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EXPERIMENTAL OBSERVATION OF MOVING DISCRETE BREATHERS IN GERMANIUM

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Keywords: ILM, breather, electric traps, germanium, DLTS

Abstract

Low energy ICP Plasma produce Atoms that arrive at a semiconductor surface with very low energy (2-8 eV) but are able to anneal defects deep inside the semiconductor [1], as shown in the figure. The number of defects before and after plasma irradiation is obtained through the well proven technique of Deep Level Transient Spectroscopy (DLTS) [2].

Several different defects were removed or modified in Sb-doped germanium, some of the them are known, such as the E center, which has the highest concentration. After eliminating other possibilities (electric field, light, heat) we now conclude that moving discrete breathers (DBs)[3], as a mechanism of long-distance energy transport, are the most likely cause. Stationary and moving breathers have been found recently by molecular dynamics in different materials with energies from 0.1 eV to a few eV [4,5]. The mechanism of annealing is an activated process, and discrete breathers have already been shown to accelerate this type of processes [6].

This would be a striking evidence of the importance of DBs in crystals and opens the way to further experiments to probe DB properties both in semiconductors and in the metals used for contacts. Most of the measurements have been done in germanium, but also it have been shown that similar effects take place in silicon.

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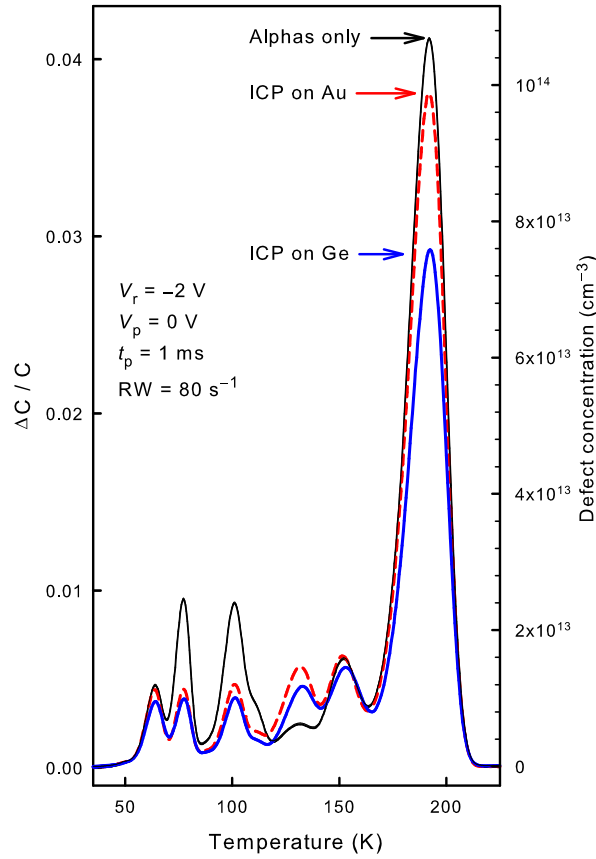


Figure 1: Three DLTS spectra performed in Sb-doped Ge after being damaged by 5 MeV α particles followed by 24 hours or room temperature annealing. The labels at the right Y-axis indicate the defect concentration at the respective peaks and are meaningless otherwise. Black (thin line): before ICP; red (dashed): after 30' ICP through an Au contact; blue (thick line): after 30' ICP directly on Ge. See text for explanation. The highest peak at 185 K corresponds to the E center defect.

BISOLECTRONS IN HARMONIC AND ANHARMONIC LATTICES

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Keywords: bisolitons, bisolectrons, anharmonic lattice, electron-lattice interaction

Abstract

It is shown that electron-lattice interaction leads to binding of two extra electrons (holes) with antiparallel spins in a molecular lattice into a bound bisoliton state at the intermediate values of electron-lattice coupling, when the adiabatic approximation is valid [1,2]. If the potential energy of the inter-site interactions in the lattice is harmonic, such bisolitons are stable at velocities less than the velocity of the sound. It is proved that the account of the lattice anharmonicity results in the formation of the bound bisolelectron state [3-4] which is stable in the whole range of its velocities up to the velocity of the sound. Such a bisolelectron propagates along the chain practically without energy dissipation and is an ideal charge carrier in quasi-one-dimensional molecular systems with moderately strong electron-lattice coupling. We show also that supersonic bisolectrons can exist in an anharmonic lattice.

According to the analytical study, the envelope function of a bisolelectron can have one or two maxima depending on the strength of the Coulomb repulsion between the electrons. This result is shown to explain the results of the numerical modeling of two electrons in an anharmonic lattice with Morse-type interactions between unit sites [5] within a wide range of the Coulomb interaction strength. It also agrees with other numerical data [6].

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SOLITONS AND CHARGE TRANSPORT IN TRIANGULAR AND QUADRATIC MORSE LATTICES

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Keywords: 2d-Morse lattices, quasi-1d and horse-shoe solitons, charge transport, sollectrons, tight-binding model

Abstract

Localized moving soliton-like excitations are considered to be potentially effective carriers for electric charges in one- and two-dimensional nonlinear lattices to model some real physical, chemical, biological substances. We study here via numerical simulations the excitation and propagation along crystallographic axes of both quasi-1d and horse-shoe supersonic solitons in triangular lattices and in quadratic lattices of particles interacting via potential Morse forces. Also soliton-like excitations are studied in quadratic lattices with additional on-site potential (cuprate-like lattices). Analysis of dispersion characteristics and solutions of the Kadomtsev-Petviashvili equation appear useful to describe properties of solitons in 2d-lattices. Then trapping of an added excess electron due to its potential quasi-electrostatic interaction with lattice particles thus forming a quasi particle soliton-electron ("sollectron") is studied in the frame of tight-binding model (TBM). It is shown that trapping of electron may be realized even if the electron is located first far enough from the soliton and its wave function is not localized ("vacuum cleaner effect").

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TRAVELLING COHERENT STRUCTURES IN THE ELECTRON TRANSPORT IN 2D
ANHARMONIC CRYSTAL LATTICES

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Keywords: Anharmonic lattice, lump solution.

Abstract

We study the feasibility of soliton-mediated electron transport in two dimensional (2D) anharmonic square crystal lattices. To this end we consider cubic and Morse anharmonic interactions in 2D lattices in the absence of the electron and numerically show the possibility of propagation of lump coherent structures similar to those in the Kadomtsev-Petviashvili (KP) equation. We finally insert the electron into the lattice to consider the electron-soliton bound state and numerically show the possibility of solectron formation.

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THE ORIGIN OF DEFECTS INDUCED IN ULTRA-PURE GERMANIUM BY
ELECTRON BEAM DEPOSITION

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Keywords: electron beam deposition, germanium, semiconductor, defects, DLTS

Abstract

Vacuum with a hydrogen partial pressure of 10^{-9} mbar in combination with static shields was used to produce electron-beam deposited (EBD) Pt Schottky barrier diodes on n-type Ge with electrically active defect concentrations lower than 10^{11} cm⁻³. Broad peaks observed in the deep level transient spectroscopy (DLTS) spectra of our diodes are indicative of surface defects while the sharp peaks that signal the presence of electron or hole traps were absent. Already in 1967, Chen et al [1] discussed a more efficient energy transfer mechanism by which an energetic electron, using a two-step process, transfers energy to the crystal lattice via a light atom (fig. 1). Energetic electrons reflected off the target as well as photons were not blocked by the shields indicating that collision products originating in the evaporator's 10 keV electron beam path with high enough energy to create vacancies were responsible for the observed EBD induced defects. This conclusion can also be drawn if n-Si is used [2].

Samples exposed to the conditions of EBD, without deposition (termed EB exposure) did not contain the same defects as the EBD samples except for the vacancy-antimony center (V-Sb), H_{0.30}. This implies that a necessary condition for the introduction of EBD defects was a thin metal layer through which energy was transferred to the germanium crystal lattice. The EB exposure defects have not yet been identified and are probably related to impurities that were accelerated into the germanium near-surface region before diffusing deeper into the material.

Acknowledgements: This project has been financed by the South African National Research Foundation.

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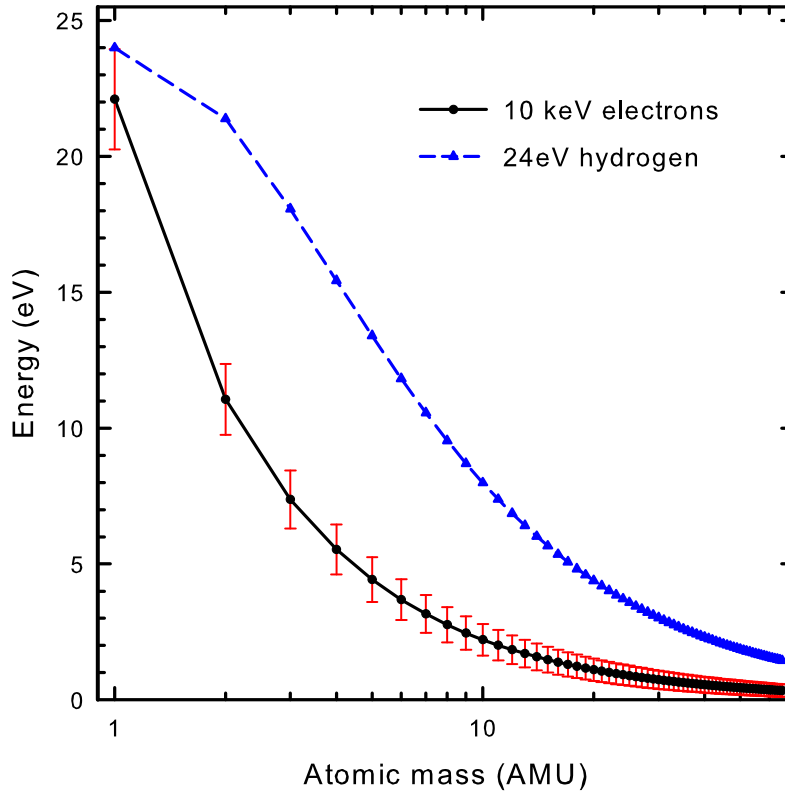


Figure 1: Maximum energy transferred during an elastic collision between a 10 keV electron or between a 24 eV hydrogen atom and particles of increasing mass. All momentum transfer calculations were performed non-relativistically where the bars denote the energy variation dependent on the relative velocity in a vacuum of the second particle.

THEORY VS. REALITY - LOCALIZED EXCITATIONS INDUCED BY OPTICAL
MANIPULATION OF PROTEINS, AS A DIFFERENT APPROACH TO LINK
EXPERIMENTS WITH THEORY

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Keywords: electron beam deposition, germanium, semiconductor, defects, DLTS

Abstract

The recent revolution in optical techniques opened the way to translationally manipulate atoms and molecules. [1] The interaction of EMF (electromagnetic field) with matter generates a new force, known as *optical force*, leading to new material properties, known as *optical matter*. In our experimental work we used high-density-green-photons, (HDGP, $\lambda = 520$ nm) beams, to optical manipulate large molecules. We succeeded to induce new optical matter in a protein molecule, which after our HDGP-manipulation, acquired antioxidant characteristics [2]. We detailed experimentally and theoretically our optical manipulation technique and dubbed the newly induced mesoscopic textures *biological optical matter* [3]. The optical manipulation of an enzyme-protein induced, unexpectedly, allosteric properties. An allosteric enzyme changes the affinity of its substrate for the enzyme active center, through binding of a small molecule (ligand) outside it. Now let us consider an enzyme in two states, (C) the natural and (*) the optical manipulated one. Let f be the concentration of a product derived from a substrate with concentration x ; in this case, the equation of evolution is:

$$\frac{\partial f}{\partial x} = -\lambda f$$

meaning that the reaction relaxes with the rate λ , $\lambda > 0$. When an external agent is at work, of strength B (like optical manipulation with HDGP) the evolution equation is:

$$\frac{\partial f}{\partial x} + \lambda f = B\lambda$$

with the solution: $f = B + (A - B) \exp(-\lambda X)$ where A is the initial concentration; we take $B > A > 0$. This is a typical inhibition-activation curve, with an efficiency level B , analogue with the allosteric kinetics.

Kinetics of α -amylase activity under optical manipulation. A connection with the phenomena of allostery appears clearly. The allosteric enzyme molecule has also two states (R & T) and an allosteric effector modifies the apparent affinity of the substrate for the allosteric enzyme active center.

As revealed by the above kinetics, in our experimental set-up, an effector- HDGP, analogue with the allosteric ligand, modifies the substrate affinity for the enzyme active center. Hence we discovered a new allostery: **the EMF acts as a different allosteric effector.**

The physical basis for this different phenomenology: the EMF, acting on large molecular structures, induces polarization effects, generating electric dipoles, which interact with each other. The computed

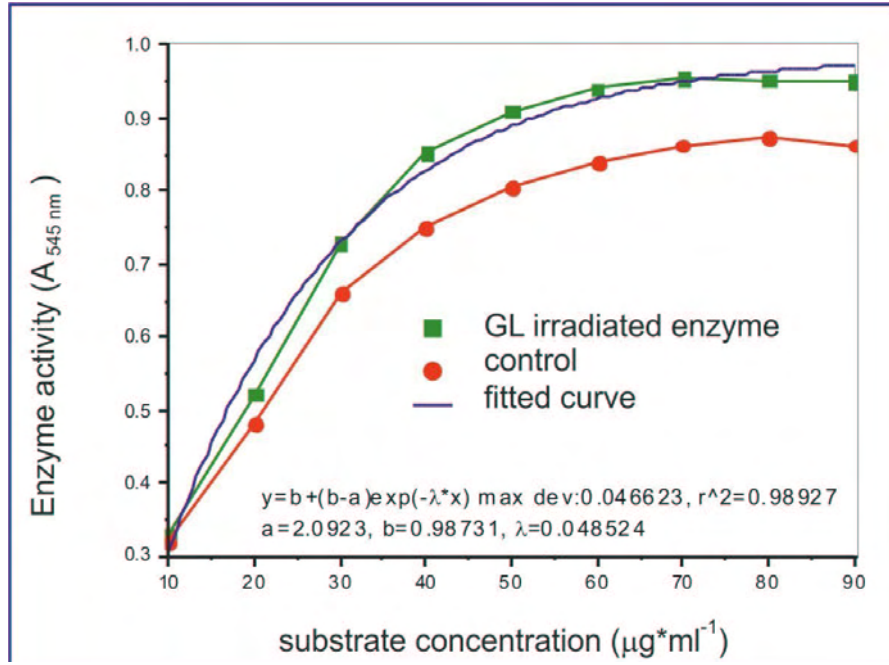


Figure 1: Kinetics of α -amylase activity under optical manipulation.

dipolar interaction energy is:

$$U = -\frac{1}{2}v^2\alpha^2\frac{E^2R^2 - 3(\mathbf{ER})^2}{R^5}$$

This is a short range force ($1/R^4$), able to bind dipoles in chains along the electric field \mathbf{E} , creating a reticular structure. We have a direct physical proof of these conjectures, obtained by AFM technique. The optical manipulated layers of enzyme molecules displayed under AFM images clear reticular areas, as compared with the randomly disposed control molecules. As a final remark let us observe that our work presents a direct link between theoretical considerations (along with their predictions) and the reality of the experimental data.

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THE AMIDE I BAND OF CRYSTALLINE ACETANILIDE:
OLD DATA UNDER NEW LIGHT

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Keywords: Acetanilide crystal, amide I band, localized states

Abstract

The crystal of acetanilide (ACN) is maintained by hydrogen-bonded networks, very similar to those that stabilize α -helices and β -sheets and for this reason it has long been considered a model for vibrational energy transfer processes in proteins [1,2]. In particular, ACN possesses an amide group (CONH) and its amide I band, with its intriguing temperature-dependent double peak, has been and continues to be the object of many investigations [3,4]. In a recent study, a semi-quantitative fit to the experimental measurements was obtained by considering that the energy of the amide I excitation saturates above a threshold value for the hydrogen bond length and that its value is also dependent on the orientation of the hydrogen bond [4]. In this talk, simulations in which the parameters of the standard models were systematically varied will be reported first in order to show that those models fail to reproduce the experimental results for the amide I band of crystalline ACN. The talk will finish with the presentation of alternative hypotheses capable of reproducing the full amide I band, together with its temperature dependence.

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MOVING DISCRETE BREATHERS IN CRYSTALS WITH NaCl STRUCTURE

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Keywords: alkali halide crystal, discrete breather, molecular dynamics

Abstract

Discrete breathers (DBs) are spatially localized nonlinear vibrational modes in defect-free anharmonic lattices [1-3]. Over the past few years, there has been increasing interest in the study of DBs in the solid state physics and materials science. Manley et al. have reported on the experimental observation of gap DBs in thermodynamic equilibrium in the NaI crystal [4], in line with the molecular dynamics simulation results published earlier by Kiselev and Sievers [5]. In [6], in the study of the phonon spectra of the NaI crystal by inelastic neutron scattering, it has been suggested the existence of ordered arrangement of DBs, which implies the possibility of energy exchange between them.

The question of whether DBs can move through crystal lattice is important for understanding their role in the formation of physical properties of crystals. Often DBs are pinned to lattice sites, but in some cases they can be mobile [7]. Moving DBs can collide with each other resulting in significant energy localization at the collision point. This energy can be spent on the creation of crystal lattice defects or on the triggering of phase transitions or fracture.

NaCl structure consists of two face-centered cubic lattices with lattice parameter a , one occupied by anions and another one by cations, displaced one with respect to another by the vector $(a/2, 0, 0)$. Each atom has six neighbors of the opposite type which are at the vertices of a regular octahedron. Each cubic translational cell consists of four anions and four cations. Interactions between atoms are described by pairwise potentials which consist of Coulomb interaction, Born-Mayer-type repulsion, and dispersive interaction [8]. For chosen parameters of potentials the equilibrium lattice parameter of the NaCl structure was found to be $a = 6.25\text{\AA}$. Computational cell used in our simulations included $8 \times 8 \times 8$ cubic translational cells, and it was subjected to periodic boundary conditions. Large difference in the atomic weights of anions and cations (10 and 100 g/mol, respectively) results in the appearance of a wide gap in the phonon spectrum. In this case the gap DBs highly localized on the light atoms and vibrating along (110) direction can be easily excited.

Initial conditions were taken in a way to excite two DBs on two light atoms neighboring along (110) direction. If the two atoms oscillate out-of-phase then no energy exchange between them is observed. Introduction of a small phase shift results in the energy exchange between the two DBs and a relay-like excitation of atoms that were not initially excited (see Figure 1).

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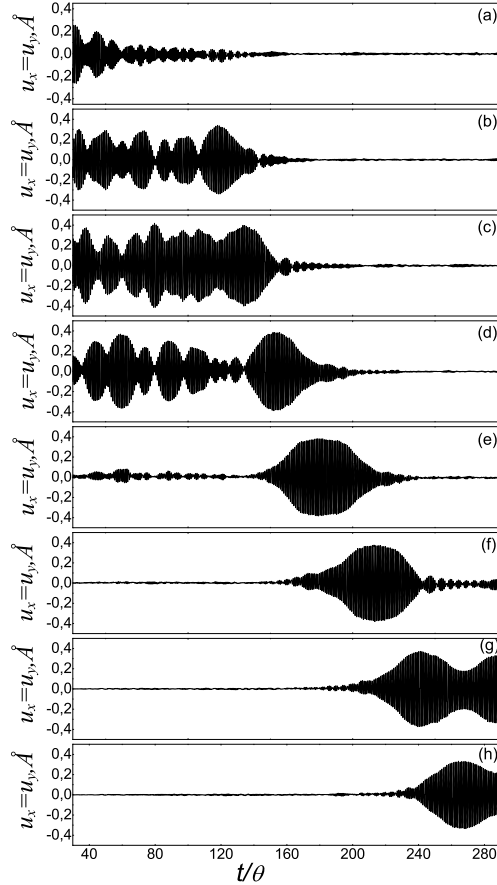


Figure 1: Displacements $u_x = u_y$ of light atoms located along (110) direction as the functions of time. Energy exchange between light atoms of the crystal resulting in motion of the DB along (110) crystallographic direction can be seen.

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MODELING OF THE ANNEALING OF RADIATION-INDUCED DEFECTS IN
GERMANIUM BY MOVING DISCRETE BREATHERS

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Keywords: ILM, breather, electric traps, germanium, DLTS

Abstract

There is an increasing interest in the mechanism and properties of non-linear lattice vibrations in crystals, which may have large lifetimes and propagation distances, and are called intrinsic localized modes (ILM) or discrete breathers (DB) [1]. In recent theoretical works by some of the present authors, existence of sessile [2] as well as mobile DBs [3] have been demonstrated in metals by means of molecular dynamics using well defined MD potentials. An important peculiarity of this phenomenon is its low energy ranging from fractions to a few eV, which makes further investigations of low-energy collision events especially appropriate for various applications. Deep Level Transient Spectroscopy or DLTS is an especially useful technique for direct experimental observation of such phenomena in semiconductors, since it allows one to detect microstructural changes deep inside the material produced by low-energy collision events at the surface, which are analyzed in the present paper. We assume that moving DB can be trapped by structural defects thus creating trapped DB (TDB), which are shown to result in the amplification of the reaction rates involving the defects. The amplification mechanism has been proposed originally to explain anomalous low-temperature reconstructive transformations in layered silicates [4]. It is based on modification of the classical Kramers escape rate from a potential well due to a periodic modulation of the well depth (or the reaction barrier height). Then, a macroscopic reaction rate (averaged over a macroscopic number of defects) can be shown to depend on the frequency of the DB collisions with a defect resulting in the TDB formation (which is proportional to the irradiation flux) and the average TDB life-time, τ_{TDB} , during which the reaction is accelerated. Besides, it depends almost exponentially on the average TDB energy, E_{TDB} . A quantitative comparison of the model with experimental data on annealing of E-centers in Germanium by low-energy Ar plasma (~ 4 eV) [5] shows an excellent agreement at the following TDB parameters: $\tau_{\text{TDB}} = 10^{-11}$ s, $E_{\text{TDB}} = 0.62$ eV, which seem to be a reasonable estimate for the life-time and the mean energy of TDB produced by moving DB with energies ranging from 0.5 to 5 eV.

Acknowledgements: VD and JFRA acknowledge the hospitality of the Institute of Physics in Tartu, Estonia. JFRA acknowledges financial support from the project FIS2008-04848.

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NUMERICAL SIMULATIONS OF NONLINEAR MODES IN MICA: PAST, PRESENT
AND FUTURE

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Keywords: nonlinear lattice excitations, numerical simulations

Abstract

Mike's work on mica goes back to the late 60's, but I first met him at the 1995 Solitons conference at Heriot-Watt. At that time, soliton research seemed to be getting more and more abstract, so it was refreshing to find an applied problem in nonlinear waves. Fortunately I had some postdoc money from the LOCNET EU collaboration, and we were able to enlist a very gifted Spanish post-doc, José Marín, to work on the hexagonal and cubic lattice problems. It is now 15 years since the original 1D and 2D calculations from this time were carried out [1-3], so I thought it might be worthwhile to review what was achieved at that time, and what were the limitations in understanding Mike's observations of tracks in real mica crystals.

I will also look at the simple 1D numerical simulations of Mike's groundbreaking transmission/ejection experiments around 2005 [4,5]. Although a number of other researchers have come up with new numerical simulations and experimental work in this area, I feel much more remains to be done to pin down the link between theory and experiments. I will review a program of work in hand to improve these results with higher dimensional and more detailed simulations.

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SOLIPLASMON RESONANCES AT METAL-DIELECTRIC INTERFACES

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Keywords: Plasmonics, Nonlinear Optics, Solitons

Abstract

Nonlinear effects are a natural scenario in the world of plasmonic resonances. The peculiarities of the dispersion properties of surface plasmonic resonances (SPP) along with the high intensities that can be achieved close to the metal/dielectric surface open the way to interesting and peculiar nonlinear phenomena. In this presentation we will review and analyze the role played by dielectric Kerr nonlinearities and how they affect the propagation of continuous wave SPPs. We will present a variational theory that will reveal itself very useful for the physical understanding of the interplay between the dispersion properties of the SPP and Kerr nonlinearities [1]. Within the previous context, the key concept of our approach will be the soliplasmon resonance, a quasi-particle constituted by a bound state of a spatial soliton and a SPP [2] (see Figure 1). By means of our variational model, we will visualize the principal physical properties of these states: dispersion properties, classification of stationary states, soliton-plasmon coupling, etc [3]. We will compare these results with those obtained by numerically solving the full nonlinear Maxwell's equations [4]. We will also take advantage of our variational model to clarify the different ways Kerr nonlinearities can affect SPP propagation by distinguishing soliplasmon resonances from different types of nonlinear plasmonic states.

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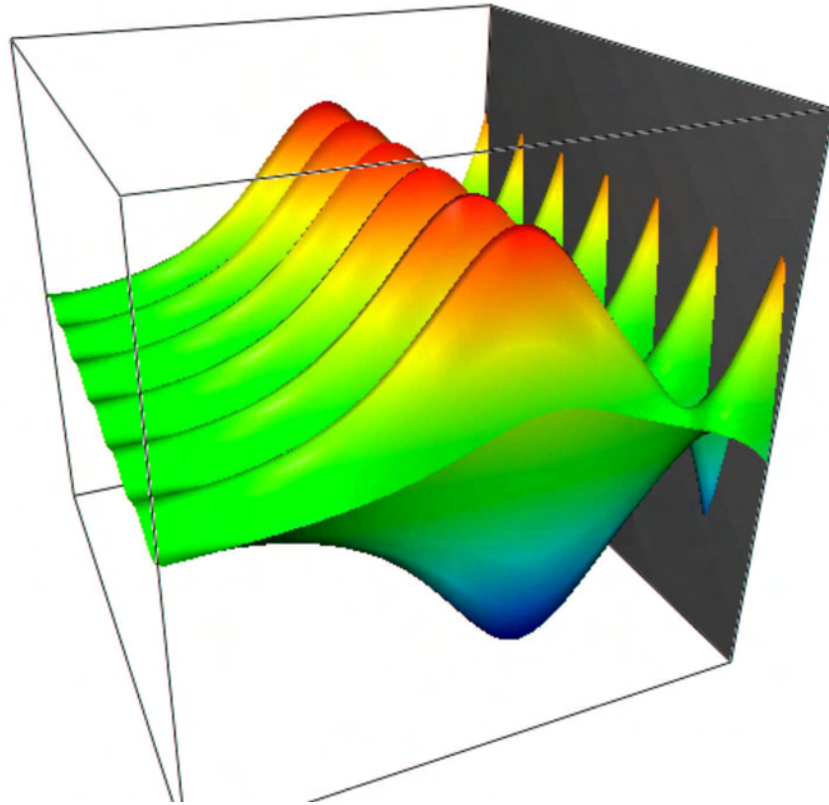


Figure 1: Characteristic example of a soliplasmon resonance propagating along a metal/Kerr interface.

ENERGY LOCALIZATION IN NONLINEAR SYSTEMS WITH FLEXIBLE GEOMETRY

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Keywords: energy localization, charge-curvature interaction, shape transformation

Abstract

Shape transformations in driven and damped micro-electromechanical arrays are considered. Closed chains of weakly coupled charge-controlled capacitors under the action of spatially homogeneous time-periodic external electric field are studied. The capacitors are modeled as electric dipoles which under an action of the external electric field periodically change their amplitude. The coupling between the vibrating dipoles and the bending degrees of freedom of the chain modifies the local bending rigidity of the chain. In the absence of driving the array takes a circular shape. When the driving intensity exceeds some critical level the circular shape of the aggregate becomes unstable and the chain takes the shape of an ellipse or, in general, of a polygon. The excitation energy is localized in such places where the chain is more flat.

Acknowledgements: I'm grateful for inviting me to the scientific committee of the conference.

EXISTENCE AND NON-EXISTENCE OF BREATHER SOLUTIONS IN DAMPED AND
DRIVEN NONLINEAR LATTICES

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Keywords: nonlinear lattices, breather solutions, localisation, pattern formation and synchronisation

Abstract

We investigate the existence of spatially localised solutions, in the form of discrete breathers, in general damped and driven nonlinear lattice systems of coupled oscillators. Conditions for the exponential decay of the difference between the maximal and minimal amplitudes of the oscillators are provided which proves that initial non-uniform spatial patterns representing breathers attain exponentially fast a spatially uniform state preventing the formation and/or preservation of any breather solution at all. Strikingly our results are generic in the sense that they hold for *any*, attractive interaction, coupling strength and on-site potential and general driving fields. Furthermore, our rigorous quantitative results establish conditions under which discrete breathers in general damped and driven nonlinear lattices can exist at all and open the way for further research on the emergent dynamical scenarios, in particular features of pattern formation, localisation and synchronisation, in coupled cell networks.

EXISTENCE, DYNAMICS AND MOBILITY OF QUANTUM COMPACTONS IN AN EXTENDED BOSE-HUBBARD MODEL

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Keywords: Compacton, extended Bose-Hubbard model, Bose-Einstein condensate

Abstract

Lattice Compactons, discrete breathers with compact support, were found for a discrete nonlinear Schrödinger (DNLS) equation extended with nearest neighbour intersite nonlinearities [1], a model originally studied with waveguide arrays in mind. These compactons were shown to exhibit very good mobility if the parameters are tuned close to the compactons stability boundary. The DNLS can also be used to model the behaviour of Bose-Einstein condensates in optical lattices, and the remarkable control over the experiments in this field of research has made it possible to study the quantum mechanics of strongly correlated atoms.

We will define the concept of a Quantum Lattice Compacton [2] and discuss the existence and dynamics, with special emphasis on mobility, of these in an extended Bose-Hubbard model corresponding to above-mentioned extended DNLS equation in the quantum mechanical limit.

The compactons is given 'a kick' by means of a phase-gradient and it is shown that the size of this phase is crucial for the mobility of the compactons. For small phase-gradients, corresponding to a slow coherent motion in the classical model, the time-scales of the quantum tunnelings become of the same order as the time-scale of the translational motion and the classical mobility is destroyed by quantum fluctuations. For large phase-gradients, corresponding to rapid classical motion, the classical and quantum time-scales separate so that a mobile, localized coherent quantum state can be translated many sites in the lattice already for small particle numbers of the order of 10.

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A CROWDION IN MICA. BETWEEN K^{40} RECOIL AND TRANSMISSION SPUTTERING

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Keywords: Kinks, lattice kinks, crowdion, silicates, muscovite, mica

Abstract

Tracks in mica muscovite which apparently are caused by some kind of lattice excitation [1] may have been produced by the recoil of K^{40} . The isotope K^{40} can decay emitting an electron or a positron with the corresponding neutrino, the recoil energy of K^{40} is of about 40 eV. The experiment by Russell and Eilbeck [2] proved the transmission of localized energy along lattice lines in the K^+ layer. The impact of an α particle on one side of a mica specimen led to the ejection of an unidentified atoms from the other side. Typical surface binding energies for silicates are between 3 and 5 eV.

We construct a 1D model for mica, taking into account that the K^+ is a repulsive one, finding supersonic kinks [3] with a large range of energies and velocities, both with next-neighbour interaction and with many neighbours. The distances between ions are extremely small, but with the introduction of the ZBL repulsive short range potential, similar kinks are found again but with reasonable ion distances [4].

However, when a substrate potential obtained from empirical potentials is introduced there is an enormous change in kink properties. Below some characteristic energy E_c and velocity V_c the kinks are dispersed in phonons. Above that energy, kinks loose energy into phonons until they achieve E_c and V_c , thereafter propagating without radiation.

This lattice kink also called crowdion has a self-selected energy E_c 30 eV, which is exactly between the recoil energy of K^{40} and the surface binding energy of atoms in silicates.

Crowdion have been found with molecular dynamics in different materials as Ni [5] showing exceptional robustness and self-focusing properties.

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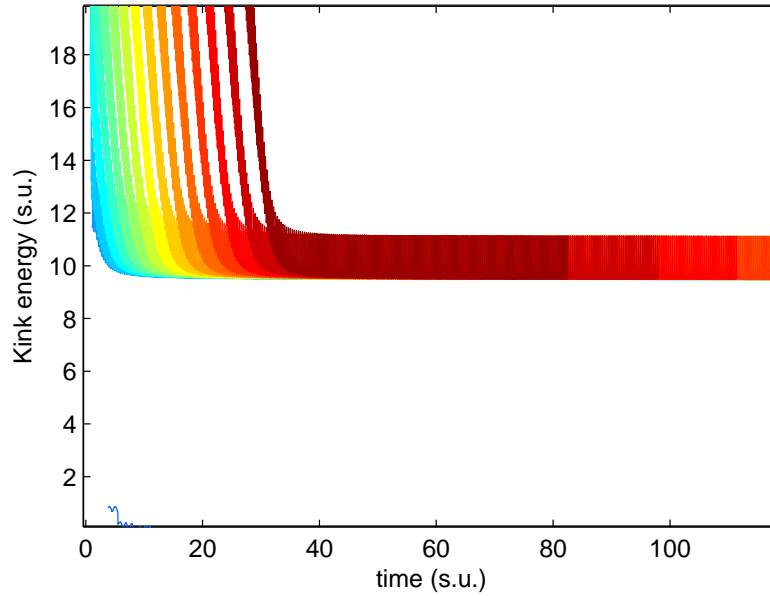


Figure 1: Large energies bring about the emission of phonons until a non-radiating lattice kink or crowdion is formed. The scaled units are equivalent to 2.8 eV.

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STRONGLY LOCALIZED MOVING DISCRETE SOLITONS (BREATHERS): NEW WAYS TO BEAT THE PEIERLS-NABARRO BARRIER

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Keywords: Peierls-Nabarro potential, discrete flat-band solitons, discrete dissipative solitons

Abstract

The question whether a nonlinear localized mode (discrete soliton/breather) can be mobile in a lattice has a standard interpretation in terms of the Peierls-Nabarro (PN) potential barrier. In particular, for any system modelled by a Discrete Nonlinear Schrödinger (DNLS) type equation, this concept can be defined as the maximum difference in energy (Hamiltonian) between solutions at fixed power (norm), centered at different lattice positions. For the most commonly studied case with on-site, cubic (Kerr) nonlinearity, the PN barrier for strongly localized solutions becomes large, rendering these essentially immobile.

Several ways to improve the mobility by reducing the PN-barrier for strongly localized modes have been proposed during the last decade, and the first part of this talk will give a brief review of two such scenarios. In 1D, one option is to utilize a competition between on-site and inter-site nonlinearities [1]. In 2D, the mobility is normally much worse than in 1D, due to the fact that also broad solitons are prone to excitation thresholds and quasicollapse instabilities. Utilizing a saturable nonlinearity was found to considerably improve the 2D mobility by reducing the PN barrier in certain parameter regimes for large power [2].

We then proceed to discuss two (if time allows) recently discovered novel mobility scenarios. The first example discussed is the 2D Kagome lattice [3], where the existence of a highly degenerate, flat linear band allows small-power, strongly localized nonlinear modes to appear without excitation threshold. The nonlinearity lifts the degeneracy of linear modes and causes a small energy shift between modes centered at different lattice positions, yielding a very small PN-barrier and mobility of highly localized modes in a small-power regime.

The second example discusses a 1D waveguide array in an active medium with intrinsic (saturable) gain and damping[4]. It is shown that exponentially localized, travelling discrete dissipative solitons may exist as stable attractors, supported only by intrinsic properties of the medium (i.e., in absence of any external field or symmetry-breaking perturbations). With a standard, on-site Kerr-nonlinearity the solitons are pinned by the PN-barrier, but decreasing the barrier with inter-site nonlinearities allows for the existence of breathing (i.e., with oscillating size) solitons as stable attractors at certain velocities, related to lattice commensurability effects. The stable moving breathers also survive in presence of weak disorder.

Acknowledgements: This project has been financed by the Swedish Research Council. This work is a collaboration with R.A. Vicencio and U. Naether (Nonlinear Optics Group, Universidad de Chile), and J.E. Prilepsky and S.A. Derevyanko (NCRG, Aston University), and was partly performed during my visits to their respective institutions, the hospitality of which I gratefully acknowledge.

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ENERGY TRANSPORT IN MOLECULAR CHAINS WITH COMBINED ANHARMONIC POTENTIALS OF PAIR INTERATOMIC INTERACTION

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Keywords: energy transport, anharmonic potentials, pair interatomic interaction

Abstract

We provide analytical and molecular dynamics simulations of heat transport in one-dimensional molecular chains with pair potential of rather general form. We show that the thermal conductivity is finite in the chains with unbounded asymmetric potentials that allow the possibility of bond dissociation. The Morse, Lennard-Jones and Coulomb potentials belong to such type of pair potentials. The convergence of the thermal conductivity is due to anomalously strong Rayleigh scattering of phonons by the fluctuations of the local bond stretching at low temperatures, and by many-particle collisions - at high temperatures. On the other hand, the chains with confining pair potential, which does not allow for the possibility of bond dissociation, possess anomalous (diverging with the chain length) thermal conductivity. We emphasize that heat transport in the symmetric or asymmetric Fermi-Pasta-Ulam potential [1] and in combined pair interatomic potentials, which contain parabolic or non-linear confining potential, is always anomalous. From our simulations we can conclude that the thermal conductivity of the one-dimensional lattice will be anomalous if the energy of the pair confining potential grows not slower than the square of the relative interatomic distance. Figure 1 shows the dependence of the thermal conductivity on the length of the molecular chain with the Coulomb potential combined with a linear confining potential, which determines the lattice period (the modified Coulomb potential), at different dimensionless temperatures (defined as in Ref. [2]), together with the results for the thermal conductivity of the exponential Toda lattice that is characterized by anomalous heat transport. The results, obtained by equilibrium and non-equilibrium molecular dynamics simulations, are consistent, which confirms their validity. The presented results can be applied to different energy-carrying low-dimensional nanomaterials, including nanowires and nanotubes.

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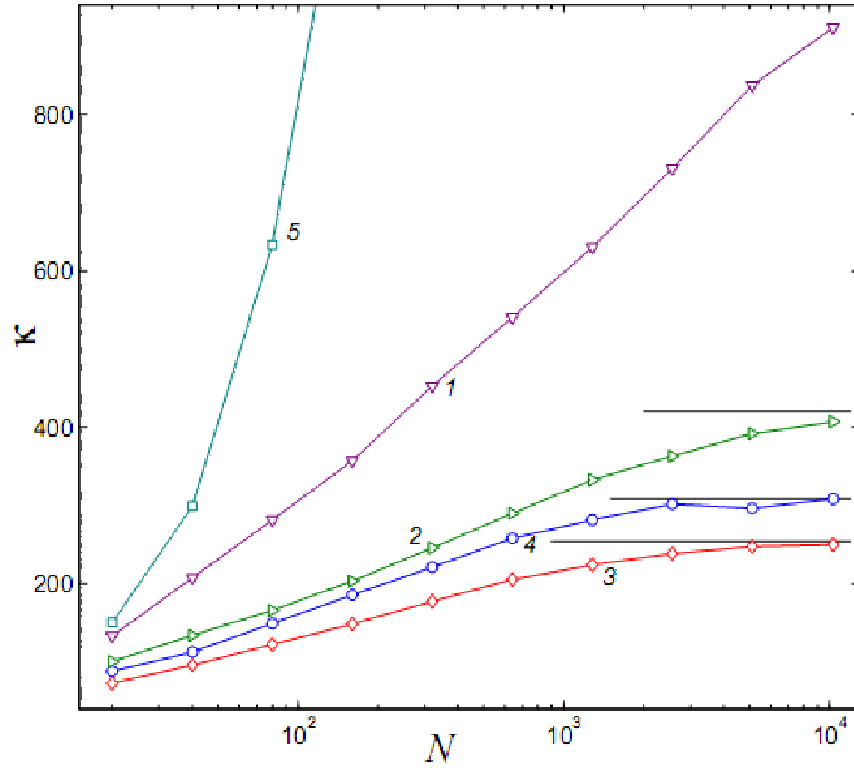


Figure 1: Thermal conductivity κ as a function of the length N of the molecular chain with the modified Coulomb potential at dimensionless temperatures $T = 0.05, 0.1, 0.2, 0.5$ (curves 1, 2, 3, 4), and with the exponential Toda potential at $T = 0.2$ (curve 5). Straight lines present thermal conductivity values, which were obtained with the use of equilibrium Green-Kubo approach.

MOBILE DISCRETE SOLITONS IN THE ONE-DIMENSIONAL LATTICE WITH THE
CUBIC-QUINTIC NONLINEARITY

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Keywords: self-focusing, Peierls-Nabarro potential, stability exchange

Abstract

We report the existence of different windows of the *self-organized mobility* for localized modes in the discrete nonlinear Schrödinger equation with the onsite cubic-quintic nonlinearities, of focusing-defocusing (competing) or focusing-focusing types:

$$i \frac{d\psi_n}{dz} + C(\psi_{n+1} + \psi_{n-1}) + \gamma|\psi_n|^2\psi_n + \nu|\psi_n|^4\psi_n = 0, \quad (1)$$

where $\psi_n(z)$ is the field amplitude at the n -th lattice site, in terms of nonlinear-optics models [1]. In the case of the competing nonlinearities ($\gamma > 0$, $\nu < 0$), the dynamical phenomenology is identified in regions where the stability *switches* between odd (onsite-centered) and even (intersite-centered) fundamental discrete solitons (in the same region, intermediate asymmetric discrete solitons exist too, cf. Ref. [1]). Unstable solitons spontaneously start oscillatory or progressive motion, if they are located, respectively, below or above a mobility threshold. Stable solitons may be set in motion by kicking, following the lines of Ref. [2].

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RECORDING PROCESS IN IRON-RICH MUSCOVITE CRYSTALS

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Keywords: mica muscovite, tracks, recording process

Abstract

Natural crystals of the layered mineral muscovite mica containing high concentrations of iron are of special interest because of their ability to record permanently the tracks of swift charged particles and quodons, which are uncharged mobile lattice excitations. The tracks present as thin ribbons of the mineral magnetite, $\text{Fe}_2\text{O}_3\text{FeO}$, that are formed epitaxially in the potassium (001)-plane of easy cleavage. Swift particles interact with a crystal at the atomic level and most of the energy of quodons is concentrated on single chains of atoms so the recording process must operate at the atomic level. As this occurs within a solid the motion of individual atoms cannot be followed. The recording process starts after a crystal has grown and becomes structurally unstable as it cools. Nucleation sites created by perturbations of the lattice allow the crystal to relax to a lower energy state. Chemical analyses of samples of muscovite showing different recording sensitivities and types of track decoration show that a high concentration of iron is essential for recording but only a minute amount of atomic rearrangement occurs. The recording process involves migration of iron and oxygen that recombine to form epitaxial ribbons of magnetite to delineate the tracks. The ability to record the motion of uncharged, highly localised lattice excitations sets tight criteria on models of the process. The reason for the variability of the recording process within a given crystal remains unknown but probably involves trace elements at concentrations below current detection thresholds.

BRIGHT SOLITONS OF ATTRACTIVE BOSE-EINSTEIN CONDENSATES CONFINED IN QUASI-1D OPTICAL LATTICE

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Keywords: Bose-Einstein Condensates, Bright Solitons, Optical Lattices

Abstract

We investigate a self-attractive Bose-Einstein condensate confined in a combination of a cigar-shaped trap and deep optical lattice acting in the axial direction by using a 1D discrete nonpolynomial Schrodinger equation (DNPSE). This 1D DNPSE, which is derived from the 3D Gross-Pitaevskii equation, admits on-site collapse unlike previously considered varieties of one-dimensional equations. We show that persistently moving bright solitons can be readily created by the application of the kick to stable on-site unstaggered solitons while staggered solitons are immobile.

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WAVE LOCALIZATION IN CHIRPED SONIC CRYSTALS

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Abstract

The study of wave propagation in periodic media has a long history in the field of vibrations and acoustics [1]. In recent years, after the pioneering works of Yablonovitch [2] and John [3], who discovered simultaneously the possibilities to control the light flow in periodic distribution of dielectric materials, an increasing interest appeared in the analogous structures to control both the elastic and acoustic waves using the well-known phononic crystals (PC). By analogy with the photonic case, these periodic arrangements present acoustic band gaps (BGs), defined as frequency ranges where vibrations, sound and phonons are forbidden. A particular case of PC, is the sonic crystal (SC) [4,5] which consist of solid scatterers embedded in a fluid host medium. In this work we consider propagation in chirped sonic crystals, systems in which the lattice constant, i.e. the distance between scatterers gradually changes along the propagation direction. We propose and experimentally demonstrate a mechanism of sound wave concentration based on soft reflections in chirped sonic crystals. The reported field enhancement occurs at around particular (bright) planes in the crystal and is related to a progressive slowing down of the sound wave as it propagates along the material. At these bright planes, a substantial concentration of the energy (with a local increase up to 20 times) was obtained for a linear chirp and for frequencies around the first band gap. A simple couple mode theory is proposed that interprets and estimates the observed effects. Wave concentration energy can be applied to increase the efficiency of detectors and absorbers

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PECULIARITIES OF THE CHANGE OF TEMPERATURE AND HEAT TRANSFER
UNDER IRRADIATION

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Keywords: Irradiation, defects, heating, self-oscillation, auto-wave

Abstract

Theoretical approach to manifestation of non-linear thermoconcentration feedback in a material under irradiation is developed. This thermo-concentration nonlinear feedback is a mechanism of instability that leads to development of self-oscillations and auto-waves. The nature of the feedback is the following.

The thermal energy of material increases under irradiation due to irradiation heating. At the same time the significant non-thermal energy is accumulated in the material as a result of accumulation of the radiation-induced defects (vacancies, interstitial atoms, their complexes etc.). The value of the non-thermal energy is equal to the energy of defects formation multiplied by the defect concentration. The accumulated energy is converted into thermal energy when the defects disappear as result of defect annealing (decay, recombination, and absorption by sinks). Rate of annealing is a strong (exponential) function of temperature. Let a small increase of the temperature arises as a result of small fluctuation. So the defect annealing increases, the energy that is stored by radiation defects is released into heat and the temperature of the material increases further. Thus the positive feed-back is formed.

Change of materials temperature and evolution of radiation damage of material are described with a system of nonlinear differential equations. The variables of the system which describe material under irradiation are densities of different radiation defects, defect characteristics and temperature of the material.

The qualitative analysis of this non-linear dynamical system is carried out. It is obtained a frequency of the self-oscillations and speed of the auto-wave. It is found conditions for which they arise and develop. The physical interpretation of obtained results is given.

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TAMING OF MODULATION INSTABILITY:
MANIPULATION, AND COMPLETE SUPPRESSION OF INSTABILITY BY
SPATIO-TEMPORAL PERIODIC MODULATION

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Keywords: Modulation instability, pattern formation.

Abstract

Modulation instability is at the basis of spontaneous pattern formation in many nonlinear spatially extended systems in Nature, technology, and everyday live. A variety of spatial patterns can be observed, like regular and stationary dissipative patterns, nonstationary (periodic and chaotic) patterns, fractal, and turbulent patterns. However in all cases, the very onset of the spatial patterns and of the spatio-temporal dynamics, the very initial break-up of the spatial symmetry, occurs via modulation instability: the homogeneous, the maximally symmetric state loses its stability with respect to the growing modes of spatial modulation. Therefore, a possibility of control and of suppression of modulation instability, i.e. a possibility of control of formation of spatial patterns in many systems, could be of a tremendous importance.

We propose, and we show, very generally, that a proper spatio-temporal periodic modulation of the parameters of the extended system can modify, and can eventually suppress the modulation instability. We show the phenomena on a model of Complex Ginzburg-Landau Equation which is a paradigmatic model for the long-wave modulation instability. We show the effect by linear stability analysis (more precisely, by a modification of Floquet analysis), as well as by direct numerical integration of the modulated Complex Ginzburg-Landau Equation in one and two space dimensions. We discuss also a possible extension of the idea beyond the long-wave instability in Complex Ginzburg-Landau Equation: we consider the other types of spatial instabilities (Turing and short-wave parametric instabilities), and we show that the developed concept of taming of spatial instabilities work also in these cases.

GAIN-DRIVEN BREATHERS IN \mathcal{PT} -SYMMETRIC METAMATERIALS

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Keywords: \mathcal{PT} -Symmetry, Discrete Breathers, Loss Compensation

Abstract

Great research efforts have been recently focused on the development and investigation of synthetic materials that exhibit a combined \mathcal{PT} -symmetry [1]. Naturally, the concepts and notions of \mathcal{PT} -symmetric systems have been extended to dynamical lattices, particularly in optics [2]. However, the realization of \mathcal{PT} -symmetric electronic circuits [3] provides a convenient platform for testing these ideas in easily accessible experimental configurations. In metamaterials, the \mathcal{PT} -symmetry relies on balanced gain and loss that also provides loss compensation [4].

It has been demonstrated that nonlinear metamaterials support localized excitations of the breather type [5,6]. A model metamaterial that combines \mathcal{PT} -symmetry with balanced gain and loss and in addition nonlinearity, made of split-ring resonators with alternatingly gain and loss in a dimer chain configuration, has been investigated numerically [7,8]. The particular structure of that class of nonlinear \mathcal{PT} -metamaterials allows the generation of novel breather excitations with very long life-times that are driven solely by the gain, in a subtle balance between gain and loss.

Gain-driven breathers can be excited in nonlinear \mathcal{PT} -metamaterials either by proper initialization of the system, or by frequency chirping of an alternating external field [9]. In the latter case, the field is applied only temporarily, in order to induce instability and create several localized waveforms that will dynamically evolve into gain-driven breathers. Importantly, the energy of fundamental gain-driven breathers is concentrated predominantly on two neighboring sites, one with gain and the other with loss, while single-site breathers cannot exist. A typical fundamental breather generated by properly initializing the \mathcal{PT} -metamaterial is shown in Fig.1, where energy oscillations that are peculiar to \mathcal{PT} -symmetric systems can be also observed.

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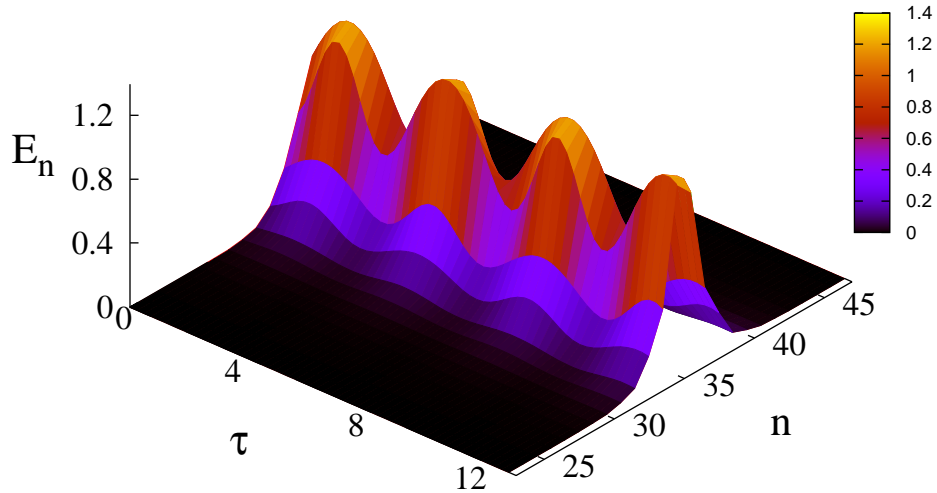


Figure 1: Spatiotemporal evolution of the energy density E_n of a gain-driven breather excitation during two periods of the breather oscillation frequency..

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MOVING BREATHER MODES IN TWO-DIMENSIONAL LATTICES

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Keywords: discrete breathers

Abstract

We investigate two-dimensional FPU lattices which model the propagation of electrical charge through nonlinear capacitors and inductors. As well as the square lattice [1], we analyse the triangular-hexagonal lattice [2] and the more open honeycomb structure [5,6]; see figure 1 for illustrations. In each case we derive the 2D NLS equations which govern the shape of a breather in the slowly-varying small amplitude limit of the system. Although these lattices are simpler than their more common 2D mechanical counterparts [3], they have a number of interesting features not present in the 1D chain. For example, there is an ellipticity constraint required for breathers to exist. In 2D there is a minimum energy threshold for breathers [4], which we show is maximised for stationary breathers, and reduces as the speed of the breather increases. Also as their speed increases, the breathers change from being circularly symmetric to ellipsoidal in profile. In addition, the generation of higher harmonic modes and the isotropy is seen to depend on the geometry of the lattice.

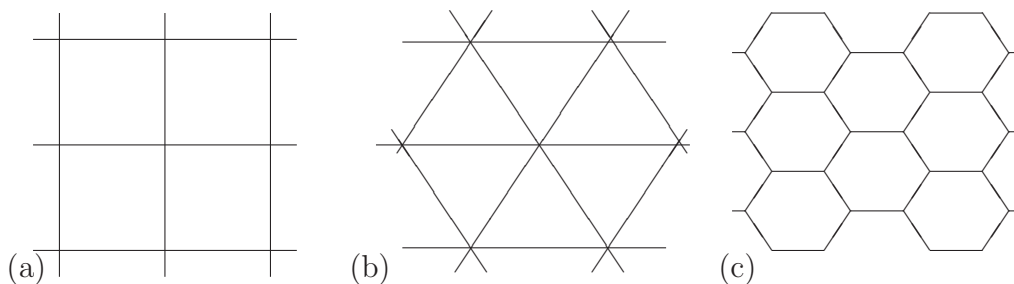


Figure 1: Illustrations of the lattice structures considered: (a) square, (b) triangular-hexagonal, (c) honeycomb.

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