rev. B **29**, 2255 (1984).