Solitons in Molecular Systems

Second Edition

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by

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SERIES EDITOR'S PREFACE

'Et moi, ..., si j'avait su comment en revenir, je n'y serais point allé.'

Jules Verne

The series is divergent; therefore we may be able to do something with it.

O. Heaviside

One service mathematics has rendered the human race. It has put common sense back where it belongs, on the topmost shelf next to the dusty canister labelled 'discarded non-sense'.

Eric T. Bell

Mathematics is a tool for thought. A highly necessary tool in a world where both feedback and non-linearities abound. Similarly, all kinds of parts of mathematics serve as tools for other parts and for other sciences.

Applying a simple rewriting rule to the quote on the right above one finds such statements as: 'One service topology has rendered mathematical physics ...'; 'One service logic has rendered computer science ...'; 'One service category theory has rendered mathematics ...'. All arguably true. And all statements obtainable this way form part of the raison d'être of this series.

This series, *Mathematics and Its Applications*, started in 1977. Now that over one hundred volumes have appeared it seems opportune to reexamine its scope. At the time I wrote

> "Growing specialization and diversification have brought a host of monographs and textbooks on increasingly specialized topics. However, the 'tree' of knowledge of mathematics and related fields does not grow only by putting forth new branches. It also happens, quite often in fact, that branches which were thought to be completely disparate are suddenly seen to be related. Further, the kind and level of sophistication of mathematics applied in various sciences has changed drastically in recent years: measure theory is used (non-trivially) in regional and theoretical economics; algebraic geometry interacts with physics; the Minkowsky lemma, coding theory and the structure of water meet one another in packing and covering theory; quantum fields, crystal defects and mathematical programming profit from homotopy theory; Lie algebras are relevant to filtering; and prediction and electrical engineering can use Stein spaces. And in addition to this there are such new emerging subdisciplines as 'experimental mathematics', 'CFD', 'completely integrable systems', 'chaos, synergetics and large-scale order', which are almost impossible to fit into the existing classification schemes. They draw upon widely different sections of mathematics."

By and large, all this still applies today. It is still true that at first sight mathematics seems rather fragmented and that to find, see, and exploit the deeper underlying interrelations more effort is needed and so are books that can help mathematicians and scientists do so. Accordingly MIA will continue to try to make such books available.

If anything, the description I gave in 1977 is now an understatement. To the examples of interaction areas one should add string theory where Riemann surfaces, algebraic geometry, modular functions, knots, quantum field theory, Kac-Moody algebras, monstrous moonshine (and more) all come together. And to the examples of things which can be usefully applied let me add the topic 'finite geometry'; a combination of words which sounds like it might not even exist, let alone be applicable. And yet it is being applied: to statistics via designs, to radar/sonar detection arrays (via finite projective planes), and to bus connections of VLSI chips (via difference sets). There seems to be no part of (so-called pure) mathematics that is not in immediate danger of being applied. And, accordingly, the applied mathematician needs to be aware of much more. Besides analysis and numerics, the traditional workhorses, he may need all kinds of combinatorics, algebra, probability, and so on.

In addition, the applied scientist needs to cope increasingly with the nonlinear world and the extra mathematical sophistication that this requires. For that is where the rewards are. Linear models are honest and a bit sad and depressing: proportional efforts and results. It is in the non-linear world that infinitesimal inputs may result in macroscopic outputs (or vice versa). To appreciate what I am hinting at: if electronics were linear we would have no fun with transistors and computers; we would have no TV; in fact you would not be reading these lines.

There is also no safety in ignoring such outlandish things as nonstandard analysis, superspace and anticommuting integration, p-adic and ultrametric space. All three have applications in both electrical engineering and physics. Once, complex numbers were equally outlandish, but they frequently proved the shortest path between 'real' results. Similarly, the first two topics named have already provided a number of 'wormhole' paths. There is no telling where all this is leading - fortunately.

Thus the original scope of the series, which for various (sound) reasons now comprises five subseries: white (Japan), yellow (China), red (USSR), blue (Eastern Europe), and green (everything else), still applies. It has been enlarged a bit to include books treating of the tools from one subdiscipline which are used in others. Thus the series still aims at books dealing with:

- a central concept which plays an important role in several different mathematical and/or scientific specialization areas;
- new applications of the results and ideas from one area of scientific endeavour into another;
- influences which the results, problems and concepts of one field of enquiry have, and have had, on the development of another.

This is the greatly modified and supplemented second edition of the first book on Davydov solitons and related matters which appeared in 1985 and is now practically sold out. The main differences are a large new chapter on the quantum theory of solitons, a thorough discussion of two component solitons and a great amount of attention paid to discussions of the physical consequences of the theory. These last two aspects have caused modifications and additions throughout the book (as compared with the first edition).

As I wrote in my preface to the first edition there is a good, albeit heuristic - there is mathematical work to be done here - argument that says that the next approximation after the linear one for (quasi) one-dimensional wave like phenomena will, inevitably, involve soliton equations. Developments since 1985 on quasi one-dimensional structures (such as protein chains), the topic of this book, have done much to bear this out, and soliton waves appear practically all the time in such structures. Examples are the soliton waves of energy transport along protein chains; these are called Davydov solitons, after their discoverer - the author of this book.

It is a pleasure to welcome this totally-up-to-date new version of this work, which is, discounting the 1st edition, still the unique comprehensive volume on the topic.

The shortest path between two truths in the real domain passes through the complex domain.

J. Hadamard

La physique ne nous donne pas seulement l'occasion de résoudre des problèmes ... elle nous fait pressentir la solution.

H. Poincaré

Never lend books, for no one ever returns them; the only books I have in my library are books that other folk have lent me.

Anatole France

The function of an expert is not to be more right than other people, but to be wrong for more sophisticated reasons.

David Butler

Bussum, 7 October 1990

Michiel Hazewinkel

Preface

The problem of electrons pairing in quasi-one-dimensional structures with the formation of bisolitons is discussed. A new bisoliton mechanism of high-T_c superconductivity of quasi-one-dimensional nonmetallic complex compounds with strong electron-phonon coupling is investigated by means of nonlinear equations. In such compounds, the coherence length is small ($\sim$ 15Å) compared $10^{-4} cm$ inherent for metals described by the BCS theory. The conditions of the generation of solitons and bisolitons at the boundary of a soft quasi-one-dimensional structure are also studied.

In a new and rather large Chapter, the basis of a quantum theory of solitons is presented which enables heat vibrations to be taken into account. The material dealing with proton conductivity via molecular chains with hydrogen bonds between molecules has been extended. The role of proton conductivity in the near-surface layers of water is also discussed.

Pekar's theory of polarons in ionic crystals is modified. The importance of an account of the spatial dispersion of optical phonons characterizing polarization of a crystal is demonstrated, if this is neglected, as has been done in all previous theories, polarons cannot move in a crystal.

In conclusion, A.A. Eremko, V.N. Ermakov, A.V. Zolotariuk, N.I. Kislukha, G.M. Pestryakov, A.I. Sergienko, and V.Z. Enol'skii who participated in the development of the original studies of the theory of solitons involved in this book, E.M. Zaika for her help in the preparation of this book for publication, and E.S. Kryachko for his English translation.

Alexander S. Davydov

Preface to the Second Edition

The first English edition of the present book was published in 1985 (also by Kluwer Academic Publishers). However, since then the theory of solitons in molecular systems has been developed considerably so that a second edition is more than justified.

This second edition is greatly modified and supplemented in view of the modern state of theory of two-component solitons in quasi-one-dimensional molecular systems. Compared with the first edition, some mathematical details have been omitted. Great attention has been paid to a discussion of the physical results of the theory outlined and its possible applications.

In molecular systems, solitons are two-component formations arising due to the nonlinear interaction of two types of quasiparticles, or fields. One should emphasize that these nonlinear formations move only with velocities less than some limiting velocity. The reasons leading to such a constraint are analyzed in the present book.

A considerable part of the book is devoted to modern approaches in the study of energy transduction and electrons in quasi-one-dimensional molecular systems and of protons in macro-molecules with hydrogen bonds. The dominant role of nonlinear phenomena in biology leading to the formation of solitons is demonstrated, and based on these concepts, some problems of modern bioenergetics are discussed. An important role of solitons in elucidating the contraction mechanism of muscles of animals, the motion of bacteria plaits, and intracellular motions are also considered.

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Introduction

For a long time linear equations have been used for describing diverse phenomena in physics, chemistry, biology, and related applications. However, these take into account only a linear response of a system to an external influence. Consequently, if the intensity of an external influence increases, the response increases at the same rate.

Fundamental to the linear equations of mechanics (Newton's equations), electrodynamics (Maxwell's equations), and quantum theory (Schrödinger's equation) is the superposition principle, which enables any physical quantity to be represented as a sum of its elementary components. For instance, white light may be considered as the sum of various monochromatic, or singe-frequency components.

Many properties of systems consisting of a large number of interacting molecules and atoms have been explained using linear equations. In particular, the introduction of the concept of collective excitations has been extremely fruitful. A collective excitation characterizes a mutual and consistent, or coherent, motion of a large number of particles. Acoustic waves in gases, liquids, and solids are examples of such collective excitations. An acoustic wave is an oscillation of particles of average density which propagates in a wavelike manner on a background of a huge number of disordered heat vibrations. Simple acoustic waves are monochromatic and are therefore characterized by a specific frequency and wavelength.

The concept of elementary excitations of different types is widely found in solid state physics, e.g. *phonons* are quanta of collective vibrations of atoms and molecules, *excitatons* are quanta of collective excitations of solids whose frequencies correspond to those of visible and ultraviolet light, and *magnons* are quanta of spin (magnetic) excitations. All these elementary excitations are described by monochromatic waves. A strongly monochromatic wave has an infinite spatial extension. For this reason, it is unable to carry energy and information. Hence, energy is transferred only by vibrational excitations which move with a given velocity and are localized within a rather small spatial region. Such localized excitations are called *wave packets* since they are formed by a large number of monochromatic waves.

In various media, the phase velocity of monochromatic waves, i.e., the velocity of motion of a constant phase, depends on the wavelength. These media are called *dispersive.* As far as the motion of a wave packet in such a media is concerned, the different monochromatic components move with different velocities, which results in an increasing spatial dimension of the wave packet. One can say that a wave packet 'runs' with a time. The effect of 'running' is one of the main difficulties connected with the transfer of energy by wave-packet-type excitations. A second noteworthy shortcoming is that a wave packet loses energy in motion. This energy is transferred to random vibrations of atoms and molecules, i.e., to heating of the medium.

It has recently been recognized that the ideal model of transport of vibrational excitations, electrons, and protons in a medium is their transfer in the form of solitary waves known as *solitons.* Unlike ordinary waves which represent a spatial periodical repetition of elevations and hollows on a water surface, or condensations and rarefactions of a density, or deviations from a mean value of various physical quantities, solitons are single elevations, such as thickenings, etc., which propagate as a unique entity with a given velocity. The transformation and motion of solitons are described by nonlinear equations of mathematical physics.

The word 'soliton' was first coined by Zabusky and Kruskal [278] in 1965 to designate briefly solitary waves corresponding to particular solutions of some nonlinear equations describing the propagation of excitations in continuous media with dispersion and nonlinearity. However, the first qualitative description of solitary waves was observed in 1834 on a surface in a shallow channel at Edinburgh, Scotland, by the naval engineer John Scott-Russell and described in 'The Report on Waves' [261]. Based on initial observations, Scott-Russell emphasized the extreme stability and auto self-organization of solitary waves. The great stability of solitons has led to numerous attempts in recent years to explain many novel phenomena in terms of solitons in different branches of physics and other sciences.

The mathematical description of solitary waves on a water surface in shallow channels was first given on a basis of the equation,

$$\left[\frac{\partial}{\partial t} + u\frac{\partial}{\partial z} + \beta\frac{\partial^3}{\partial x^3}\right] u = 0, \quad u = u(x,t). \tag{1}$$

proposed in 1895 by Korteweg and de Vries (KdV equation) [213].

Interest in solitary waves has considerably increased due to related studies in plasma physics. In 1958, Sagdeev [104,105], showed that solitary waves, similar those observed on a water surface, could propagate in plasma in a strong magnetic field. Kadomtsev and Karpman [73] have given a complete review of magnetic and ionic-acoustic solitons in plasmas, and have considered in particular the nonlinear Schrödinger equation whose one-dimensional analogue has the form

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + G|\psi|^2\right]\psi(z,t) = 0,$$

where G is a nonlinearity parameter and where $\hbar^2/2m$ is associated with dispersion. This equation is used for describing the self-focus phenomena in nonlinear optics, one-dimensional self-modulation of a monochromatic wave in plasma, etc.

Some problems in the theory of superconductivity and ferromagnetism lead to the sine-Gordon equation (see Chapter X):

$$\left[\frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial t^2}\right]\psi(z,t) = \sin\psi(z,t).$$

Besides the equations mentioned above, are known many other nonlinear equations involving dispersion, whose solutions have a form of stable solitary waves due to the mutual compensation of nonlinear and dispersion effects. The formation of waves in a continuum described by nonlinear equations is related to a spontaneous breakdown of the local symmetry of a homogeneous system, i.e., with self-localization of the excitation energy, electric charge density, or other physical quantities.

The exceptionally important peculiarity of nonlinear equations is that they cannot be studied by means of a linearization procedure, even with subsequent treatment of small nonlinearities via perturbation theory based on expansion into normal linear modes. Nonlinear equations lead to nonlinear phenomena, such as *solitons, kinks, breathers,* and others which are impossible to obtain within finite-order perturbation treatment. These nonlinearities are fundamental as quasiparticles of linear theories, they give important information relating to the properties of appropriate media, and they play an important role in energy processes, in energy and charge transfer phenomena, and in structural transitions.

Solitary waves possess some remarkable properties which make it possible to compare them with particles. For instance, the conservation of shape and velocity after interaction is a particle-like property. It is, in fact, such properties which prompted Zabusky and Kruskal to call them *solitons* [278].

Together with ordinary extended waves, the solitary-like excitations are inherent to many nonlinear dynamical systems. Their analytical description is, however, well developed for one-dimensional systems only. In the one-dimensional case the nonlinear equations mentioned possess an infinite number of conservation laws and admit exact solutions via the so-called *method of inverse scattering* for the auxiliary linear operator. This method originated in the work of Gardner et al. [229], and was further developed by Zakharov, Faddeev, Novikov, Calogero, Marchenko, and others. The book by Zakharov et al. [66] is devoted to a complete treatment of this method. In the mathematical literature, the description 'soliton' is used only with respect to the localized solutions of completely integrable one-dimensional systems. Localized excitations described by incompletely integrable nonlinear equations are usually called *solitary waves.*

In the description of real systems, one cannot restrict the treatment to completely integrable equations alone, since the latter correspond to idealized dynamical systems. This neglects phenomena relating to the existence of boundaries and other degrees of freedom, dissipation, and small physically relevant perturbations due to surrounding bodies (complete isolation is, in fact, impossible). Unstable solitary waves can be used for a description of realistic systems if their lifetimes are larger compared with the time inherent for the phenomenon under study.

Here, the term 'soliton' is applied in a broader sense, i.e., to describe any self-localized excitations propagating without substantial change of form and velocity, due to a dynamical balance between nonlinearity and dispersion.

In solid state physics, approximate ideas of elementary excitations, as quasiparticles described by plane waves or, strictly, by wave packets, are of a current interest. General solutions of many linear phenomena are expressed in terms of such linear or quasilinear modes. One can suggest that solitons should play the same role in nonlinear dynamics.

The present book is devoted to the study of nonlinear phenomena occurring in quasi-one-dimensional molecular structures and their explanation in terms of solitons. However, we would like to begin our treatment of nonlinear phenomena by the example of the classical solitary waves observed by John Scott-Russell [261] in 1834 on a water surface in a shallow rectangular channel. As mentioned before, surface waves in such a channel are described by a dimensional equation of the type (1) given by Korteweg and de Vries (for short, KdV equation).

The function $u(x,t)$ in eqn. (1) characterizes a deviation from an average magnitude of velocity density, or any other real classical quantity, which is useful for a description of diverse phenomena in physics. The KdV equation is applied particularly to the study of ion-acoustic [271], magneto-hydrodynamical waves in plasma [203,207], acoustic waves in an anharmonic lattice [265-270,275,277], and many other phenomena. A complete treatment of the KdV equation is presented in the reviews of Kadomtsev and Karpman [73] and Toda [267], in the monograph by Karpman [74], and in other works.

In a particular case, when the function $u(x,t)$ in eqn. (1) characterizes a velocity in a continuum, we redesignate it by $\Phi(x,t)$ and rewrite eqn. (1) as follows

$$\Phi_t + 6g\Phi\Phi_x + \beta\Phi_{xxx} = 0, \quad \Phi = \Phi(x,t). \tag{2}$$

Henceforth, we shall use subindices of functions for denoting the appropriate derivatives. The nonlinear equation (2) describes a perturbation which propagates in a medium with nonlinearity and dispersion,

$$\omega(q) = c_0 q - \beta q^3, \tag{3}$$

where c_0 is the phase velocity of small vibrations described by a plane wave with wavenumber q in the limit $q \to 0$.

Neglecting the nonlinear term, $g = 0$, one can transform eqn. (2) into the linear one,

$$\Phi_t + \beta\Phi_{xxx} = 0, \tag{4}$$

which is traditionally called the linearized KdV equation. It is noteworthy that eqns. (2) and (4) are written within the coordinate frame x,t where a phase velocity c_0, involved in the dispersion (3), vanishes. Within this coordinate frame moving with velocity c_0, eqn. (4) possesses a particular solution of a plane-wave type,