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Modeling Mesoscopic Phenomena in Extended Dynamical Systems

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Abstract

This is the final report of a three-year, Laboratory-Directed Research and Development project at the Los Alamos National Laboratory (LANL). We have obtained classes of nonlinear solutions on curved geometries that demonstrate a novel interplay between topology and geometric frustration relevant for nanoscale systems. We have analyzed the nature and stability of localized oscillatory nonlinear excitations (multi-phonon bound states) on discrete nonlinear chains, including demonstrations of successful perturbation theories, existence of quasiperiodic excitations, response to external statistical time-dependent fields and point impurities, robustness in the presence of quantum fluctuations, and effects of boundary conditions. We have demonstrated multi-timescale effects for nonlinear Schrodinger descriptions and shown the success of memory function approaches for going beyond these approximations. In addition we have developed a generalized rate-equation framework that allows analysis of the important creation/annihilation processes in driven nonlinear, nonequilibrium systems.

1. Background and Research Objectives

Two of the important lines along which complexity in nonlinear condensed matter has evolved over the last decade are complex dynamics of coherent structures in problems with competing length and/or time scales and partial differential equations (PDEs) with length and time scales controlled by additive or parametric forcing and damping. We are now at last able to also tackle the fundamental concern of combining nonlinearity with disorder and noise. This opportunity raises major issues for applications of mathematics—particularly stochastic nonlinear PDEs—and a new role for the synergistic combination of analysis and scientific computing. Our intent was to develop the necessary analytical and numerical technology base for several emerging themes in nonlinear condensed matter and materials science. Our principal concern was to address aspects of coherence and chaos as they appear in PDEs and

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coupled systems of ordinary differential equations (ODEs) representative of current condensed matter physics and materials science.

Condensed matter is almost always concerned with spatially extended dynamical systems. Many such systems show aspects of low-dimensional phase spaces and attractors. This is most typically due to the formation and dynamics of collective or coherent structures in strongly nonlinear systems, controlling "mesoscopic" behavior. Nonlinear mode reduction is therefore essential. Examples are "soliton" or "solitary wave" modes appearing in condensed matter as dislocations, vortices, domain walls, etc. On the one hand, we have developed a variety of nonlinear collective coordinate and nonlinear spectral analysis techniques to identify and isolate the dynamics of such coherent structures in weak perturbations from integrable systems. On the other hand, many condensed matter problems are in a heavily overdamped regime, e.g., convection cells, charge-density waves, and flux motions in superconductors. A Lyapunov free energy functional can often be defined in such diffusive cases, lending itself to Landau symmetry/normal form analysis of steady states -- the equivalent of ground or metastable space-time attractors. These attractors may be, e.g., periodic patterns (such as a periodic array of rolls in a convection cell); the study of the bifurcations of these patterns under increasing stress has been an important chapter in modern applied mathematics.

Competitions of length scales or symmetries lead to stationary patterns in space that can be constant, periodic, quasi-periodic, or even totally irregular ("structural chaos"). The instability of such patterns under increasing stress can be approached by perturbation theory, leading typically to complex Ginzburg-Landau (CGL) equations coupled to the periodic reference state. The unstable phase modes may then be traveling waves or localized "defects," which can nucleate transitions from one pattern to another. A key topic for mathematical and computational science in this area is the mechanism determining patterns in space and time in systems with competing length and frequency scales. Some analytical progress has been made for evolutionary PDEs of CGL type via the inertial manifold concept. The competing length and time scales correspond to the optimal (lowest dimensional) set of modes spanning the manifold. There are intimate relationships between space and time in that ground state spatial structures (i.e., stationary solutions) lead directly to the frequency scales observed as a system relaxes from a nonequilibrium configuration or as it responds to external forces. If the ground state is spatially constant, it becomes unstable through spatially extended modes; if it is nonconstant (because of competing length scales), the unstable modes are spatially localized and will saturate in the underlying nonlinearity into coherent structures, whose dynamics controls the time scales observed macroscopically. If the ground state is chaotic, then the complexity of environments for the coherent structures increases correspondingly and leads to many ("glassy") time scales. We have developed a number of nontrivial model problems

drawn from condensed matter that demonstrate this coupling of space and time and provide examples of "self-organized criticality" and "mesoscopic complexity."

The mathematical field of stochastic nonlinear PDEs enters the present setting when noise and disorder appear in combination with nonlinearity and sometimes also lattice discreteness. For example, noise is a natural way of approximating the effects of the neglected states in a collective coordinate representation. The presence of noise may have dramatic effects on the solutions: The combined effects of noise and nonlinearity may be additive and synergistically enhance each other, or they may be mutually destructive; also, the distribution (color) of space or time scales plays empirically important, but as yet poorly understood, roles.

2. Importance to LANL's Science and Technology Base and National R&D Needs

The Laboratory's condensed matter and materials science research in several of its technical divisions and centers offers the possibility of controlled, laboratory-scale experiments on well-characterized electronic and structural systems. This capability has increasingly fostered a symbiotic relationship between experiment, simulation, and analysis that has directly tested and illuminated general problems in dynamical systems theory. Nonlinear condensed matter systems are typically modeled by nonlinear PDEs at various physical scales. Lattice discreteness is intrinsically relevant in many solid state contexts, so that coupled ODEs must be addressed. Equations such as the sine-Gordon (SG), nonlinear Schrödinger (NLS), and CGL have been studied intensively because of their direct relevance to condensed matter and materials science: surface physics, convection cells, acoustics, magnetism, optics, Josephson junctions and transmission lines, electronically active materials, etc.

The general numerical and analytical techniques and strategies developed in the Los Alamos Center for Nonlinear Science (CNLS) and similar interdisciplinary units around the world have now matured to the point where applications to nonlinear and nonequilibrium processes in specific disciplines are both possible and necessary. Our aim has been to use recent problems in condensed matter physics and materials science to motivate a choice of issues of general concern in nonlinear mathematics and to develop appropriate analytical and numerical techniques. Our primary focus was to develop a mathematical physics technology base for handling compelling new issues in nonlinear dynamical systems theory. However, we were careful to take strong guidance from, and transfer results to, specific applications being studied experimentally at Los Alamos and elsewhere. Projects of this type with which we had (and still have) close associations include self-trapping (polaron formation) in low-dimensional electronic materials, nonlinear optical materials and transmission lines, convection cells, surface growth, vortex dynamics in layered magnetic materials, microstructural materials

and process modeling, textures in elastically phase-transforming materials, Josephson junction arrays and coupled transmission lines, flux flow in superconductors, quantum dots and arrays (nanotechnology), and semiconductor modeling. Nonlinear and nonequilibrium processes are increasingly fundamental to a description of modern materials. Indeed, an understanding of these processes is crucial as we move into an age of purpose-designed novel electronic and structural materials characterized by strong nonlinearity and disorder, with reduced and anisotropic geometries and with competing interactions (length, frequency, etc.).

3. Scientific Approach and Accomplishments

We have studied perturbation theory and nonlinear collective coordinates in the periodically, randomly, and parametrically driven nonlinear Schrödinger, sine-Gordon, and similar equations in $(1 + 1)$ and higher dimensions. We investigated creation and lifetime of coherent structures, established effective transport coefficients for these systems, and tested predictions of reduced models against full simulations to provide calibration for a mesoscale materials modeling strategy. We used spectral codes and stochastic dynamics codes on, e.g., the CM-5. We also studied quantum chaotic problems, including memory function descriptions of such systems with spatial and temporal noise.

We have followed specific investigations of analytic and numerical techniques and applications for collective modes interacting via disorder, (thermal and quantum) noise, nonlinearity, and lattice discreteness: nonlinear collective coordinates. We have applied the techniques we have developed to quantify collective coordinates and their role in pattern formation and complex dynamics. These include analytical methods in one and two dimensions (1-D and 2-D) and also inverse spectral transform codes developed (with E. Overman, OSU) for 1-D sine-Gordon and nonlinear Schrödinger equations. These approaches have proved to be excellent for following the dynamics of individual collective structures. We have used them to study (a) Hamiltonian chaos due to disorder and (b) the sine-Gordon equation with dissipation and external driving of the form $f(kx - \omega t)$, where $f(x)$ is periodic. This introduces the following: (a) competition of two length scales dynamically; (b) explicit evaluations of Melnikov and multifractal $[I(a)]$ tests for chaos in collective coordinates; (c) coupling the spectral code to Langevin equations to derive and test Fokker-Planck descriptions of extended dynamical systems in a small number of collective coordinates; (d) comparing the spectral code results with approximate analytical schemes based on nonlinear mode reduction decompositions; and (e) using collective coordinates as a basis for defining geometrical (e.g., Berry) phases in spatially extended systems.

We have also used collective coordinate techniques to do the following: (a) study fluxon collective coherence and phase locking in a long Josephson junction subject to high frequency pumping fields (phase locking is observed numerically and is consistent with our analysis, even when the drive frequency is 16 times the fluxon oscillator frequency); (b) predict and confirm numerically that a resonance mechanism can produce stable moving solitons in a discrete (1+1)-dimensional nonlinear Schrödinger equation in the presence of dissipation and as AC driving in the form of a standing wave; and (c) demonstrate that threshold driving strengths exist, above which a stable breathing mode exists in the damped (1+1)-dimensional cubic nonlinear Schrödinger equation driven by a two-frequency AC drive. There is again good agreement with direct numerical simulation. Our collective variable reductions of the Landau-Lifshitz equations governing classical spin dynamics in (2+1)-dimensions have been extended to include image "charges" in finite systems. This gives an excellent description of the dynamics of vortex-vortex and vortex-antivortex collective structures, estimates of vortex mass, etc.

We have studied aspects of stochastic PDEs (and coupled ODEs), addressing mathematical issues motivated by condensed matter and materials science problems. One specific project involved studying noise and disorder in problems of coupled fields. Such problems (e.g., in nonlinear optics, self-trapping in plasmas, polaron formation) are frequently approached by adiabatically slaving one field to the other; however, disorder in space or time leads to additional scales that must be incorporated in multiscale reduction techniques. For instance, the NLS equation results from adiabatic slaving in ordered systems. On some length- and time-scales, disorder simply translates into coefficient disorder in the NLS equation; however, on other scales, completely new equations must be analyzed.

For a second project, concerning the competition between Anderson localization (due to disorder) and self-trapping (due to nonlinearity) in the NLS equation itself, we will consider effects of both additive and parametric perturbations on the continuum NLS equation and an integrable discrete version due to Ablowitz and Ladik, with various boundary conditions (periodic, free, absorbing). We have also found bifurcations as the strength of nonlinearity and disorder are varied, and these were explored by several techniques including direct numerical solution of the time-dependent PDE, nonlinear spectral analysis, collective coordinate approximations with which to describe smoothing of the disorder and effective single-particle dynamics, and renormalization group (RG) scaling approaches. We have discovered that there are striking effects of lattice discreteness in the NLS (and related equations), including soliton trapping on maxima of potential variations and bounded motion on linearly increasing potentials. The existence of oscillatory local (breather-like) solutions in

nonlinear equations, stabilized by lattice discreteness, is strongly debated currently for applications in molecular crystals, DNA dynamics, etc.

We have extensively studied the discrete (1+1)-dimensional nonlinear Schrödinger equation in a form that interpolates continuously away from the integrable (Ablowitz-Ladik) limit. We have demonstrated that the integrable limit retains integrability in a spatially uniform external electric field with arbitrary time-dependence. In the static electric field limit, the system exhibits a periodic evolution that is a surprising nonlinear counterpart of linear-Schrödinger-equation Bloch oscillations. We have further shown that localization can be dynamically induced by a harmonic time-dependence, as a consequence of parametric resonances at certain field strengths. The nonlinear Bloch oscillations and dynamic localization are found numerically to be a property of the discreteness and not limited to the integrable limit of our model -- in the nonintegrable case, energy is localized at the resonance conditions, but chaotically so.

Noise in general has color. A particularly important example is the monochromatic case, a periodic modulation of parameters or external perturbations. We have found that coherent structures have a particle-like robustness if their length scale is either small or large compared to the disorder scale -- the effects on the soliton dynamics can then be treated within an effective Fokker-Planck or RG scaling scheme. On the contrary, if the length scales are comparable, nonperturbative effects dominate -- periodic transitions between different coherent patterns, random destruction and refocusing of the soliton, excitation of selected radiation, or even permanent soliton dispersion. These events are analogous to homoclinic points in single particle chaos and dominate transport coefficients. The periodic case exhibits the key elements of the competition for arbitrarily colored noise. We have numerically observed a rich spectrum of dynamics as either the soliton amplitude (relative to the periodic potential amplitude) or velocity are varied. Preliminary results for random potentials show that high velocity solitons can ride over the disorder ahead of all radiation emission but that slower solitons emit tails of coherent pulses and are eventually trapped.

A complementary problem concerns the competition between nonlinear modulation or self-focusing into solitons (from distributed initial energy or following the soliton destruction above) and linear (Anderson) localization driven by disorder. Unlike corresponding linear problems, this competition is controlled by at least two relevant variables, e.g., energy and amplitude. We have studied scaling regimes using RG and numerical techniques for both classical and quantum mechanical cases. In the quantum case, we used exact diagonalization and coherent state approximations to probe "quantum chaos" through fractal wave function structure as a function of integrability and $\hbar$ -- it is particularly important to understand quantization of homoclinic and unstable orbits.

We have also undertaken a study of the NLS equation with sinusoidal additive driving. This work demonstrated the possibility for a statistical mechanics description of the soliton creation and annihilation processes in the dissipative, strongly driven NLS systems. We have shown by analyzing statistical mechanics quantities and by constructing a phenomenological stochastic theory that the soliton annihilation/creation process has sub-Poissonian character and is dominated by two-solitons and large amplitude radiation. A generalized rate-equation theory has been formulated.

We have also undertaken studies of the (1+1)-dimensional discrete nonlinear Schrödinger equation in the presence of random disorder to study collapse of initially flat data. The indications are that scaling toward linear (Anderson) localization occurs at low initial data amplitudes, crossing over toward nonlinear (soliton) scaling at large amplitudes with complex multi-attractor dynamics in the crossover region. We have also considered the validity of semiclassical and scaling approximations typically invoked to justify discrete nonlinear Schrödinger descriptions in coupled quasiparticle-boson quantum systems. Using exact numerical techniques on a few site chains, together with memory function analysis, we have shown that there exists a hierarchy of time-scales that rationalizes collective "tunneling" in such models. We find that the discrete nonlinear Schrödinger equation is only valid in a very limited antiadiabatic regime, whereas semiclassical approximations become exact in a nontrivial adiabatic limit.

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