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DAVID W. MCLAUGHLIN

Department of Mathematics
and
Program in Applied and Computational Mathematics
Princeton University
204 Fine Hall
Princeton, New Jersey 08544

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6. AUTHOR(S)
David W. McLaughlin

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Program in Applied and Computational Mathematics
Princeton University
204 Fine Hall, Washington Road
Princeton, New Jersey 08544-1000

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The principal investigator, together with a post-doctoral fellows Tetsuji Ueda and Xiao Wang, several graduate students, and colleagues, has applied the modern mathematical theory of nonlinear waves to problems in nonlinear optics and to equations directly relevant to nonlinear optics. Projects included (i) the interaction of laser light with nematic liquid crystals and (ii) chaotic, homoclinic, small dispersive, and random behavior of solutions of the nonlinear Schroedinger equation. In project(i) the extremely strong nonlinear response of a continuous wave laser beam in a nematic liquid crystal medium has produced striking undulation and filamentation of the laser beam which has been observed experimentally and explained theoretically. In (ii), qualitative properties of the nonlinear Schroedinger equation (which is the fundamental equation for nonlinear optics) have been identified and studied. These properties include optical shocking behavior in the limit of very small dispersion, chaotic and homoclinic behavior in discretizations of the partial differential equation, and random behavior.

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Abstract

The principal investigator, together with a post-doctoral fellows Tetsuji Ueda and Xiao Wang, several graduate students, and colleagues, has applied the modern mathematical theory of nonlinear waves to problems in nonlinear optics and to equations directly relevant to nonlinear optics. Projects included (i) the interaction of laser light with nematic liquid crystals and (ii) chaotic, homoclinic, small dispersive, and random behavior of solutions of the nonlinear Schroedinger equation. In project(i) the extremely strong nonlinear response of a continuous wave laser beam in a nematic liquid crystal medium has produced striking undulation and filamentation of the laser beam which has been observed experimentally and explained theoretically. In (ii), qualitative properties of the nonlinear Schroedinger equation (which is the fundamental equation for nonlinear optics) have been identified and studied. These properties include optical shocking behavior in the limit of very small dispersion, chaotic and homoclinic behavior in discretizations of the partial differential equation, and random behavior.

1 Technical Report

Under this research grant, the modern mathematical theory of nonlinear waves has been applied to problems in nonlinear optics. Projects include (i) the interaction of laser light with nematic liquid crystals and (ii) chaotic, homoclinic, small dispersive, and random behavior of solutions of the nonlinear Schroedinger equation.

In project (i), liquid crystals possess an *extremely strong* coefficient of nonlinearity, a property which has led our interdisciplinary group [McLaughlin, Ueda, and Wang (Program in Applied and Computational Mathematics); Braun, Faucheux, and Libchaber (Department of Physics, Princeton University); Muraki and Shelley (Courant Institute, New York University)] to use this particular nonlinear medium to study the basic physics of the interaction of light with matter. This group has used experimental, mathematical, and numerical methods in its investigations. Specifically, the extremely strong nonlinear response of a continuous wave (cw) laser beam in a nematic liquid crystal medium has produced striking undulation and filamentation of the cw beam which has been observed experimentally and explained theoretically.

In project (ii), qualitative properties of the nonlinear Schroedinger equation (NLS) have been discovered and investigated. This equation is the fundamental equation of nonlinear optics. Properties investigated include optical shocking behavior in the limit of very small dispersion, chaotic and homoclinic behavior in discretizations of NLS, and random behavior.

In the following, we describe these projects in more detail. A bibliography, together with a list of publications, is included.

1.1 Light Interacting with Nematic Liquid Crystals

The scientific importance of this laser light -liquid crystal study arises from its extremely large coefficient of nonlinearity which enables one to investigate very strong nonlinear effects with low power, cw lasers. Our interest is in the behavior of the spatially localized, coherent structures in this system –that is, in the formation, undulation, and interaction of self-focused filaments in this cw system. These strongly nonlinear effects are distinctly different from traditional NLS (Kerr) nonlinear optics. Finally, one strength of this project is its genuine interdisciplinary nature – with components from experimental and theoretical physics, as well as from theoretical and computational mathematics.

For most materials, the coefficient which describes the strength of the light-matter interaction is very small, and high powered pulsed lasers are required to generate interesting nonlinear effects. In contrast, in nematic liquid crystals [36] the nonlinear coefficient can be extremely large ($10^6 - 10^{10}$ times greater than in a typical optical media such as CS_2), thus permitting experimental investigation of a strongly self-focused optical system using moderate power (1-10 W) lasers. While weakly nonlinear optical systems are adequately described by nonlinear Schroedinger (NLS) equations, the mathematical theory of nematic optics involves *strong* coupling between the electromagnetic and nematic director (molecular orientation) fields. One of our principle results is to show that this coupling produces an unusual optical system with striking behavior.

In our theoretical and numerical study, we have focused upon the *experimental results* [3] [4] on light nematic interactions in cylindrical geometries, where the experiment observes the self-focusing of a laser beam in a nematic-filled capillary tube. The cylindrical configuration permits effective cooling, as well as a striking longitudinal visualization of the transverse structures, a view which is invaluable for corroboration of experiment and theory. Critical features of the experimental observations include the formation of a focal spot, the onset of transverse beam undulations, and, most striking, a beautiful longitudinal view of the formation and interaction of multiple beam filaments.

In *theoretical work* [4] [28] under previous Air Force support, we have developed a *coupled nonlinear field* description of the essential physics of nematic self-focusing. This theory begins from the time-dependent theory for liquid crystal optics which, in the absence of fluid flow, involves the Maxwell equations for the electric field $\vec{E}$ coupled to a nonlinear parabolic equation for the director $\vec{n}$, a field of unit vectors which describes the local molecular orientation [11]. We immediately idealize to a time independent director field, a time- averaged electric field, and a two-dimensional (planar) geometry. We then nondimensionalize, scaling all lengths on the transverse width of the "tube", and the electric field intensity on the "Frederiks transition length" [11]. With this scaling the experimental value of the (dimensionless) optical wave number is very large – $k \simeq 1.4 \times 10^4$. Thus, we replace the Maxwell equations by their geometrical optics approximation.

Under this Air Force Grant, we have completed both our numerical [30] and our asymptotic [29], [31] studies of this two dimensional model.

In [30], we have studied numerically the full behavior, including "boundary layer" effects near the front of the nematic filled tube. These numerical experiments were initiated by the natural broad Gaussian profile of the incoming laser beam. This numerical study rather faithfully reproduces all of the qualitative features of the physical experiment. (Quantitative agreement cannot be expected because of the two-dimensional idealization.) These features include the formation of multiple self-focused focal spots, the behavior of these focal spots as a function of the input laser intensity, and the breakup of the beam into two filaments. In addition, these numerical experiments identify caustics in the self focusing process as the source of the filaments which were observed in the numerical experiments, and show that the phenomena is very similar to behavior in the small dispersion limit of optical shocking (which is described below).

In our asymptotic studies *under this Air Force grant*, we have completed and substantially improved the scalar analysis [29], and we have extended that analysis to polarized fields [31]. In [29] we have completed for the scalar model a very systematic mathematical derivation of the "outer-inner" equations which describe the subtle weakly nonlinear, coupled geometric optics behavior, and show that both undulation and filamentation are captured in this asymptotic limit. In [31], we have extended this model to a vector polarized system. In the latter work, intrinsic curvalinear coordinates were introduced and used to clarify and to simplify significantly the effects of undulation on the analysis.

1.2 Properties of the NLS Equation

1.2.1 Small Dispersive Behavior

This work continues our earlier study, under previous Air Force support, of the behavior of nonlinear waves in the limit of small dispersion [27], [15], [8]. *Under this Air Force Grant*, we have completed our studies of small dispersive behavior for the case of defocusing nonlinearity [16], and have made progress in the more difficult focusing case [8], [5]. (Very recently, Bronski has significantly advanced this study [6].)

These studies consider the NLS equation,

$$\begin{aligned} iq_t &= -\epsilon^2 q_{xx} \pm q\bar{q}q, \\ q(x,0) &= A_{in} \exp \frac{i}{\epsilon} S_{in}(x), \end{aligned}$$

in the limit ($\epsilon \to 0$) of vanishing dispersion. In the defocusing (+) case, this limit is closely related to the physical phenomena of "optical shocking"

[33] [32]. In [16], we have completed a detailed study of the defocusing case, adapting the methods which Lax and Levermore developed for the integrable KdV equation to the integrable defocusing NLS case. In [8], [5] the behavior in the focusing (-) case is considered for very weak $0(\epsilon)$ nonlinearities using numerics, together with a form of weakly nonlinear geometrical optics. (Since obtaining his Ph.D. under my supervision, Bronski has initiated a study of the integrable spectral theory of focusing NLS. In that study [6] he has obtained some striking properties of the behavior of the spectrum for small ϵ which will be crucial in understanding the limit in the focusing case.)

1.2.2 Chaotic Behavior of NLS

Under previous Air Force support, as surveyed in [26] and [24] we have shown that long time behavior can be chaotic in the damped- driven NLS equation,

$$iq_t = q_{xx} + 2\,[\,q\bar{q} - \omega^2]\,q \;+\; i\epsilon\,[\hat{D}q - 1]. \tag{1.1}$$

Here the constant $\omega \in (\frac{1}{2}, 1)$, ϵ is a small positive constant, and $\hat{D}$ is a *bounded* negative definite linear operator on a function space of even, 2π periodic functions. In the simplest chaotic state, the wave form is spatially coherent, and the chaos is temporal and consists in a single solitary wave in interaction with the (long wavelength) mean. Under even boundary conditions, the solitary wave can only be located at the center ($x = 0$), or at the edge ($x = \pi$). In the chaotic state it jumps, irregularly, between these two spatial locations.

Mathematically, numerical observations of this type of "jumping" (for maps and odes) can be made precise by showing the existence of an invariant set on which the motion is topologically equivalent to a Bernoulli shift on two symbols – C (center) and E (edge); that is, the motion is as random as a sequence of "coin tosses". Our goal is to extend this mathematical analysis to the damped-driven NLS pde.

Such analysis begins with homoclinic orbits for the unperturbed system. In the case of the NLS pde, and integrable discretizations thereof, we [26], [23] [18] [19] have shown (under earlier Air Force support) the existence of a rich class of integrable homoclinic orbits. These orbits possess complicated spatial structure, including spatially localized excitations near the center ($x = 0$) and near the edge ($x = \pi$). The next step in the analysis is to establish the persistence of these homoclinic orbits under the damped-driven perturbation, and the final step is to use these persistent homoclinic orbits to construct a "symbol dynamics".

Under this Air Force Grant, we have completed [20], [21] these two steps for a particular discretization of the perturbed NLS pde. The discretization that we choose is a finite difference scheme in space x which, in the unperturbed ($\epsilon = 0$) case produces an integrable discrete system of $2N + 2$ coupled ode's. We work at arbitrary, but finite, N.

In [20] we prove, for this perturbed discrete system, the persistence of a symmetric pair of homoclinic orbits – one with spatial structure at the center and the other with spatial structure at the edge. Our arguments combine Melnikov analysis with a geometric form of singular perturbation theory. This geometric structure enables us to carry out rigorous "shooting arguments" in this high dimensional setting.

With this pair of persistent homoclinic orbits, my former graduate student Y. Li and S. Wiggins [21] have shown that perturbed, discrete NLS belongs to a class of dynamical systems which generically possess an invariant set with a Bernoulli shift dynamics.

These arguments for persistent homoclinic orbits and a shift dynamics were carried out for this discretization of the NLS pde in order to provide a model for the analysis of the pde itself. During this grant, substantial progress has been made on the second step (persistent homoclinic orbits) of this pde program.

Under this Air Force Grant, work has also been completed on a conservative perturbation of NLS pde [9]. In this work, two distinct difference schemes are viewed as long wavelength perturbations of the integrable NLS equation. These produce a conservative perturbation of NLS, for which numerical experiments [1], [25] display chaotic response. In [9] we have initiated a Melnikov study of persistent homoclinic orbits for this conservative perturbation of NLS.

To conclude this subsection on chaotic behavior in NLS pde's, we emphasize that our work in this area of chaos in pde's begins with numerical experiments which display chaotic behavior. Then we use mathematical analysis to establish specific features of the chaotic wave which have actually been observed numerically. This close relation between numerical experiments and analysis is central to all of our work on this Air Force Grant.

1.2.3 Random Behavior of NLS

McLaughlin, working primarily with Michael Shelley and a graduate student, Jared Bronski, has been studying the effects of randomness on nonlinear propagation. For example, does the random phenomenum of *localization* survive nonlinearity? Can many instabilities in a deterministic system produce an effective randomness and, if so, how can the effect be described analytically? How does random initial data propagate in a nonlinear deterministic NLS system?

Localization is the striking effect that in a one dimensional, linear media of infinite length, any amount of randomness prohibits propagation [2]. For linear Schroedinger equations with random potential, the phenomena is well known and has been established rigorously in the mathematical physics literature [35]. In the presence of both nonlinearity and randomness [14], almost nothing is known mathematically [12] [13] [17]. Some time ago, Shelley [34] carried out some careful numerical studies of discrete NLS in the presence of a random potential, which show striking, yet distinct, phenomena in the defocusing, linear, and focusing cases.

Our group has concentrated upon behavior in nonlinear Schroedinger systems, sometimes in the presence of random potentials and sometimes in a deterministic setting with many instabilities. In particular, we are investigating the combined effects of nonlinearity and randomness.

The work of Devillard and Souillard [12] is one of the few rigorous results on nonlinear localization. They consider time harmonic solutions to a nonlinear Schroedinger equation with a random potential subject to the fixed output boundary conditions;

$$\begin{aligned} i\psi_t &= -\psi_{xx} + V(x,\omega)\psi + \beta|\psi|^2\psi \\ \psi(x,t) &= \exp(-ik^2 t)F(x). \end{aligned}$$

so that F satisfies the ODE

$$k^2 F = -F_{xx} + V(x,\omega)F + \beta|F|^2 F,$$

They are able to show that in the fixed output formulation localization occurs a.s. - that the transmission approaches 0 as $L \to \infty$. The decay of F is algebraic (like L^{-1}) in the case of a focusing nonlinearity rather than exponential as is the case with localization in the linear ($\beta = 0$) case.

Having established localization, a fair question to ask is whether these particular solutions which exhibit localized behavior are physically observable. The numerical experiments of Shelley, et. al. looked at the full time evolution of a plane wave incident on a nonlinear, random slab. They found the evolution of an incident plane wave differed markedly from a time-harmonic solution. In the focusing case ($\beta < 0$) the solution at long times consisted of many soliton-like wave packets bound to local minima of the random potential. The temporal spectrum of the long time solution was far from monochromatic. While interesting, these observations were not unexpected given intuition from solitons for focusing nonlinearity.

In the defocusing case ($\beta > 0$) the long time result was much more interesting - the wave function at long times shaped itself to look like the random potential. More precisely the long time behavior of an incident plane wave with frequency k^2 was

$$\beta|\psi(x,t)|^2 \approx k^2 - V(x)$$

so that there was no localization. Interestingly the temporal spectrum, after an initial transient, settled down to something nearly monochromatic. The nonlinear evolution somehow selected an atypical time harmonic solution. The numerical results of Shelley, Newell and Caputo [10] seem to indicate that the time harmonic solutions considered by Devillard and Souillard may not be dynamically unstable and are thus probably not physically observable.

Under this Air Force Grant, Bronski completed his thesis [5] in which he established this instability. He carried out a linear stability analysis and showed that the unstable eigenvalues are isolated (point spectrum) and correspond to eigenfunctions which vanish at infinity. He obtained explicit bounds which show that any unstable eigenvalues must lie in a certain bounded region of the complex plane determined by F and V, similar to the Howard semi-circle in the theory of hydrodynamic stability. He currently lacks any sufficient condition which would guarantee the existence of unstable eigenvalues; however, by numerically solving the eigenvalue problem, he has shown that in the typical situation both the focusing and the defocusing case have unstable eigenvalues. This is interesting since neither defocusing nonlinearity nor randomness are by themselves sufficient to cause an instability. It is only through the interaction of the two terms that instabilities arise.

Bronski also has developed an intuitive description of the origin of these instabilities. This intuition originates from resonances in a nearby, selfadjoint eigenvalue problem. More importantly, Bronski has also developed an intuitive understanding of the why the defocusing case saturates at an atypical periodic profile, and why this atypical profile is stable. Thus, this work provides considerable intuition about the interaction of nonlinearity with randomness.

Most recently, we have been performing numerical experiments with many realizations of the initial data. These are important to provide statistical information about the distribution of unstable eigenvalues, as well as more information about their typical configurations. These numerical experiments are in progress, and will be published in [7]

In addition, *under this Air Force* grant, Bronski and McLaughlin [5] have investigated the averaged longwave behavior of NLS when the initial data involves many instabilities. An effective equation for the long wave behavior was derived, using the formal "renormalization group" approach [37] [39].

Finally, *under this Air Force grant*, McLaughlin, working with A. Majda and E. Tabak, has been using a carefully designed equation in the NLS class to study weak turbulence formalism [38] for the random initial value problem. The particular equation was chosen to permit closed form analysis, and at the same time, tractable numerical simulations. This work is in progress, and will be published in [22].

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PERSONNEL ASSOCIATED WITH RESEARCH EFFORT

[1.] **Xiao Wang** - Princeton University, Visiting Research Collaborator, 10/1/93 - 12/31/93

[2.] **Tetsuji Ueda** - Princeton University Post-Doctoral Fellow, 10/1/93 - 9/30/94

GRADUATE STUDENTS AFFILIATED WITH RESEARCH EFFORT

[1.] **Jared Bronski** - Princeton University, Program in Applied and Computational Mathematics. (Worked on semiclassical limits and random behavior for nonlinear Schroedinger Equations; Ph.D. November 1994. Thesis - "Aspects of Randomness in Nonlinear Wave Propagation") Awarded an NSF Postdoctoral Fellowship.

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[2.] **Jonathan Callet** - Princeton University, Program in Applied and Computational Mathematics. (Working under joint supervision of Andrew J. Majda and David W. McLaughlin on weak turbulence theory for nonlinear wave equations; completed 3rd year of graduate study.)

[3.] **Yuchi Chen** - Princeton University, Program in Applied and Computational Mathematics. (Worked on diffusively coupled bistable optical devices; currently unenrolled, candidacy continues. Ph.D. expected spring 1996.)