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LOCALIZATION AND ENERGY TRANSFER IN NONLINEAR SYSTEMS

June 17-21, 2002, San Lorenzo de El Escorial, Madrid, Spain.

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Conference Objectives

This is the third conference organized in the framework the European LOCNET Project (Localization by Nonlinearity and Spatial Discreteness and Energy Transfer in Crystals, Biomolecules and Josephson Arrays, RTN1 – 1999 – 00370).

The Conference will be focused on main lectures in each area to introduce the main concepts and stimulate the discussions.

Registration: The amount of Registration fee is 150 euro.

Support: The Organizing Committee applied to provide financial support for young researchers, eventually invited speakers from outside the Network and the publication of proceedings. Up to now, we are not able to confirm it.

Accommodation:

The package starts with the dinner on Sunday, 16 June 2002, and ends with breakfast on Saturday, 22 June 2002.

Full board accommodation in single room: 480 euro.

Full board accommodation in a shared double room: 360 euro.

Registration deadline: February 28, 2002.

A touch about accommodation: San Lorenzo de El Escorial is 49 kilometres from Madrid. It is close to Sierra de Guadarrama at a height of 1.055 metres. The town is a pleasant and peaceful spot during the year and becomes a lively cultural centre during the summer. Its picturesque surroundings heighten to a greater extent the powerful architecture of the Monastery built by King Philip II to house also the Royal Palace and the Pantheon for the kings of Spain.

All conference sessions will be held at the Florida Hotel booked to host the Conference. The hotel overlooks the Monastery and it is located in the best area of the town centre.

More information about the town and surroundings in <http://www.escorialvirtual.com> (Spanish site).

Updates on Conference news on WWW: <http://conody.fdi.ucm.es/pr/conf2002>

All communications regarding the Conference must be sent to

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1 A Nonlinear Dynamical Model for Ultrafast Catalytic Transfer of Electrons

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Abstract

Electron transfer is an ubiquitous elementary process of chemical reactions. It is expected that the required time for an electron transfer between different molecules is minimum at the so called Marcus inversion point in the space of parameters. However, it is precisely in the vicinity of this inversion point that the standard adiabatic (or Born Oppenheimer) approximation used for this theory, breaks down.

Then, we use the complex amplitudes of the electronic wave-functions on the different sites as Kramers variables. The strong coupling of the electronic charge to the many nuclei, ions, dipoles, etc ... of the environment, is modelled as a strongly coupled thermal bath better considered classically. The effective dynamics of a quantum electron hopping between different sites can be described after elimination of the bath variables by a Discrete Nonlinear Shroedinger equation with norm preserving dissipative terms and Langevin random noises (at finite temperature).

Our model recovers the standard Marcus results far from the inversion point where atomic thermal fluctuations adiabatically induce the electron transfer. Close to the inversion point in the non adiabatic regime, electron transfer may become ultrafast (and selective) at low temperature essentially because of the nonlinearities when they are appropriately well tuned. We demonstrate and illustrate numerically that a *weak* coupling of the Donor site with an extra appropriately tuned (catalytic) site, can trigger an ultrafast electron transfer to the acceptor site at zero degree Kelvin while in the absence of this catalytic site no transfer at all would occur (the new concept of Targeted Transfer initially developped for discrete Breathers is extended to polarons and applied for this theory).

Among other applications, this theory should be relevant for describing the ultrafast electron transfer observed in the photosynthetic reaction center of living cells.

2 Nonlinear Charge Transport Mechanism in Periodic and Disordered DNA

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Abstract

We study the transport of charge due to polarons in a model of DNA, which takes in account the three-dimensional helical structure of DNA, and the coupling of the electron wave function with the H-bond distortions and the twist motions of the base pairs.

Stationary states are constructed using a nonlinear map. Perturbations of the ground states lead to moving polarons which travel long distances along the DNA molecule. The influence of parametric and structural disorder due to the impact of the ambient is considered, showing that the moving polarons survive to a certain degree of disorder.

References

- [1] T.D. Holstein, *Ann. Phys. NY* 8, 325, 343 (1959).
- [2] P.W. Anderson, *Phys. Rev.* 109, 1492 (1958).
- [3] M. Peyrard and A.R. Bishop, *Phys. Rev. Lett.* 62, 2755 (1989).
- [4] L.V. Yakushevich, *Quart. Rev. Biophys.* 26, 201 (1993).
- [5] M. Barbi, S. Cocco and M. Peyrard, *Phys. Lett. A* 253, 358 (1999).

3 Overdamped Inertial Dynamics of Frenkel-Kontorova Models

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Abstract

We consider the overdamped inertial dynamics of a chain of particles with convex interactions in a tilted periodic potential. In particular we prove that if for a given mean spacing there are no rotationally-ordered equilibria then there is a globally attracting periodically sliding solution. The key is a novel preserved partial order.

References

- [1] Claude Baesens and Robert MacKay, Overdamped inertial dynamics of tilted Frenkel-Kontorova models, preprint.

4 Low Frequency Dynamics in N-Methylacetamide and L-Alanine

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Abstract

N-Methylacetamide (NMA) and L-Alanine are molecular crystals with networks of intermolecular hydrogen bonds. Both have some internal or external modes displaying unusual temperature dependence of their intensity, and overtone peaks. In both cases, these anomalous temperature behavior have been correctly taken into account within the theory of the vibrational polaron, following the models developed first by A. Davydov, and then by J. Krumhansl and A. Scott. However, we have detected, for the first time, new structural instabilities in both systems by precise DSC. In L-Alanine single crystals, Raman measurements confirms this breaking of symmetry. The origin of this instability could be the switching of the N-H...O bond between two neighbouring molecules accompanying the re-orientation of the NH₃⁺ group, preserving the macroscopic symmetry. It is worth to note that the anomalous intensity increase of the NH₃⁺ torsional mode with decreasing temperature could as well been understood like the rise of a new order parameter. The dynamics of the methyl groups in NMA has been shown very sensitive to the local environment. The controversial A-Amide mode observed in the mean IR, could be as well interpreted as the new order parameter of the ordered phase occurring below ? 240K, in agreement with DSC and previous NMR data. A very low frequency new dispersive mode has also been observed by QENS and is under discussion. These results suggest analogies between breathers theories and three dimensional non-linear lattice dynamics of crystals with structural phase transitions.

5 Breathers in 1D Lattices and 2D Homoclinic Orbits

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Abstract

On this poster, I will present a numerical method for finding spatially localized and time-periodic solutions to Klein-Gordon lattice equations in one dimension. This method is based on an approximation recently proposed by G.P. Tsironis [3] and adds to it a second assumption, together linking breather solutions to homoclinic orbits of a 2-dimensional map. It drastically improves the rotating wave approximation [1, 2] and enriches Tsironis' method by the direct link to homoclinic orbits. The homoclinic orbits are good starting points for a Newton-Raphson iterative scheme to find breather solutions of the original equations of motion (although a rigorous mathematical proof that these numerical solutions are indeed true breathers is still lacking). Homoclinic orbits can be found easily using the methods of [4]. Results are presented for both the hard ϕ^4 potential and the Morse potential.

References

- [1] See e.g. A.J. Sievers and S. Takeno, *Phys. Rev. Lett.* 61 (1988) 970.
- [2] T. Bountis et al., *Phys. Lett. A* 268 (2000) 50.
- [3] G.P. Tsironis, *J. Phys. A* 35 (2002) 951.
- [4] J.M. Bergamin, T. Bountis and M.N. Vrahatis, "Homoclinic orbits of invertible maps", submitted for publication (2002).

6 The Window Josephson Junction: a Coupled Linear Nonlinear System

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Abstract

We investigate the interface coupling between the 2D sine-Gordon equation and the 2D wave equation in the context of a Josephson window junction using a finite volume numerical method and soliton perturbation theory. The geometry of the domain as well as the electrical coupling parameters are considered. When the linear region is located at each end of the nonlinear domain, we derive an effective 1D model, and using soliton perturbation theory, compute the fixed points that can trap either a kink or antikink at an interface between two sine-Gordon media. This approximate analysis is validated by comparing with the solution of the partial differential equation and describes kink motion in the 1D window junction. Using this, we analyze steady state kink motion and derive values for the average speed in the 1D and 2D systems. Finally we show how geometry and the coupling parameters can destabilize kink motion.

References

- [1] D.W. McLaughlin and A.C.Scott, *Phys. Rev. A.* 18 (1978) 1652.
- [2] A. Benabdallah, J. G. Caputo and N. Flytzanis, *Physica D*, vol 161 79-101 (2002).
- [3] *Finite volumes for complex applications II: problems and perspectives*, R. Vilsmeier, F. Benkhaldoun and D. Hanel Eds., Hermès, (1999).

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7 Analysis of the Breathers in Single Plaquette of Josephson Junction

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Abstract

We present a theoretical study of *inhomogeneous* dynamic (resistive) states in a single plaquette consisting of three Josephson junctions. These breather states are found to exist in a large range of control parameters (dc bias γ , anisotropy η and self inductance β_L). We perform an analytical analysis of these states, and their stability and resonance behaviour. Numerical calculations confirm our results and show that instabilities arise due to resonant interactions between the breather and electromagnetic oscillations (EOs) mediated by the breather state. These instabilities manifest themselves by various nonlinearities, resonant steps and voltage jumps in the current-voltage characteristics. Resonant interactions of such a breather state with electromagnetic oscillations manifest themselves by resonant current steps and voltage jumps in the current-voltage characteristics. An externally applied magnetic field leads to a variation of the relative shift between the Josephson current oscillations of two resistive junctions. By making use of the rotation wave approximation analysis and direct numerical simulations we show that this effect allows to effectively control the breather instabilities, e. g. to increase (decrease) the height of the resonant steps and to suppress the voltage jumps in the current-voltage characteristics.

References

- [1] A. Benabdallah, M. V. Fistul and S. Flach, *Physica D*, vol 159, 202-214, (2001).
- [2] M. V. Fistul, S. Flach and A. Benabdallah, *Phys. Rev. E*, vol 65, 046616 (2002).
- [3] Poster of Francesca Pignatelli.
- [4] E. Trías, J. J. Mazo, A. Brinkman and T. P. Orlando, *Physica D*, vol 156, 98.

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8 Discrete Breather Scattering from a Lattice Junction

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Abstract

We study the scattering of a moving discrete breather (DB) on a junction in a Fermi-Pasta-Ulam (FPU) chain consisting of two segments with different mass of the particles. We consider four distinct cases: (i) a light-heavy (abrupt) junction in which the DB impinges on the junction from the segment with lighter mass, (ii) a heavy-light junction, (iii) an up mass-ramp in which the mass in the heavier segment increases continuously as one moves away from the junction point, and (iv) a down mass-ramp. Depending on the mass difference and DB characteristics (frequency - i.e., amplitude - and velocity) the DB can either reflect from, or transmit through, or get trapped at the junction or on the ramp. For the heavy-light junction, the DB can even split at the junction into a reflected and a transmitted DB. The latter is found to subsequently split into two or more DBs. For the down mass-ramp the DB gets accelerated in several stages, with accompanying radiation (phonons). These results are rationalized by calculating the Peierls-Nabarro barrier for the various cases. We also point out implications of our results in realistic situations such as electron-phonon coupled chains.

9 A Renormalization Approach For the Quantum Frenkel-Kontorova Model

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Abstract

We will show a generalization of the classical Transition by Breaking of Analyticity in the Frenkel-Kontorova model [1] (a discrete sine-Gordon) to non-zero Planck's constant and temperature. This analysis is based on the study of a renormalization operator for the case of irrational mean spacing (see [2] and [3] for classical case) using Feynman's functional integral approach.

References

- [1] S. Aubry & P. Y. Le Daeron, *Physica D* 8 (1983) 381
- [2] R. S. MacKay, *Physica D* 50 (1991) 71
- [3] R. S. MacKay, *J. Stat. Phys.* 80 (1995) 45

10 Collapse Dynamics in Spatially Inhomogeneous Non-linear Schrödinger Equation Models.

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Abstract

Collapse of (2+1) and (1+1) dimensional beams in the inhomogeneous two-dimensional cubic and the one-dimensional quintic nonlinear Schrödinger equation is analyzed numerically and analytically. It is shown that in the vicinity of a narrow attractive linear potential, the collapse may be delayed or arrested. Self-guiding light in layered nonlinear media will also be considered.

11 Genetic Algorithms and Breather Generation.

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Abstract

We present a useful method of breather construction based on the genetic algorithms technics. Pseudo-analytical solutions in the form of elliptic functions for a large class of physically relevant nonlinear lattices is obtained. The method we introduce may be applied equally to optic and acoustic chains, and is presented here explicitly for a soft ϕ^4 lattice.

References

- [1] Rajendra Saha, Pinaki Chaudhury, S.P. Bhattacharyya, “Direct Solution of Schrodinger equation by genetic algortihm: test cases”, Phys. Lett. A, 291, (2002) pp 397.
- [2] D. E. Goldberg, “Genetic Algorithms in Search, Optimization and Machine Learning”, Addison Wesley, Reading , MA, (1989).

12 What Drives Protein Folding and Function?

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Abstract

Proteins act as the machines of life, they drive essentially all the physical and chemical processes that go on in living cells: they catalyse reactions, pass signals and provide basic structure. Although they are 100 million times smaller than man-made machines they can perform similar tasks, such as transport molecules from one part of a cell to another and act as motors. The way they function is still very obscure but it is known that they perform their functions by going from one well defined conformation into another. Two basic questions remain unanswered: first, how do proteins acquire a well defined structure out of the many possibilities that are potentially available (the protein folding problem)? Secondly, how do they change conformation? While macroscopic machines are triggered by classical actions, the triggers of protein machines are quantum mechanical, typically they are chemical reactions and the binding of ions or small molecules. The main question is thus how these localized actions eventually lead to the concerted motions of the 100's or even 1000's of atoms that constitute conformational changes [1]. Here the difficulties with the current view, according to which the native structure of proteins corresponds to the minimum of their (free) energy [2], are highlighted. In contrast, and following in the footsteps of Davydov [3] and Scott [4], it is proposed that vibrational energy transfer is the real driver of protein folding and function [5].

References

- [1] M. Gerstein and A.M. Lesk and C. Chothia, *Biochemistry* 33, 6739 (1994).
- [2] Anfinsen, C.B. *Science* 181, 223–233 (1973).
- [3] A.S. Davydov, *Solitons in Molecular Systems* Kluwer Academic Publ., Dordrecht, 2nd edition, 1991.
- [4] A. Scott, *Phys. Rep.* 217, 1–67 (1992).
- [5] L. Cruzeiro-Hansson and P. A. S. Silva, *J. Biol. Phys.* 27, S6-S9 (2001).

13 Interaction of Moving Discrete Breathers with Impurities

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Abstract

The influence of an impurity in the movement of discrete breathers in Klein–Gordon chains is analyzed. By means of numerical simulations, it is observed that the moving breather can cross the impurity, can be reflected by it, or can be trapped originating a quasi-periodic breather. The existence of the trapping phenomenon is explained through the *Nonlinear Local Mode hypothesis*. It provides with a necessary condition in order that the moving breather can be trapped and consists in that: (1) there must exist a resonance with a breather centred in the impurity (the Nonlinear Local Mode); (2) there must not exist a linear local mode whose wave vector is different from the nonlinear local mode's one. This hypothesis has been confirmed in several models with different implementations of the impurity.

The behaviour of the interaction in Klein–Gordon chains is similar to the observed within the NLS approximation [1]. However, the origin of the trapping is different to the NLS case, where the resonance must imply a linear local mode.

References

- [1] K Forinash, M Peyrard y BA Malomed. Interaction of discrete breathers with impurity modes. *Physical Review E*, 49:3400, 1994.
- [2] J Cuevas, F Palmero, JFR Archilla y FR Romero. Moving discrete breathers in a Klein–Gordon chain with an impurity. Nlin.PS/0203026.
- [3] Z Fei, YuS Kivshar y L Vzquez. Resonant kink-impurity interactions in the sine–gordon model. *Physical Review A*, 45:6019, 1992.

14 Isochronicity, Equidistant Spectrum and Discrete Breathers

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Abstract

The proof of existence of classical discrete breathers in Hamiltonian networks of coupled oscillators given by MacKay and Aubry [1] requires the onsite potential not to be isochronous. This means that the frequency of a single oscillator has to vary with its energy (or its action). On the other hand, a recent proof of existence of quantum discrete breathers by MacKay [2] requires the levels of the spectrum of the onsite potential not to be equidistant. These two conditions seem to be naturally related to each other. Nevertheless, we show by examples that neither isochronicity generates equispaced energy levels nor an equidistant spectrum implies that the corresponding potential is isochronous in general. These results raise several interesting questions regarding breathers existence and continuation. For instance breathers exist in weakly coupled classical isochronous oscillators.

References

- [1] R.S. MacKay and S. Aubry, *Nonlinearity*, 7 (1994) 1623-1643.
- [2] R.S. MacKay, *Physica A*, 288 (2000) 174-198.

15 Some Exact Results for Quantum Lattice Problems

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Abstract

We study the exact eigenvalue spectrum for a variety of quantum lattice models including the Quantum Discrete Nonlinear Schrödinger Model, the Quantum Ablowitz-Ladik model, and the Quantum Salerno model. These results extend previous work [1, 2], by considering larger number of quanta and bigger lattices.

References

- [1] A C Scott, J C Eilbeck and H Gilhøj, *Quantum lattice solitons*, *Physica D* **78**, 194-213, (1994)
- [2] M Salerno and J C Eilbeck, *A general method to solve Hamiltonians with infinite-range interactions*, *Phys. Rev. A.* **50** 553–556 (1994).

16 Two Examples of Quantum Rotational Dynamics of Methyl Groups in Crystals: The sine-Gordon and Coupled pair Theories

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Abstract

For light quantum rotors like methyl groups, the intrinsic periodicity of the angular coordinate imposes strict topological degeneracy and rotational tunnelling is observed in many crystals at low temperature. Owing to the large cross-section of H atoms for incoherent neutron scattering, tunnelling transitions for CH₃ rotors are best observed with the inelastic neutron scattering (INS) techniques. Multi-component spectra due to dynamical coupling are observed in some cases and different models were proposed to account for local or collective rotational dynamics or coupling between rotation and translation of the center of mass. Unfortunately, the hope that advanced quantum chemistry methods could provide realistic modelling of the effective potentials experienced by methyl rotors is not yet fulfilled.

Rotational dynamics in two prototypical systems will be presented. In the lithium acetate dihydrate, LiCH₃COO;2H₂O, neutron diffraction experiments allow us to demonstrate that methyl dynamics are represented with pairs of strongly coupled rotors [1]. This is in marked contrast to the case of the 4-methylpyridine crystal for which methyl rotation is well represented with the quantum sine-Gordon theory for infinite chain of coupled rotors [2]. These dynamics are tentatively related to the crystal structures.

References

- [1] B. Nicolaï, F. Fillaux and A. Cousson, in preparation.
- [2] F. Fillaux and C. J. Carlile, Phys. Rev. B, 42 (1990) 5990.

17 Wave Scattering by Discrete Breathers.

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Abstract

We study the influence of internal discrete breather dynamics on wave scattering. Especially interesting are one-dimensional systems as paradigmatic models of long molecules. The breather state being a localized excitation generates a time-dependent localized scattering potential for plane waves. We identify several typical scattering setups where the internal time dependence of the breather is of crucial importance.

The first class concerns systems with both vibrational and rotational excitations. The wave scattering by rotational excitations is strongly suppressed as compared to vibrational ones. This is due to the fact that the time-averaged scattering potential cuts the molecule into two noninteracting parts. At the same time the rotational excitation provides with a leading order scattering channel at a frequency of the sum of the plane wave frequency and the breather frequency.

The second class concerns systems with gaps in the plane wave spectrum, generated e.g. by a molecule deposited on a substrate. In such cases, especially when the breather frequency is located in the gap, resonant interactions between plane waves and local quasilevels allow a strong, even total reflection.

Our results are related to the ongoing discussion of anomalous heat conductivity in on-dimensional systems. Another application concerns the availability of active tunable transmitters in the range of 10-100 GHz on the basis of coupled small Josephson junctions. Finally our method can be slightly modified to account for the resonant electron tunneling in molecular wires in the additional presence of laser fields, which can be used to control and tune the resistance of the wire.

18 Broken Symmetries and Directed Collective Energy Transport in spatially extended systems

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in representation of Mikhail Fistul

Abstract

We study the appearance of directed energy current in homogeneous spatially extended systems coupled to a heat bath in the presence of an external ac field $E(t)$. The systems are described by nonlinear field equations. By making use of a symmetry analysis we predict the right choice of $E(t)$ and obtain directed energy transport for systems with a nonzero topological charge Q . We demonstrate that the symmetry properties of motion of topological solitons (kinks and antikinks) are equivalent to the ones for the energy current. Numerical simulations confirm the predictions of the symmetry analysis and, moreover, show that the directed energy current drastically increases as the dissipation parameter reduces. Our results generalize recent rigorous theories of currents generated by broken time-space symmetries to the case of interacting many-particle systems.

19 A Centre Manifold Technique for Computing Discrete Breathers

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Abstract

For a large class of infinite one-dimensional nonlinear lattices time-periodic oscillations can be viewed as solutions of an ill-posed nonlinear recurrence relation on a loop space. We give simple spectral conditions under which all small-amplitude solutions lie on an invariant finite-dimensional centre manifold. This result reduces the problem locally to the study of a finite-dimensional mapping and provides an exact version of the rotating-wave approximation method (which can be viewed as a tangent-space approximation). The reduced mapping may possess homoclinic orbits to 0 corresponding to discrete breathers. We show how to compute the centre manifold and the reduced mapping at an arbitrary order.

References

- [1] G. James *Centre manifold reduction for quasilinear discrete systems*, submitted to *J. Nonlinear Science* (2002)
- [2] G. James, *Existence of breathers on FPU lattices*, *C.R.Acad.Sci.Paris*, t. 332, Série I (2001), p. 581-586.
- [3] A.J. Sievers and S. Takeno, *Intrinsic localized modes in anharmonic crystals*, *Phys. Rev. Lett.* 61 (1988), p.970-973.
- [4] G. Iooss, *Bifurcation of maps and applications*, *Math. Studies* 36 (1979), Elsevier-North-Holland, Amsterdam.

20 Breather-Phonon Resonances and Oscillatory Instabilities in Anharmonic Lattices

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Serge Aubry, Anna Maria Morgante, Georgios Kopidakis

Abstract

We will review recent results [1]-[5] concerning different aspects of breather-phonon interactions in anharmonic lattices. Depending on the available time, some or all of the following topics will be discussed:

(i) [1, 2] Using a multiscale perturbational approach, we analyze the nonlinear interaction between breathers and small perturbations, and identify fundamental lowest-order mechanisms for breather growth and decay through generation of radiating higher harmonics.

(ii)[3, 4] We identify nonlinear standing-wave phonons as exact multibreather solutions, which are typically unstable through oscillatory instabilities. Depending on whether the phonon wave vector is larger or smaller than $\pi/2$, the long-time dynamics resulting from these instabilities yields either formation of persistent breathers, or thermalization.

(iii)[5] When a higher harmonic of the breather frequency enters the linear phonon band, an exact 'phonobreather' solution with non-zero tail appears. We show that for small finite systems, where the phonon frequencies are sparsely distributed, practically localized exact solutions ('phantom breathers') exist with frequencies in-between the phonon frequencies. For particular parameter values the tails may completely vanish, and the phantom breathers decay exponentially for the whole system size.

References

- [1] M. Johansson and S. Aubry, *Phys. Rev. E* 61, 5864 (2000).
- [2] M. Johansson, *Phys. Rev. E* 63, 037601 (2001).
- [3] A.M. Morgante, M. Johansson, G. Kopidakis, S. Aubry, *Phys. Rev. Lett.* 85, 550 (2000).
- [4] A.M. Morgante, M. Johansson, G. Kopidakis, S. Aubry, *Physica D* 162, 53 (2002).
- [5] A.M. Morgante, M. Johansson, S. Aubry, G. Kopidakis, *J. Phys. A: Math. Gen.* 35 (2002).

21 Breathers in Simple Models of Polymers with Secondary Structure

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Abstract

The search for breather solutions in simple models of polymers with a secondary structure might be regarded as a first step towards an understanding of the role that local excitations might play for the functionality of proteins. A minimal model should include the following two features: (a) a one-dimensional system (chain) is embedded in d -dimensional space ($d > 1$), (b) inter-particle interactions involve at least d neighbours in order to obtain a secondary structure. We use a simple model proposed by Zolotaryuk *et al.* [1]: a chain of masses embedded in two-dimensional space, where the masses interact by means of linear nearest-neighbour and next-nearest-neighbour forces. The secondary structure of the system gives rise to effective nonlinearities and therefore, despite the linearity of the forces, breather solutions might exist.

Numerical tests confirm the existence of breathers in this system. Although existent, the simplest type of breathers involving only one frequency seems to be of minor relevance for the dynamics of the system, whereas multifrequency breathers might play their part.

References

- [1] A. V. Zolotaryuk, P. L. Christiansen, and A. V. Savin, *Two-dimensional dynamics of a free molecular chain with a secondary structure*, Phys. Rev. E 54:3881–3894 (1996).

22 Dark and Bright Compactlets

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Abstract

We report our recent studies of bright and dark compactlets (i.e. solutions which are strictly constants outside a given interval) in discrete nonlinear Klein-Gordon (KG) and nonlinear Schrödinger (NLS) chains. We analyze classes of nonlinear lattice models which can support *exact* compactlet solutions. Temporal behaviour and lattice patterns of compactlets of the respective lattices are studied. Classification of such solutions and description of their stability are provided. Particular sets of KG and NLS nonlinearities of relevance to applications are studied.

23 Electromagnetic Wave Diode Based on a Nonlinear Photonic Crystal

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Abstract

We proposed a new concept of a diode-like device based on the nonlinear 1D photonic crystal which exhibits nonreciprocal properties with respect to the direction of propagation of the incident wave. The nonreciprocity is achieved due to the second-harmonic generation (SHG) in the left part of the dual periodic structure that possesses $\chi^{(2)}$ nonlinearity and Bragg reflection of the fundamental harmonic in the right component of a dual structure. We have shown that for an appropriate frequency of the fundamental signal which lies within the band gap such a device can act as a light diode that operates at the frequency of the second harmonic with the amplitude that is predicted to be significantly stronger than fundamental signal for sufficiently large intensity of the incident wave.

24 Stationary Energy Transport in Nonlinear Lattices

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Abstract

Deriving macroscopic phenomenological laws of irreversible thermodynamics from simple microscopic models is one of the tasks of non-equilibrium statistical mechanics. We consider stationary energy transport in crystals with reference to simple mathematical models consisting of classical oscillators coupled on a lattice. The role of lattice dimensionality on the breakdown of the Fourier's law is discussed and some universal quantitative aspects are emphasized: the divergence of the finite-size thermal conductivity is characterized by universal laws in one and two dimensions.

References

- [1] S. Lepri, R. Livi, A. Politi, *Thermal conduction in classical low-dimensional lattices*, preprint cond-mat/0112193, submitted to **Phys. Reports** (2002).
- [2] S. Lepri, R. Livi, A. Politi, *Heat conduction in chains of nonlinear oscillators*, **Phys. Rev. Lett.** 78, 1896 (1997).
- [3] S. Lepri, *Memory effects and heat transport in one-dimensional insulators*, **Eur. Phys. J. B** 18 441 (2000).

25 Quantum Targeted Energy Transfer in DNLS and Klein-Gordon Dimers

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Abstract

It has been shown earlier that it is possible to tune two weakly coupled classical anharmonic oscillators in order that when injecting a selected amount of energy on the first one, it is completely transferred to the second one and oscillates back and forth. This effect of Targeted Energy Transfer (TET) is obtained because the variable frequencies of the two oscillators remain almost equal during the transfer. TET to occur requires a coupling larger than a certain critical coupling which can be small.

The purpose of the present work is to study the same effect with quantum oscillators. We consider first TET in an integrable DNLS dimer. It is found that conditions for quantum TET are the same as for the corresponding classical dimer. However, a damping of the energy oscillations between the two oscillators is observable as a consequence of the quantum dispersion of the initial wave packet.

We next consider a quantum Klein-Gordon dimer in which classical TET occurs. It is found that quantum TET persists with a damping of the energy oscillations as in the quantum DNLS case but now the critical coupling for having TET increases as the number of bosons decreases. This effect is interpreted as a consequence of the non integrability of the classical model.

26 Discrete Breathers in 2D Josephson-junction Arrays

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Abstract

We predict theoretically and confirm numerically the existence of discrete breathers (intrinsic localised modes) in the dynamics of a two-dimensional Josephson-junction array biased by radio-frequency fields. The solutions are linearly stable in the framework of the Floquet theory and robust in the presence of thermal fluctuations. We have also discussed the conditions for realizing an experimental detection of these modes.

27 Kink Ratchet Potentials

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Abstract

A fluxon in a Josephson-junction parallel array behaves like a single particle in a periodic pinning potential. Different configurations of critical currents and cell areas result in different profiles for the fluxon potential. We analyze the minimal conditions to achieve an effective potential in which mirror symmetry is absent, namely a fluxon ratchet potential. Following one of such configurations we have designed circular arrays and probed some of the fluxon properties. Theoretical predictions are nicely fulfilled by the experiments.

References

- [1] Ratchet potential for fluxons in Josephson-junction arrays. F. Falo, P.J. Martínez, J.J. Mazo, and S. Cilla. *Europhys. Lett.* 45(6), 700-706 (1999).
- [2] Depinning of kinks in a Josephson-junction ratchet array. E. Trías, J.J. Mazo, F. Falo y T.P. Orlando. *Phys. Rev. E* 61, 2257-2266 (2000)
- [3] Fluxon ratchet potentials in superconducting circuits. F. Falo, P.J. Martínez, J. J. Mazo, T. P. Orlando, K. Segall and E. Trías. *Appl. Phys. A* 75, 263-269 (2002)

28 Breather Scattering in the Dissipative Driven Frenkel-Kontorova Model

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Abstract

In the dissipative and driven Frenkel-Kontorova model discrete breathers can be obtained by a simple continuation procedure which consists in slowly varying the strength C of the inter-particle coupling and taking full advantage of the attractor property of the breather solution. Varying C several bifurcations are encountered [1]. In particular, spontaneously moving breathers are found for C within a certain range. Having obtained these moving breathers, their behaviour in collisions can be studied. Colliding breathers can rebound, form a bound state, or one or both of the colliding breathers can be destroyed. Numerical scattering experiments indicate a very sensitive and irregular dependence of the qualitative outcome of the scattering on the initial conditions. If Gaussian white noise is coupled to the system, this sensitivity also shows: Even very weak noise can change the qualitative result of a scattering process.

References

- [1] Marín J. L., Falo F., Martínez P. J., and Floría L.M., Phys. Rev. E 63 66603 (2001).

29 Transfer dc Magnetization in ac Quantum Driven Spins

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Abstract

We consider $s = 1/2$ spins in the presence of a constant magnetic field in z -direction and an AC magnetic field in the $x - z$ plane. A nonzero DC magnetization component in y direction is a result of broken symmetries. A pairwise interaction between two spins is shown to resonantly increase the induced magnetization by one order of magnitude. We discuss the mechanism of this enhancement, which is due to additional avoided crossings in the level structure of the system.

References

- [1] F. Bloch ,Phys. Rev. 102, 104 (1956).
- [2] N. Bloembergen, *Nonlinear optics* W. A. Benjamin Inc., (1965).
- [3] S. Flach, O. Yevtushenko, and Y. Zolotaryuk, Phys. Rev. Lett. 84, 2358 (2000).
- [4] O. Yevtushenko, S. Flach, Y. Zolotaryuk, and A. A. Ovchinnikov, Europhys. Lett. 54, 141 (2001).
- [5] S. Flach and A. A. Ovchinnikov, Physica A 292,268 (2001).

30 Breathers in Josephson Junction Ladders: Resonances and Electromagnetic Waves Spectroscopy

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Abstract

We present a theoretical study of the resonant interaction between dynamical localized states (*discrete breathers*) and linear electromagnetic excitations (EEs) in Josephson junction ladders. By making use of direct numerical simulations we find that such an interaction manifests itself by *resonant steps* and various sharp switchings (*voltage jumps*) in the current-voltage characteristics. Moreover, the power of ac oscillations away from the breather center (the *breather tail*) displays singularities as the externally applied dc bias decreases. All these features can be mapped to the spectrum of EEs that has been derived analytically and numerically. Using an improved analysis of the breather tail, a spectroscopy of the EEs is developed. The nature of breather instability driven by localized EEs is established.

References

- [1] E. Trias, J. J. Mazo and T. P. Orlando, Phys. Rev. Lett. 84, 741 (2000).
- [2] P. Binder, D. Abraimov, A. V. Ustinov, S. Flach and Y. Zolotaryuk, Phys. Rev. Lett. 84, 745 (2000).
- [3] A. E. Miroschnichenko, S. Flach, M. V. Fistul, Y. Zolotaryuk, and J. B. Page, Phys. Rev. E 64, 066601 (2001).
- [4] M. Schuster, P. Binder and A. V. Ustinov, Phys. Rev. B 65, 016606 (2002).
- [5] M. V. Fistul, A. E. Miroschnichenko, S. Flach, M. Schuster and A. V. Ustinov, cond-mat/0111460 (2001).

31 A Breather Existence Result for Diatomic FPU Chains with Arbitrary Mass Ratios

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Abstract

We present a mathematically rigorous proof for the existence of breathers in diatomic FPU chains with arbitrary mass ratios. This completes an existence result proved by Livi, Spicci and MacKay for large mass ratios ([3]). The proof doesn't use the concept of anticontinuous limit and is based on a discrete centre manifold reduction. For interaction potentials satisfying a hardening condition, we find breathers with frequencies slightly above the optic band, or in the gap slightly above the acoustic band. When the potential satisfies the opposite softening condition, we obtain breathers with frequencies in the gap slightly below the optic band. This result is in agreement with numerical simulations by Kiselev, Bickham and Sievers ([4]).

References

- [1] G. James and P. Noble, *Breathers on diatomic FPU chains with arbitrary masses*, preprint 2002, University of Toulouse.
- [2] G. James, *Centre manifold reduction for quasilinear discrete systems*, submitted to *J. Nonlinear Science* (2002).
- [3] R. Livi, M. Spicci and R.S. Mackay, *Breathers on a diatomic FPU chain*, *Nonlinearity* 10 (1997), p. 1421-1434.
- [4] S.A. Kiselev, S.R. Bickham and A.J. Sievers, *Anharmonic gap mode in a one-dimensional diatomic lattice with nearest-neighbor Born-Mayer-Coulomb potentials and its interaction with a mass-defect impurity*, *Phys Rev B* 50 (1994), number 13, p. 9135.

32 Vortices in Bose-Einstein condensates: Nonlinear phenomena

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Abstract

One of the hottest topics in the field of Bose-Einstein condensation (BEC) with many connections with nonlinear science and the general theory of topological defects is that of vortices [1]. The interest on vortices in BEC is related to the fact that its existence is one of the most spectacular manifestations of superfluidity and are related to the existence of persistent currents in the system, which have been observed in experiments with Bose-Einstein condensates [2]

I will describe recent results on

1. Existence, nucleation, stability and dynamics of vortices in normal and rotating systems [3].
2. Structural stability of vortices and formation of vortex lattices [4].
3. Vortices in multi-component systems [5].

References

- [1] See e.g. A. Svidzinsky, A. L. Fetter, *Jour. Phys. B* **13**, R135 (2001), and references therein.
- [2] M. R. Matthews *et al.*, *Phys. Rev. Lett.* **83**, 2498 (1999); K. W. Madison, *et al.* *Phys. Rev. Lett.* **84**, 806 (2000); J. R. Abo-Shaeer, *et al.* *Science* **292**, 476 (2001).
- [3] J. J. García-Ripoll, V. M. Pérez-García, *Phys. Rev. A*, **60** 4864 (1999); **63** 041603(R) (2001); **64** 053611 (2001). V. V. Konotop, V. M. Pérez-García *ibid* **62**, 033610 (2000).
- [4] J. J. García-Ripoll, G. Molina-Terriza, V. M. Pérez-García, and L. Torner, *Phys. Rev. Lett.* **87**, 140403 (2001).
- [5] J. J. García-Ripoll, V. M. Pérez-García, *Phys. Rev. Lett.* **84**, 4264 (2000); V. M. Pérez-García, J. J. García-Ripoll, *Phys. Rev. A* **62** 033601 (2000).

33 Cooling non-linear lattices towards energy localisation

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Abstract

We study the phenomenon of spontaneous energy localisation which occurs when thermalised non-linear lattices are put in contact with a $T = 0$ bath [1]. This process leads to the birth of discrete breathers and the localisation pathway is reminiscent of modulational instability of the band-edge linear modes [2]. In particular, after a transient stage where a collection of short-lived localised objects strongly interact among each other [3, 4], a *residual pseudo-stationary* state is reached. The latter is characterised by the presence of discrete breathers and its energy decays exponentially with a huge time constant. We find that the distribution of breather energies is markedly different in 1D and 2D. In fact, in 1D the residual state is invariably a single-breather state, whereby in 2D one observes a collection of stationary localised vibrations. We study the distribution of the breather energies in the residual state, which carry important information regarding the breather-breather interactions during the transient. Moreover, from the analysis of such distributions, we show how the presence of an energy threshold [5] for energy localisation in more than 1D makes the spontaneous formation of breathers a thermally-activated process.

References

- [1] G. P. Tsironis and S. Aubry, *Phys. Rev. Lett.* **77** (26) 5225 (1996).
- [2] F. Piazza, S. Lepri and R. Livi, *J. Phys. A*, **34**, 9803 (2001).
- [3] R. Reigada, A. Sarmiento and K. Lindenberg, *Phys. Rev. E* **64** 066608 (2001).
- [4] R. Reigada, A. Sarmiento and K. Lindenberg, *Physica A* **305**, 467 (2002).
- [5] S. Flach, K. Kladko and R. S. MacKay, *Phys. Rev. Lett.* **78** 1207 (1997).

34 Observation of Breather-like States and Resonances in a Single Josephson Cell

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Abstract

Experimental observation of broken symmetry states (breather-like) in a small Josephson system, consisting of a cell with three small Josephson junctions, will be presented. The measurements were performed at different temperatures in such a way as to control the damping of the system. The experimental regions of existence of the breather-like states at different values of damping are found to be in accordance with the theoretical ones, evaluated by a simplified dc model. Increasing the damping of the system the rotation frequency of the breather-like is decreased so that we could study the breather-like in the range of the frequencies of the electromagnetic oscillations. In this condition we observed different resonant behaviours in the current-voltage characteristics, due to the interaction between breather-like and electromagnetic oscillations in the cell. We will show also the experimental dependence of these different resonant steps to external frustration. Comparison of measured data with the previous theoretical studies by [1, 2] will be reported.

References

- [1] A. Benabdallah, M. V. Fistul, S. Flach, *Physica D* 159 (2001) 202.
- [2] M. V. Fistul, S. Flach and A. Benabdallah, *Phys. Rev. E* 65, 046616 (2002)

35 Energy Activation and Thermostability NADP-isocitrate Dehydrogenase from Rat Heart Mitochondria under Oxidative stress Conditions

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Abstract

As well known, the energy transfer during catalytic action enzymes has nonlinear character, and this process determinates effectiveness and stability of enzyme system functioning, that is significant at norm and especially at oxidative stress conditions. The role of NADP- isocitrate dehydrogenase (NADP-IDH, E.C. 1.1.1.42.) in regulation of free radical processes intensity in myocardium at ischemia is considered to NADPH supply for glutathione reductase/glutathione peroxidase (GR/GP-system) antioxidative system functioning because the enzyme plays a key role in NADPH generation in rat cardiomyocytes. Investigations of energy activation and thermostability of electrophoretically homogeneous preparations of NADP-IDH purified from rat heart mitochondria, using differential centrifugation, desalinization on Sephadex G-25, ion-exchange chromatography on DEAE-cellulose and gel - chromatography on Sephadex G-150 were conducted. The temperature optimum over the range tested (10 0 C ? 70 0 C) was found at 40 0C and 50 0C for NADP-IDH from ischemic and normal rat myocardium. An Arrhenius plot of the data from 10 0C to 40 0C for NADP-IDH purified from ischemic heart showed a breakpoint at 30 0 C, resulting in activation energy values of 7352 kkal between 10 and 30 0 C and 5936 kkal between 30 and 40 0C. Whereas the breakpoint in the Arrhenius plot for enzyme preparations from normal myocardium is absence and the activation energy value, calculated in temperature range 10 0C - 50 0C was 6593 kkal. From the data of comparative study of thermostability and light diffusion values at the temperature range 10 0C - 70 0C it can be concluded, that NADP-IDH from ischemic heart under temperature interval 45 - 60 0C has more lower thermostability as compared with the enzyme from normal tissue. The deactivation of NADP-IDH from ischemic heart at 70 0C accompanied with the further increase of light diffusion level, evidently, was associated with enlarge of protein surface due to dissociation or conformational unfolding. Therefore, the presence of breakpoint on the Arrhenius plot, higer activation energy value and light diffusion level, lower temperature optimum and thermostability of the enzyme preparations under ishemical conditions indicate that NADP-IDH, operating in ischemic mitochondria is more unstable with respect to temperature. Thus, that the obtained specific features of NADP-IDH under ischemia might be have significance for interrelation of NADP-IDH and GR/GP-system functions in mitochondria of rat heart.

36 The Parametrically Modified Sine-Gordon Equation: an Special Case Between the Integrable and Non-Integrable Models

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Abstract

We present a numerical study of the spectral properties of the linearized problem around the kink solution in the parametrically modified sine-Gordon equation (pmsG) [1],

$$\phi_{tt} - \phi_{xx} = -\frac{\partial U}{\partial \phi}, \quad -\infty < x < \infty,$$

$$U(\phi, r) = \frac{(1-r)^2 [1 - \cos(\phi)]}{1 + r^2 + 2r \cos(\phi)}, \quad |r| < 1.$$

The spectrum of this problem is related to integrability properties [2]. In the absence of an internal mode (IM), which happens for $r = 0$ (sine-Gordon equation), this system is integrable and the interactions between solitons are elastics. Due to the appearance of an IM ($r < 0$) the collisions between solitary waves become inelastic, so the pmsG is non-integrable. However, for $r > 0$, there is no internal mode to explain the inelasticity in the collision process in the still non-integrable pmsG equation. In this talk we investigate the inelasticity of the collisions in the absence of the IM by analyzing the linear spectrum [3].

References

- [1] M. Remoissenet and M. Peyrard. J. Phys. C: Solid State Phys. 14, L481, (1981). Phys. Rev. B 26, 2886 (1982).
- [2] M. Peyrard and D. K. Campbell. Physica 9D, 33, (1983).
- [3] Niurka R. Quintero and P.G. Kevrekidis. Physica D: Nonlinear Phenomena.

37 Dynamics of Discrete Breather in Flexible Chains.

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Abstract

We present the study of discrete breather dynamics in curved polymer-like chains consisted of masses connected via nonlinear springs. For chains with strong angular rigidity, we find that breather motion is strongly affected by the presence of bended regions of the polymers, while the breathers themselves show a very strong resilience and remarkable stability in the presence of geometrical changes. For more flexible chains modelled via second neighbour interactions we find that chain geometry typically does not destroy the localised breather states but, contrary to the angularly rigid chains, it induces some small but constant energy loss. Furthermore, we find that a curved segment acts as an active gate reflecting or refracting the incident breather and transforming its velocity to a value that mostly depends on the DB frequency. We analyse the physical reasoning behind these seemingly general breather properties

38 Experimental Investigations of Rotobreathers in Josephson Ladders

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Abstract

We present experimental and numerical studies of localized rotational states (discrete breathers) in a one-dimensional rotor lattice, the Josephson ladder. The latter is formed by an array of Josephson tunnel junctions arranged along the spars and rungs of a ladder.

With an externally applied time-constant uniform bias (force), the localized dynamic states persist even in the presence of dissipation, while their rotational frequency is dependent on the magnitude of the bias. This allows for a systematic experimental study of the properties of the localized rotational states.

For matching rotational frequencies, we observe strong resonant interaction between the dc-bias supported localized states and the spatially extended linear electromagnetic excitations (phonons) of the lattice. Under certain conditions, we find resonant breather-like states displaying *incommensurate* dynamics.

Additionally, we investigate the possibility of applying time-periodic external bias to support the localized rotational states. Preliminary experimental results will be reported.

References

- [1] M. Schuster, P. Binder, and A. V. Ustinov, “Observation of breather resonances in Josephson ladders”, *Phys. Rev. E* 65, 016606, 2002.
- [2] M. V. Fistul, A. E. Miroshnichenko, S. Flach, M. Schuster and A. V. Ustinov, “Incommensurate dynamics of resonant breathers in Josephson junction ladders”, *Phys. Rev. B* 65, 174524 (2002).

39 Theoretical Analysis of Travelling Discrete Breathers in FPU

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Abstract

In this paper we present briefly a method of collective coordinates describing the slow Hamiltonian dynamics in approximate periodic solutions of Hamiltonian systems [1]. The method enables one to analyse approximate travelling discrete breathers in oscillator networks as soon as a continuous family of (possibly approximate) discrete breathers depending on a translation coordinate is known. We consider two cases related to the Fermi-Pasta-Ulam chain (FPU). Firstly, a family of weakly localised DB can be constructed for FPU, from the existence results of G. James [2]. In this case we give an analytical estimate of the velocity of DB which is very close to the group velocity. Moreover we demonstrate that the corresponding Peierls-Nabarro barrier (defined in [1] for discrete breathers) is negligible in this case. Secondly, we give preliminary results for the case of strongly localised DBs in FPU which is dealt with by considering a family of compacton-like DBs. The latter have been shown to exist, at least approximately, when the potential is purely anharmonic and is an homogeneous function [3]. Our analytic results are illustrated by numerical simulations.

References

- [1] R.S. MacKay and J-A Sepulchre, Effective Hamiltonian for traveling discrete breathers, *J. Phys. A: Math. and Gen.* 35 (2002) (to appear).
- [2] G. James, Existence of breathers on FPU lattices, *Comptes Rendus Acad Sci Serie I*, 332 (2001) 581–6.
- [3] Y. S. Kivshar, Intrinsic localized modes as solitons with a compact support, *Phys. Rev. E* 48 (1993) R43-45.

40 Controlling the Energy Flow in Nonlinear Lattices: A Model for a Thermal Rectifier

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Abstract

We address the problem of heat conduction in 1-D nonlinear chains [1]. We consider the Peyrard-Bishop model [2], which was originally developed to describe the basic features of the DNA molecule. We discuss the possibility of controlling the heat flux along the 1-D system; we show that, acting on the parameter which controls the strength of the on site potential inside a segment of the chain, we induce a transition from conducting to insulating behavior in the whole system. Quite remarkably, the same transition can be observed by increasing the temperatures of the thermal baths at both ends of the chain by the same amount. The control of heat conduction by nonlinearity opens the possibility to propose new devices such as a thermal rectifier. We show some numerical results that confirm the existence of such a rectifying effect[3].

References

- [1] F.Bonetto, J.L.Lebowitz and L. Ray Bellet in A. Fokas, A. Grigoryan, T. Kibble and B. Zegarlins Eds., *Mathematical Physics 2000*, Imperial College, London 2000, and math-phys/0002052; S. Lepri, R. Livi and A. Politi, cond-mat/0112193.
- [2] M.Peyrard and A.R. Bishop, *Phys. Rev. Lett.* 62, 2755 (1989); T. Dauxois, M.Peyrard and A.R. Bishop, *Phys. Rev.E* 47, 684 (1993).
- [3] M.Terraneo, M.Peyrard and G.Casati, *Phys. Rev. Lett.* 88, 094302 (2002).

41 Critical Dynamics of DNA denaturation

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Abstract

The dynamics of the Peyrard-Bishop model of DNA denaturation is examined. Numerical simulations reveal that, as the transition is approached from below, the Fourier spectrum of the displacement autocorrelations $S(k, \omega)$ exhibits (i) a "soft" phonon peak at the corresponding frequencies of the high-temperature phase, if the wavevector k is larger than the inverse correlation length, and (ii) a central peak, which becomes dominant at long wavelengths and critically narrow near the instability. Results can be analyzed in terms of a memory function which consists of a low-frequency relaxational contribution, and a broad band due to oscillations.

42 Statistical Properties of Discrete Breathers

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Abstract

We present some ideas regarding the equilibrium thermodynamics of breather systems. In order to handle the complexity of the phase space of the nonlinear we clone the original system and perform statistics on the cloned ensemble. We demonstrate numerically in the context of a pseudospin model that ergodicity is broken and time correlation functions are equivalent to certain restricted averages over phase space variables.

43 The non-locality and fractional derivatives

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We present some non local wave equation and the relation with fractional derivatives. The fractional calculus represents a mathematical tool to deal with non local effects in time or space.

References

- [1] Fractional diffusion equations with internal degrees of freedom. L. Vazquez. Journal of Computational Mathematics. 2002 in press.
- [2] Fractionally coupled solution of the diffusion equation. L.Vazquez, Rui Vilela Mendes. Applied Mathematics and Computation. 2002 in press.
- [3] Hamiltonian systems with fractional time derivatives. G. Turchetti. D. Usero. L. Vazquez. 2002 in pres. Tamsui Oxford Journal of Mathematical Science. 2002 in press.

44 Noise-induced Pattern Recovery in Neural Networks.

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Abstract

A network of FitzHugh-Nagumo oscillators is trained, following a Hebbian learning rule, to store a set of disconnected patterns in an associated way. The stored patterns can be recalled by noise alone if the delays of the synaptic transmissions are properly fixed. In the retrieval of the associated patterns it is determinant the strength of the synapsis transmission. Unppaired tuning of this parameter may result in too much or too little excitability and therefore in missfunctioning of the network.