International Workshop on Nonlinear Energy Localization in Crystals and Related Media

December 2-3, 2016
Kyoto International Exhibition Hall "Miyako Messe," Kyoto, Japan

Organizer

Yusuke Doi, Osaka University, Japan
Masayuki Kimura, Kyoto University, Japan

Support

Toyota Physical and Chemical Research Institute
The Kyoto University Foundation

Book of Abstracts

International Workshop on Nonlinear Energy Localization in Crystals and Related Media

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Kyoto, JAPAN

Scope

In this workshop, theoretical, numerical and experimental problems on nonlinear energy localization called discrete breather (DB)/intrinsic localized mode (ILM) in materials and related discrete structures are discussed. The topics focused in the workshop are:

- Basic theory of DB in mathematical models
- Molecular dynamics simulations of DB's dynamics in crystals
- DB in optical physics
- Observation of DB in experiment
- Thermal transport in nonlinear discrete systems
- Nonlinear dynamics in metamaterials and MEMS

Organizers

Yusuke Doi, Osaka University, Japan

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Supports

Toyota Physical and Chemical Research Institute

(Specially Promoted Project "Study on noble condensed matter theory based on nonlinear energy transportation")

The Kyoto University Foundation

Venue

Kyoto International Exhibition Hall "Miyako Messe"

9-1 Okazaki Seisyoji-cho, Sakyo-ku, Kyoto 606-8343 JAPAN

Session Schedule

2016.12.2 (Fri.)

9:40-9:50 Opening

9:50-10:30 **Search of discrete breathers in unstrained graphene**
Sergey V. Dmitriev (Institute for Metals Superplasticity Problems of Russian Academy of Sciences), Ivan P. Lobzenko, Andrey A. Kistanov, Elena A. Korznikova

10:30-10:55 **Variety of discrete breathers in fcc crystals**
Elena A. Korznikova (Institute for Metals Superplasticity Problems of Russian Academy of Sciences), Andrey A. Kistanov, Sergey V. Dmitriev

10:55-11:05 break

11:05-11:30 **Properties of discrete quasibreathers and Rosenberg modes in graphene by means of classical and quantum molecular dynamics**
Ivan Lobzenko (Toyota Technological Institute), George Chechin, Alexandr Chetverikov, Sergey Dmitriev

11:30-11:55 **Role of intrinsic localized modes in atomic structures: trigger of stone-wales defect formation in carbon nanotubes**
Takahiro Shimada (Kyoto University), Takayuki Kitamura

11:55-13:20 Lunch

13:20-14:00 **Mobile breather scattering in a 2D hexagonal crystal lattice**
J. Chris Eilbeck (Heriot-Watt University)

14:00-14:40 **Localized nonlinear excitations in silicate layers**
Juan F.R. Archilla (University of Sevilla)

14:40-15:05 **Mobile discrete breathers and symmetry of pairwise interaction in crystals**
Yusuke Doi (Osaka University), Akihiro Nakatani

15:05-15:30 **Moving Intrinsic Localized Modes and Its Behavior at Junction between Two Different Lattices**
Masayuki Kimura (Kyoto University), Ryo Tsujisaka, Yoshiharu Taniguchi, Yasuo Matsushita, and Takashi Hikihara

15:30-15:50 Break

15:50-16:15 **Defects in single-walled carbon nanotubes investigated by atomic force microscopy and its related techniques**
Yuji Miyato (Osaka University), Kei Kobayashi, Hirofumi Yamada

16:15-16:40 **Existence and stability of odd and even parity discrete breathers in Fermi-Pasta-Ulam lattices**
Kazuyuki Yoshimura (Tottori University)

Evening Banquet

2016.12.3 (Sat.)

10:00-10:40 **Confining interparticle potential makes both heat transport and energy diffusion anomalous in one-dimensional phononic systems**
Yuriy A. Kosevich (Semenov Institute of Chemical Physics, Russian Academy of Sciences), Alexander V. Savin

10:40-11:20 **Non-universal heat correlation functions and their anomalous scaling in one-dimensional systems**
Daxing Xiong (Fuzhou University), Jun Zhang

11:20-11:45 **Contact geometric approaches to nonlinear RLC circuit lattices in contact with heat bath**
Shin-itiro Goto (Kyoto University)

11:45-13:20 Lunch

13:20-14:00 **Wave Propagation in Origami-based Mechanical Metamaterials**
Hiromi Yasuda (Washington University), Jinkyu Yang

14:00-14:25 **Making of air-levitation-type coupled oscillator array and experiments on excitation of intrinsic localized modes**
Yosuke Watanabe (Osaka University), Mai Nishimoto, Chika Shiogama

14:25-14:50 **Traveling Intrinsic Localized Modes in Nonlinear Driven Damped Lattices**
M. Sato (Kanazawa University), S. Shige, T. Mukaide and A. J. Sievers

14:50-15:00 Closing

Poster Presentation

P1 **Molecular dynamics simulation of intrinsic localized modes in two types of carbon nanotube**
Guanghui Sun (Osaka University), Yusuke Doi, Akihiro Nakatani

P2 **Existence condition and stability of rotating intrinsic localized modes in FPU-β chain with fixed boundaries**
Atsuki Mitani (Kyoto University), Masayuki Kimura, Shinji Doi

P3 **Frequency response of localized modes in one dimensional resonant circuit array with an impurity**
Takuya Fujimoto (Kyoto University), Masayuki Kimura, Shinji Doi

Abstracts

Search of discrete breathers in unstrained graphene

Sergey V. Dmitriev [A], **Ivan P. Lobzenko** [B], **Andrey A. Kistanov** [C], **Elena A. Korznikova** [D]

Institute for Metals Superplasticity Problems of RAS, 450001, Khalturina str., 39 Ufa, Russia

e-mail: [A] dmitriev.sergey.v@gmail.com, [B] ivanlobzenko@gmail.com, [C] andrei.kistanov.ufa@gmail.com, [D] elena.a.korznikova@gmail.com

Graphene is one atom thick carbon layer with unique combination of physical and mechanical properties promising for many applications. Nonlinear lattice dynamics of graphene has been addressed in recent theoretical and experimental works. In particular, several studies have been done on the possibility to excite discrete breathers (or intrinsic localized modes), which are long-lived, spatially localized nonlinear vibrational modes. In the present work, based on the molecular dynamics simulations and ab initio simulations, we discuss the possibility to excite discrete breathers (DBs) in unstrained graphene. The main problem here is to find proper initial conditions that lead to excitation of long-lived spatially localized vibrational modes. Our main approach is to begin with the study of amplitude-frequency dependence for various short-wavelength extended phonon modes in the nonlinear regime. For those modes whose frequencies at large amplitudes leave the small-amplitude phonon spectrum we apply bell-shape functions to cut-off a localized mode, i.e., a DB. It is concluded that the results are strongly dependent on the interatomic potentials used in the simulations. Our preliminary conclusion is that it is very difficult to find a DB with in-plane atomic motion, which is supported by the earlier studies [1]. Particularly, we could not confirm the results of the work [2] where the existence of DBs in unstrained graphene was reported. However, following the recent work [3] we were able to excite several DBs with out-of-plane atomic oscillations. Our study calls for additional studies based on ab initio calculations to prove or disprove the existence of DBs in unstrained graphene.

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Variety of discrete breathers in fcc crystals

Elena A. Korznikova[A], **Andrey A. Kistanov**[B], **Sergey V. Dmitriev**[C]

Institute for Metals Superplasticity Problems of RAS, 450001, Khalturina str., 39 Ufa, Russia

e-mail: [A] elena.a.korznikova@gmail.com, [B] dmitriev.sergey.v@gmail.com, [C] andrei.kistanov.ufa@gmail.com

Discrete breathers (or intrinsic localized modes) are spatially localized and periodic in time vibrational modes in defect-free nonlinear lattices, e.g., in crystals. Existence and properties of discrete breathers (DBs) in various crystals attract growing interest of researchers working in solid state physics and materials science. Experimental detection of DBs is a challenging problem and today the main tool for their study is atomistic simulations.

Many metals and ordered alloys have face-centered cubic (fcc) lattice and, for this reason, the study of DBs in such lattice is of practical importance. The first report on DBs in pure metals, including fcc Ni, was done in [1]. The authors found a rod-like DB which spans over a dozen of atoms in one close-packed atomic row. Later it was shown that, e.g., two-dimensional Morse crystal supports at least two types of DBs of different symmetry [2]. This finding poses the question: how many different types of DBs can be excited in three-dimensional crystals? In this work, the results of molecular dynamics simulations are reported to demonstrate that fcc crystals can support a variety of DBs, some of them are stable, others are unstable and typically transform in time to a stable DB.

Presented results demonstrate that even crystals with simple structure such as fcc can support more than one stable DB.

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Properties of discrete quasibreathers and Rosenberg modes in graphene by means of classical and quantum molecular dynamics

Ivan Lobzenko[A], Sergey Dmitriev[B], George Chechin[C], Alexandr Chetverikov[D]

[A]Toyota Technological Institute, 2-12-1 Hisakata, Tempaku-ku, Nagoya, 468-8511 Japan

[B]Institute on Metal Superplasticity problems, 39 Stepan Khalturin street, Ufa 450001 Russia

[C]Research Institute of Physics, Southern Federal University, 194 Stahki Ave.,Rostov-on-Don 344090, Russia

[D]Saratov State University, 83 Astrakhanskaya Street, Saratov, 410012 Russia

e-mail: [A]ivan.lobzenko@gmail.com, [B]dmitriev.sergey.v@gmail.com, [C]gchechin@gmail.com, [D]chetvap@rambler.ru

The density functional method was used for the simulation of symmetry determined nonlinear normal modes [1] and discrete breathers in graphene without strain applied. Along with quantum approach the classical molecular dynamics was used to obtain such dynamical properties of modes as lifetime and frequency on amplitude dependency. It is shown that dynamical properties of nonlinear objects are strongly dependent on the phenomenological potential used for molecular dynamics simulation. Results derived from classical modeling using Tersoff [2], AIREBO [3] and Savin [4] set of the phenomenological potentials are compared with *ab initio* calculation results (by means of density functional method). Such comparison allow to conclude on the legitimacy of the use of Savin potential for modeling nonlinear high amplitude dynamical objects in graphene.

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Role of Intrinsic Localized Modes in Atomic Structures: Trigger of Stone-Wales Defect Formation in Carbon Nanotubes

Takahiro Shimada[A] **and Takayuki Kitamura**[B]

[A,B]Department of Mechanical Engineering and Science, Kyoto University, C3, Kyoto-daigaku Katsura, Nishikyo-ku, Kyoto 615-8540, Japan

e-mail: [A]shimada@me.kyoto-u.ac.jp, [B]kitamura@kues.kyoto-u.ac.jp

The crucial role of intrinsic localized modes (ILMs) or discrete breathers (DBs) in the atomic scale as a trigger of defect nucleation was studied using molecular-dynamics simulations for a (5,5) armchair carbon nanotube (CNT) under axial tension. A localized vibration at a pair of neighboring atoms was found to be the ILM, which simultaneously produces an intense concentration of kinetic energy, even in the structurally homogeneous CNT. The excited ILM was gradually amplified by the nonlinearity of C-C interaction. The amplified ILM, then, drove the breaking of the on-site C-C bond, which leads to the Stone-Wales transformation producing a topological defect consisting of two pentagons and two heptagons coupled in pairs. This signifies that mechanical instability can be activated by the ILMs. Such mechanism is expected to apply to other mechanical instabilities, e.g., as an origin of phase transformations in silicon under hydrostatic pressure.

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Mobile breather scattering in a 2D hexagonal crystal lattice

J. Chris Eilbeck

Department of Mathematics and Maxwell Institute, Heriot-Watt University,
Riccarton, Edinburgh EH9 2LN, UK

We continue our previous studies [1,2] to look at mobile discrete breather-breather *scattering* in a 2D hexagonal crystal lattice model. The system has only one dimensionless parameter, the ratio of the well depths of the interaction potential and the on-site potential, and we investigate the dependence of the breather 2D properties on this parameter value. High values lead to larger spatial displacements in adjacent chains of atoms and thus increase a 2D nature of the quasi-one-dimensional breather solutions. This effect is further investigated during the breather-breather collisions by following the constrained energy density function in time of a set of randomly excited mobile breather solutions. Inline collisions can lead to 60° scattering, and collisions of mobile and stationary breathers at relative angles can lead to a wide variety of states.

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Localized nonlinear excitations in silicate layers

Juan F.R. Archilla

Group of Nonlinear Physics, University of Sevilla,

ETSI Informática, Avda. Reina Mercedes s/n; 41012-Sevilla, Spain, Email: archilla@us.es

Recently the subject of localized nonlinear excitations that leave fossil tracks in silicate layers [|1] have received renewed attention because it was realized that the dark tracks are produced by positive charge and that also negative localized charge transport can be detected [2,3]. This discovery opens the way to understanding an intermediate mechanism for charge transport between ohmic conductivity and superconductivity, called hyperconductivity, for which also there was experimental evidence from long ago in polymers [4] and it is also presently subject of renewed experimental, theoretical and engineering interest [5]. The transport of charge by nonlinear excitations also opens the way to experimentation, which is currently underway at Sevilla University trying to detect significant changes in the extremely low conductivity of mica muscovite when nonlinear localized vibrations are excited through the interaction of alpha irradiation or plasma ions.

In the present communication a review of the present state of the theoretical and experimental research will be presented together with simple but realistic models of nonlinear excitation in silicate layers presenting the different forms of localized excitations with their energies and stability, as kinks [6] and breathers, tentatively relating them to the different observed tracks and the possible relationship with charge transport.

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Mobile discrete breathers and symmetry of pairwise interaction in crystals

Yusuke Doi[A] and Akihiro Nakatani[B]

[A,B]Department of Adaptive Machine Systems, Osaka University, 2-1 Yamadaoka, Suita 5650871, Japan

e-mail: [A]doi@ams.eng.osaka-u.ac.jp, [B]nakatani@ams.eng.osaka-u.ac.jp

Mobile discrete breathers (DBs) or intrinsic localized modes (ILMs) are energy transport phenomena peculiar to nonlinear discrete systems [1,2]. Especially the mobile DB in crystal is an important problem for understanding nonlinear dynamics on an atomic scale in crystals [3,4]. In theoretical systems such as Fermi-Pasta-Ulam (FPU) β lattices, the mobile DBs does not propagate smoothly [5]. For example, the mobile DBs which are kicked by initial perturbations tends to lose its velocity. The velocity of precise numerical solutions of the mobile DBs deviates around its averaging velocity. Recently, a new lattice called a pairwise interaction symmetric lattice (PISL) which supports smooth propagation of the mobile DBs has been proposed [6]. In this work, we discuss an extension of PISL to the generic nonlinear lattice including higher nonlinear terms and long-range interactions which appear in pairwise interaction potentials for describing dynamics of crystal.

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Moving Intrinsic Localized Modes and Its Behavior at Junction between Two Different Lattices

Masayuki Kimura,[A※] Ryo Tsujisaka[B], Yoshiharu Taniguchi[B], Yasuo Matsushita[C], and Takashi Hikihara[A]

[A]Department of Electrical Engineering, Kyoto University, Katsura, Nishikyo-ku, Kyoto 615-8510 Japan
[B]Department of Electronic Systems Engineering, The University of Shiga Prefecture, 2500 Hassaka-cho, Hikone 522-8533 Japan
[C]Advanced Mathematical Institute, Osaka City University, 3-3-138 Sughimoto, Sumiyoshi-ku, Osaka 558-8585 Japan
e-mail: ※kimura.masayuki.8c@kyoto-u.ac.jp

Energy localized state in an anharmonic crystal is known as intrinsic localized mode (ILM) or discrete breather (DB). They are first identified as a spatially localized and temporary periodic solution in Fermi–Pasta–Ulam (FPU) lattice [1]. ILM is usually static in space. However, it is known that perturbing an unstable ILM causes a moving energy localization, namely, a moving ILM [2, 3]. Moving ILM can be considered as a carrier of kinetic energy in lattice. Controlling the energy flow in lattice [4, 5] is important for phonon engineering [6], which enables us to manage heat flow in nano-meter scale devices.

In this work, we first investigate moving ILMs in a mixed lattice of FPU and nonlinear Klein–Gordon lattice, which is derived from a micromechanical cantilever array [7]. Numerically rigorous solutions of moving ILMs are obtained by finding fixed points on the nonlinear map consisting of a Poincaré map and a shift map. The relationship between the velocity and the energy of movement of moving ILM is shown numerically. By using the obtained solutions of moving ILM, we investigate behaviors of moving ILMs at a junction of two different lattices at which a parameter of the lattice is changed step-like. Three different behaviors, namely, reflection, transmission, and acceleration are observed at the junction. The behaviors depend on the energy of movement of moving ILM, parameter gap at the junction, and the direction of the moving ILM. Phenomenologically, an effective energy barrier causes those behaviors. In this work, the barrier height is investigated with respect to parameter gaps. In addition, we demonstrate that the energy barrier can rectify the moving ILM.

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Defects in single-walled carbon nanotubes investigated by atomic force microscopy and its related techniques

Yuji Miyato[A], Kei Kobayashi[B] and Hirofumi Yamada[B]

[A]Dept. of Systems Innovation, Osaka University, 1-3 Machikaneyama, Toyonaka 560-8531, Japan

[B]Dept. of Electronic Science & Engineering, Kyoto University, Katsura, Nishikyo, Kyoto 615-8510, Japan

e-mail: [A]imiyato@sup.ee.es.osaka-u.ac.jp

The electronic transport characteristics of single-walled carbon nanotubes (SWNTs) depend on not only their chirality but also defects. The Stone-Wales defect is known as one of the typical point defects formed in the SWNT lattice, and could be induced from intrinsic localized modes [1]. It is important to investigate property of the defect in order to understand the roles in the electronic transport. We focused on the measurement of local characteristics on SWNTs by using the atomic force microscopy (AFM) and its related techniques, such as Kelvin probe force microscopy (KFM), AFM potentiometry (AFMP) and scanning gate microscopy (SGM). Figure 1 shows one of the measurement results, which was taken by SGM. The SGM image corresponds to distribution of the current change through the SWNT channel, caused by local gating from the probe tip at each tip position during the scan. The current change was observed around the specific point of the SWNT channel as shown in Fig.1 (b). It indicated that a defect was located at this point, and that the electronic transport of the SWNT was mainly dominated by this defect. Thus, AFM techniques are very useful to study the local properties of defects.

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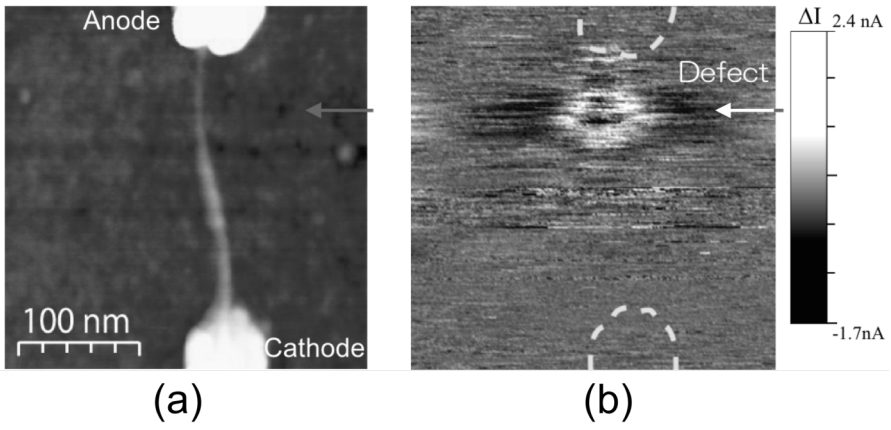

Fig. 1. (a) AFM topographic and (b) SGM images of an SWNT connected to two gold electrodes. In the SGM image, the channel current was mapped during the scan, while applying the bias voltage of 2 V between the electrodes and the tip bias voltage of -3 V.

Existence and stability of odd and even parity discrete breathers in Fermi-Pasta-Ulam lattices

Kazuyuki Yoshimura

Department of Information and Electronics, Graduate school of Engineering, Tottori University

4-101 Koyama-Minami, Tottori 680-8552, Japan

e-mail: kazuyuki@eecs.tottori-u.ac.jp

Discrete breathers (DBs) are spatially localized and time-periodic solutions in nonlinear lattices [1,2]. Two types of fundamental DB modes are known, which have different symmetries in their spatial profiles, i.e., odd and even parity symmetries. The odd and even parity modes are called Sievers-Takeno (ST) mode and Page (P) mode, respectively. In a strongly localized regime, the ST and P modes have the approximate normalized profiles (…, 0, -1/2, 1, 1/2, 0, …) and (…, 0, -1, 1, 0, …), respectively. A fundamental issue concerning DB is existence proof and stability analysis of these modes. However, no existence proof has been given in the strongly localized regime, and also there has been no rigorous result for their stability.

We consider the Fermi-Pasta-Ulam (FPU) lattices described by the Hamiltonian

$$H = \sum_{n=-N}^{N} \frac{1}{2} p_n^2 + \sum_{n=-N}^{N} V(q_{n+1} - q_n)$$

with the periodic boundary conditions. The potential function is assumed to have the form

$$V(X) = W(X, \mu) + \frac{1}{k} X^k$$

where $X \in \mathbf{R}$ and μ is a set of parameters. We place the assumptions (P1)-(P3) on V: (P1) $k \geqq 4$ is an even integer; (P2) W is C^2 with respect to X and μ; (P3) $W(X, 0)=0$. The present potential function includes the case of polynomial potential functions. Under these assumptions, we have proved the existence of ST and P modes in the FPU lattices. Moreover, we have proved that the ST mode is spectrally unstable while the P mode is spectrally stable.

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Confining interparticle potential makes both heat transport and energy diffusion anomalous in one-dimensional phononic systems

Yuriy A. Kosevich and Alexander V. Savin

Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin str., Moscow 119991, Russia

e-mail: yukosevich@gmail.com, asavin00@gmail.com

We provide molecular dynamics simulation of heat transport and energy diffusion in one-dimensional molecular chains with different interparticle pair potentials at zero and non-zero temperature. We model the thermal conductivity (TC) and energy diffusion (ED) in the chain of coupled rotators and in the Lennard-Jones chain either without or with the confining parabolic interparticle potential. The considered chains without the confining potential have normal TC and ED at non-zero temperature, while the corresponding chains with the confining potential are characterized by anomalous (diverging with the system length) TC and superdiffusion of energy. Similar effect is produced by the anharmonic quartic confining pair potential. We confirm in such a way that, surprisingly, the confining pair potential makes both heat transport and energy diffusion anomalous in one-dimensional phononic systems. We show that the normal TC is always accompanied by the normal ED in the thermalized anharmonic chains, while the superdiffusion of energy occurs in the thermalized chains with only anomalous heat transport.

Non-universal heat correlation functions and their anomalous scaling in one-dimensional systems

Daxing Xiong and Jun Zhang

Department of Physics, Fuzhou University, Fuzhou, Fujian, 350108, China

email:phyxiongdxfzu.edu.cn, t10077@fzu.edu.cn

The investigation of heat correlation functions and their scaling behaviors is currently a hot topic in the theoretical research field of thermal transport [1-3]. In this talk we will show some present results on this topic, especially those in certain linear/nonlinear integrable/non-integrable one-dimensional (1D) systems. We will give at least numerical evidences that these heat correlation functions show non-universal shapes [4], and their scaling exponents would undergo a crossover [5, 6] between different universal exponents as predicted by theories [1-3]. In some nonlinear non-integrable systems, we are trying to relate the non-universality and crossover of heat spreading to the properties of discrete breathers (DBs). We would like to show such a viewpoint: the different types of DBs, especially the intra-band and extra-band ones, would have distinct effects on heat correlation functions shapes and also their scaling behaviors.

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Contact geometric approaches to nonlinear RLC circuit lattices in contact with heat bath

Shin-itiro Goto[A]

[A]Department of Applied Mathematics and physics, Graduate School of Informatics,
Kyoto University, Yoshida-Honmachi, Sakyo-ku, 606-8501, Japan
e-mail: [A]goto.shinichiro.5r@kyoto-u.ac.jp

Contact geometry is known to be the odd-dimensional cousin of Symplectic geometry [1], and has been studied from purely mathematical viewpoints. Aside from such viewpoints, contact geometry has also been applied to various mathematical sciences including theory of dissipative mechanical systems, control theory, electromagnetism, thermodynamics, and so on. Recently it was shown in Ref. [2] that information geometry, known as a geometrization of mathematical statistics, and electric circuit theory can be unified with contact geometry by noticing that cumulant generating functions in mathematical statistics and electromagnetic energy functions in circuit theory are convex. Furthermore, hidden mathematical structures were revealed, and entropy production was calculated for some electric circuits without any voltage source. One also notices that the application of contact geometry is not restricted to conservative systems, and that dissipative systems can be analyzed with contact geometry. We then feel that contact geometric methods can deal with conservative (dissipative) nonlinear lattice systems consisting of (R)LC circuit elements, and some mathematical tools developed in contact geometry can be applied to such lattice systems. It is then expected that this analysis can reveal hidden mathematical structures of lattice systems.

In this talk attention is drawn to some applications of contact geometry to nonlinear lattice systems that are consisting of electrical circuit elements whose nonlinearity can be designed with conductors. In particular, after reviewing basics of contact geometry, we talk about our contact geometric formulation of such nonlinear lattice systems, entropy production of lattices in contact with heat bath, similarities among our geometric theory of such lattice systems, thermodynamics and information geometry.

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Wave Propagation in Origami-based Mechanical Metamaterials

Hiromi Yasuda[A] and Jinkyu Yang[A]

[A]Department of Aeronautics and Astronautics, University of Washington,
Guggenheim Hall, Seattle, WA 98195, USA
e-mail: [A]jkyang@aa.washington.edu

We study unique wave propagation in mechanical metamaterials which are composed of origami-based unit cells, specifically Tachi-Miura Polyhedron (TMP) and Triangulated Cylindrical Origami (TCO). The TMP is a bellows-like origami structure, which is known as rigid origami. This means that the deformation of the TMP takes place only along its crease lines, while all facets remain rigid during folding/unfolding. On the other hand, the TCO can be observed as a buckling pattern of a thin-walled cylinder, and it can support both axial and rotational motions. First we simplify these two origami structures to understand their folding behaviors. We introduce a two-bar linkage model to characterize the mechanical response of the TMP under compressive loading, whereas the TCO is modeled as a truss-like structure by removing all facets and replacing crease lines by linear spring elements. Using these simplified models, we examine the static mechanical properties, e.g., force-displacement relationship and total potential energy, of origami cells. By manipulating the initial shape of the structure, we show the tunability of these mechanical properties. Based on the static analysis, we then design origami-based mechanical metamaterials which consist of multiple origami-based unit cells stacked vertically. Our analysis shows that both TMP- and TCO-based system can support a unique type of nonlinear waves under compressive impact, so called rarefaction waves which are characterized by a tensile wave front despite the application of compression. In addition to the rarefaction wave, the origami-based systems exhibit the formation of frequency band structures if two distinctive origami-based unit cells (e.g., different initial folding angles) are stacked in an alternating way. By leveraging these unique behaviors, the origami-based mechanical metamaterials have great potential for engineering devices such as impact absorbers and mechanical wave filters.

Making of air-levitation-type coupled oscillator array and experiments on excitation of intrinsic localized modes

Yosuke Watanabe [A], **Mai Nishimoto** [A] **and Chika Shiogama** [B]

[A] Graduate School of Engineering Science, Osaka University, 1-3 Machikaneyama, Toyonaka 560-8531, Japan

[B] School of Engineering Science, Osaka University, 1-3 Machikaneyama, Toyonaka 560-8531, Japan

e-mail (Watanabe): watanabe@me.es.osaka-u.ac.jp

To demonstrate and observe excitation of intrinsic localized modes (ILMs) [1-3] in macro scale, a mechanical apparatus of coupled oscillator chains has been constructed with designing new nonlinear springs. The experimental apparatus consists of twenty identical oscillators, nonlinear springs, a long and straight air track with a blower and a driver for forcing the chains at one end. The oscillators are connected with neighboring ones through the springs and the chains are supported above the air track. The relation of restoring force of the spring to deflection is approximately cubic and symmetrical with respect to the equilibrium position in the apparatus with appropriate tensions. One end of the chains is fixed and the other is driven sinusoidally in the direction of the chains at a frequency. It has been observed that, driving with a frequency above the cutoff, localized oscillations can be excited intermittently at the driven end and they are propagated along the chains at a constant speed. The FFT shows that the peak of the spectrum of the oscillations is located in the region where linear wave propagations are prohibited, therefore, the localized oscillations can be regarded as the mobile type of ILMs [4, 5].

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Traveling Intrinsic Localized Modes in Nonlinear Driven Damped Lattices

M. Sato[A], S. Shige[A], T. Mukaide[A] and A. J. Sievers[B]

[A]Graduate School of Natural Science and Technology, Kanazawa University
Kanazawa, Ishikawa 920-1192, Japan

[B]Laboratory of Atomic and Solid State Physics, Cornell University
Ithaca, New York 14853-2501, USA

e-mail: msato153@staff.kanazawa-u.ac.jp

In a nonlinear lattice, a nonlinear localized excitation called intrinsic localized modes (ILMs) exist. Traveling ILMs can be generated at a driven-damped condition with a propagating driver. A clean, regular traveling ILM is observed at a certain range of the driver frequency. At ends of the stable frequency region, bifurcations take place. Overall structure of the bifurcations is similar to that observed for a stationary ILM in a micromechanical cantilever array when the driving amplitude is small, while at a higher driving amplitude a resonance effect modifies the higher frequency bifurcation.