CHAOS2024 - *Hybrid*

17th Chaotic Modeling and Simulation International Conference

11 - 14 June, 2024, Chania, Crete, Greece

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Book of Abstracts.

Special Session on
Localized Excitations in Nonlinear Lattices

Organizers: Jānis Bajārs and Juan FR Archilla

Special Session on Localized Excitations in Nonlinear Lattices (LENL) in CHAOS2024, Chania, Crete, Greece, June 11-14, 2024.

Program CHAOS2024

17th Chaotic Modeling and Simulation International Conference,

Chania, Crete, , Greece, 11 – 14 June, 2024 Hybrid

Special and Contributed Sessions: Tuesday, June 11,2024: 11:30-14:00 (EEST)

Room 2

Invited session: LENL: Localized Excitations in Nonlinear Lattices.

Chair: Jānis Bajārs and Juan FR Archilla
11:30-14.00 SCS1

Development of Nonmonotonically Propagating Annealing of Defects with Oscillating Temperature at the Wave Front
Pavel Selyshchev

Effects of Self-correlated Gaussian Noise on the Emergence of Robust Breathers in the Ac-driven, Dissipative sine-Gordon Model
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Nonlinear Energy and Charge Transport in Silicates. Experiments and Semiclassical Models
Juan F.R. Archilla, JānisBajārs, Yusuke Doi, Masayuki Kimura

Numerical Integration of Thermostated Semiclassical Hamiltonian Lattice Equations
JānisBajārs, Juan F.R. Archilla

Soliton Dynamics in an Oscillating Magnetic Field
Larissa Brizhik

Thermalization slowing down for weakly nonintegrable many-body dynamics
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Traveling Localized Vibrations in a Magnetically Coupled 2-DOF Resonators
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Path to equilibrium of breathers in nonlinear lattices
Juan FR Archilla, Jānis Bajārs, Sergej Flach

Development of nonmonotonically propagating annealing of defects with oscillating temperature at the wave front.

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Abstract: The most practical and fairly effective methods for recovering materials after irradiation is annealing of radiation defects namely disappearing of defects induced by heating, for example by means of recombination, etc. One of modes of annealing is a self-propagating annealing with constant speed and constant propagating profiles of temperature and defect density [1]. This annealing mode has the form of "stepped" distributions of temperature and defect density running at a constant speed. Before the wave front, the density of defects is constant and non-zero, and the temperature is equal to the ambient temperature. Behind the front, the density of defects is practically zero, and the temperature is increased. Annealing of defects occurs in the "annealing zone" - a narrow region of the "step" of the wave front.

Numerical investigation of this mode finds that for some set of parameters there are modes with oscillations of propagation speed and front of temperature profile. It has been found that oscillations of temperature takes place in the "annealing zone". In the annealed region, temperature disturbances have a form of temperature waves that follow temperature fluctuations in the "annealing zone." In the unannealed region, the temperature drops monotonically - temperature fluctuations do not have time to establish themselves due to the movement of the temperature front because an increase in temperature in the unannealed region leads to the annealing of defects in it and a displacement of the front of the wave. Temperature surges correspond to an increase in the steepness of the front of the defect annealing wave and an increase in the speed of its propagation.

It has been have established that these this mode develops due to thermo-concentration feedback, leading to instability of the mode with constant speed. The phenomenon was described using the theory of bifurcations. A criterion for the instability is obtained. An approximate analytical solution, which describes characteristic features for the post-bifurcation mode, is constructed.

Keywords: Defect annealing. Nonlinear feed-back. Self-propagating wave. Instability. Bifurcation.

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Effects of self-correlated Gaussian noise on the emergence of robust breathers in the ac-driven, dissipative sine-Gordon model

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Abstract: It has recently been established that thermal noise and harmonic forcing can cooperatively excite sine-Gordon breathers robust to dissipation. So far, this phenomenon has been therefore explored assuming a Gaussian noise source, delta-correlated both in time and space [1,2]. Given the potential implications of the present ideas, e.g., for the experimental observation of breathers in extended Josephson systems, it is particularly important to address the effects of more realistic noise sources with finite correlation time and/or correlation length. Here we show that breathers still emerge under this broader class of noise sources. Furthermore, we find that the correlation time and the correlation length offer control over the probability of observing breathers, a fact which can be very useful for the design of protocols aimed at detecting these elusive nonlinear excitations [3].

Keywords: Perturbed sine-Gordon model. Breathers. Self-correlated Gaussian noise.

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Nonlinear Energy and Charge Transport in Silicates. Experiments and semiclassical models.

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Abstract: Experiments with silicates bombarded by alpha particles show the transport of charge and energy without the need of an electric field, the energy and momentum provided by the alpha particles. We construct two semiclassical models to model the observed phenomena, a phenomenological one, used as a test model to develop and refine the theory, and other obtained from physical principles and empiric potentials. For the latter the propagation of charge is difficult to achieve, but there are exact neutral excitations, transporting energy. We also present provisional results on the thermalized lattice.

Keywords: Nonlinear excitations. Charge transport. Energy transport. Semiclassical lattices. Silicates.

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MK: JSPS Kakenhi (C) No. 21K03935

Numerical integration of thermostated semiclassical Hamiltonian lattice equations

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Abstract: In this work, we develop computationally efficient splitting methods for semiclassical Hamiltonian lattice equations, where crystal lattice models are described by classical Hamiltonian dynamics, whereas an extra charge (electron or hole) is modeled as a quantum particle within the tight-binding approximation. Such models are of significant scientific importance. A particular application is hyperconductivity, i.e., the experimental observation of charge transport without the presence of an external electric field when a silicate is bombarded with alpha particles. The charge is carried by nonlinear lattice excitations. In the present work, the canonical equations for a semiclassical Hamiltonian describing the coupled lattice-charge dynamics are coupled to a gentle stochastic thermostat, which drives the system to the canonical distribution at a prescribed temperature with minimal perturbations to the Hamiltonian trajectories while at the same time ensuring the conservation of the charge probability. The properties of the proposed splitting methods are explored and numerically demonstrated on a phenomenological semiclassical Hamiltonian lattice model.

Keywords: semiclassical Hamiltonian dynamics; splitting methods; lattice models; stochastic thermostats; charge transfer; nonlinear localized excitations.

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Soliton dynamics in an oscillating magnetic field

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Abstract: The talk is dedicated to 50 years of the Davydov's soliton [1]. The influence of oscillating magnetic field on the soliton dynamics is investigated [2]. It is shown that such dynamics is described by the system of coupled nonlinear equations, which in the continuum adiabatic approximation can be reduced to the modified nonlinear Schroedinger equation. Soliton dynamics is shown to depend essentially not only on the amplitude and frequency of the magnetic field, but also on its orientation. In the magnetic field parallel to the molecular chain axis soliton propagation is a composition of the "free" soliton coherent movement along the molecular chain and electron cyclotron oscillations in the perpendicular plain with the effective cyclotron frequency and mass, In the case of magnetic field perpendicular to molecular chain axis, soliton propagation along the chain is described by the modified nonlinear Schroedinger equation with the term in the right hand side, which is determined by the magnetic field. This equation is solved using the nonlinear perturbation theory [3]. It is shown that soliton parameters are functions oscillating in time with the frequency of the main harmonic, given by the frequency of the external field, and its higher multiple harmonics. Such complex soliton dynamics in the oscillating external magnetic field affects charge transport and, therefore, the processes, this transport is involved in, such as electroconductivity in low-dimensional systems used in micro- and nanoelectronics [4] or redox processes in living organisms [5].

Keywords: Davydov soliton, magnetic field, low-dimensional system, perturbation theory, mechanism of therapeutic effect of oscillating magnetic field

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Thermalization slowing down for weakly nonintegrable many-body dynamics.

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Abstract: We observe different universality classes in the slowing down of thermalization of many-body dynamical systems upon approaching integrable limits. We identify two fundamentally distinct long-range and short-range classes defined by the nonintegrable perturbation network spanned amongst the (set of countable) actions of the corresponding integrable limit. Weak two-body interactions (nonlinearities) induce long-range networks in translationally invariant lattices. Weak lattice coupling (hopping) instead induce short-range networks. For classical systems we study the scaling properties of the full Lyapunov spectrum. The long-range class results in a single parameter scaling of the Lyapunov spectrum, with the inverse largest Lyapunov exponent being the only diverging time control parameter and the rescaled spectrum approaching an analytical function. The short-range class results in a dramatic slowing down of thermalization and a rescaled Lyapunov spectrum approaching a non-analytic function. An additional diverging length scale controls the exponential suppression of all Lyapunov exponents relative to the largest one. For quantum spin chains we compute ergodization time scales within the framework of the Eigenstate Thermalization Hypothesis and the Lyapunov time from operator growth methods using Krylov Complexity. The comparison of both time scales confirms the existence of the above universality classes for quantum many body dynamics as well.

Keywords: Chaos, Thermalization, Nonintegrable Perturbations, Lyapunov Spectrum, Scaling, Universality, Eigenstate Thermalization Hypothethis, Krylov Complexity, Quantum Spin Chains

Traveling Localized Vibrations in a Magnetically Coupled 2-DOF Resonators

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Abstract: A magnetically coupled 2-DOF resonators is fabricated to observe traveling localized vibrations and to study their characteristics experimentally. The 2-DOF resonator consists of an elastic rod and a permanent magnet. The magnet is attached to the top of the rod. Several rods are equally spaced and arranged in one dimension. The edge of the array is externally excited by a shaker. The amplitude and frequency of the shaker are carefully adjusted, and then traveling localized vibrations are successfully generated. We will discuss the condition of the amplitude and the frequency for generating the traveling localized vibrations.

Keywords: Intrinsic Localized Mode, Discrete Breather, Coupled Resonator Array, Nonlinear Vibrations and Waves in Lattices

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Path to equilibrium of breathers in nonlinear lattices

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Abstract: A simple parameter that characterizes the degree of localization in a lattice is the participation number *P*, defined as the ratio between the square of the total energy and the sum of the squares of the local energies. It takes values between 1 when all the energy is in one particle and N, when all the particles have the same energy. An approximate deduction proves that at thermal equilibrium $<P>=N/2$, where *N* is the number of particles in the system. Numerical simulations result in a slightly larger value. However, we can take it as a parameter indicating that the system is very close to thermal equilibrium as the variance or *P* is anyway relatively large.
We produce a thermalized state at thermal equilibrium with a given average energy per particle $h=E/N$, where *E* is the total energy of the system. Then, we add a localized energy E_b to a single site, mimicking the interaction of an incident particle as a neutron. We call the localized excitation a *discrete breather* [1,2], as it tends to perform localized oscillations during some time in the thermalized environment. We let the system evolve until $P=N/2$ after some time that we call the *thermalization* time t_{th}. We perform many simulations which lead to many different values of t_{th}, as it should be expected because the initial conditions are very different, including but not limited to the value of *P*.

We observe that t_{th} decreases exponentially with the energy delivered E_b both for hard and soft quartic potentials, a result previously observed in [3] for the DNLS. This suggests that the conservation of the norm in the DNLS is not necessary for the exponential behavior of the thermalization time. The similitude of the exponents with both hard and soft potentials is striking, and we are repeating the study for some different systems as the Frenkel-Kontorova lattice, and models for Josephson-junction arrays, with the objective of determining the generality of the phenomenon.

Keywords: Nonlinear lattices. Breathers. Thermal equilibrium. Lifetime.

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