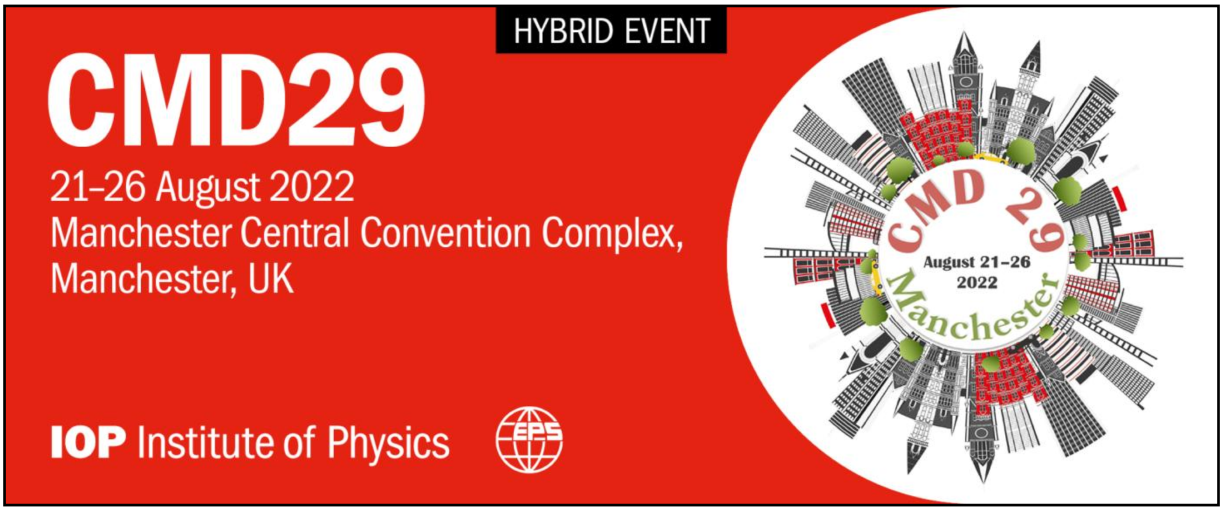

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Book of Abstracts for the mini-coloquium: LONE 2022: Localized nonlinear excitations in condensed matter. Theory and experiments.

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Keywords: nonlinearity, localization, crystals

Summary: If the displacements from the equilibrium positions of some atoms in a crystal are large enough, the linear description is no longer valid. Stationary and travelling solutions are no longer phonons and very often can remain localized a long time. They can be of different types as kinks, solitons, breathers and others. If they transport electric charge they are known as polarobreathers, solectrons and other terms.

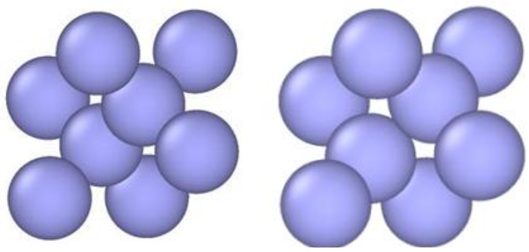
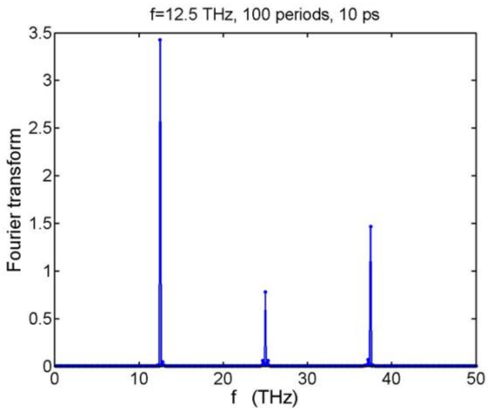
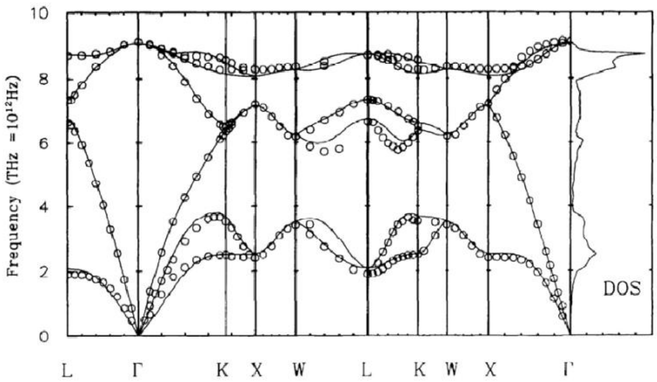


Figure 1. A breather in germanium

The reason for localization is that the frequencies and momenta of a localized excitation do not overlap with the phonon frequencies and momenta. As an example, Figure 1 shows a stationary breather in Ge that involves the out of phase vibration of two atoms and their six neighbours. Figure 2 plots its Fourier spectrum. The single fundamental frequency and its harmonics reveal the periodicity and the nonlinear character of the vibration. The frequencies are well above germanium phonon bands.





Mathematically, the proof of existence of stationary breathers is well established [1]. Moving breathers, typically have a single frequency in the moving frame, where solitons and kinks do not vibrate [2]. Breathers have been obtained using molecular dynamics [3] and ab initio molecular dynamics [4]. They can experience elastic scattering in simulations [5]. Experimentally, moving localized excitations can be stimulated by ion bombardment [6] and if they transport charge, the current can be measured [7]. Their signature appears in neutron spectroscopy [8].

We need more theory to predict properties that can be measured and more measurements where nonlinear localization appears. Among them: spectroscopy, interaction with defects and phase transitions, electric currents, carrier density, production by plasmas and ions. This is the objective of the minicolloquium.

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Programme LONE 2022: Localized nonlinear excitations in condensed matter. Theory and experiments.

Abstracts

Novel thermalization classes of weakly nonintegrable many-body systems

Sergej Flach

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter IX, August 25, 2022, 11:30 AM - 12:30 PM

We propose a novel framework to characterize the thermalization of many-body dynamical systems close to integrable limits using the scaling properties of the full Lyapunov spectrum. We investigate macroscopic weakly nonintegrable lattice dynamics beyond the limits set by the KAM regime. We perform our analysis in two fundamentally distinct long-range and short-range integrable limits which stem from the type of nonintegrable perturbations - weak two-body interactions (nonlinearities) versus weak lattice coupling (hopping). Long-range limits result in a single parameter scaling of the Lyapunov spectrum, with the inverse largest Lyapunov exponent being the only diverging time control parameter and the rescaled spectrum approaching an analytical function. Short-range limits result in a dramatic slowing down of thermalization which manifests through the rescaled Lyapunov spectrum approaching a non-analytic function. An additional diverging length scale controls the exponential suppression of all Lyapunov exponents relative to the largest one.

Engineering electrical lattices to support resonant, gap, or edge localized modes

Lars English

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter IX, August 25, 2022, 11:30 AM - 12:30 PM

The unit cell properties, crystal structure, and coupling characteristics of electrical lattices can be tailored to make them hosts for a variety of nonlinear localized excitations. Here we explore three examples through experimental measurements and numerical simulations: (a) resonant localized modes in a lattice with second-neighbor interactions exhibiting oscillatory wings, (b) bright and dark localized modes in the bandgap of a diatomic lattice, and (c) edge localized modes in a finite two-dimensional honeycomb lattice near the Dirac points in frequency.

Charge transport in materials by mobile nonlinear inter-atomic interactions called quodons.

Francis Michael Russell

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter X, August 25, 2022, 2:00 PM - 3:30 PM

The transmission of charge by mobile, highly-localized, nonlinear lattice excitations through various materials including polymers and metals is reported. The excitations, called quodons, are created by collisions of swift particles with a material. Filters made of PTFE allow separation of conduction-currents from quodon-currents. This allows study of the existence and propagation of quodons in metals and semiconductors. Demonstration of ability of quodons to propagate across interfaces of different materials revealed their pervasiveness. This suggested the structure and stability of a quodon is not critically dependent on the structure of the material. The cause and sources of free-charges in a material that are trapped by quodons are revealed in time-resolved spectra of the quodon-currents. It was found that significant fractions of quodon-currents can be short-circuited or blead to ground by insulators used in coaxial cables and connectors. This can result in complete loss of quodon-current to ground by even a short length of coaxial cable connecting to a current meter. This loss can be minimized by use of magnetic levitation or vertical hanging of samples from a current-meter. However, this does not eliminate loss to ground potential by insulating material used in the input connector of a current meter. These losses pose a serious problem in exploiting the exceptional properties of quodons for practical applications to power transmission systems. So far, transmission of quodons can only be stopped by inserting in a circuit, or a supporting structure, a gap containing a gas or vacuum. This limitation is not surprising as quodons are similar to phonons as both involve inter-atomic interactions. This suggests the possibility of using multiple layers of materials of very different density and atomic mass to impede quodons. Nevertheless, it is possible to construct a practical source of quodons to exploit their ability to anneal defects or, at higher intensities, cause structural damage to organic materials such as DNA. One such device is described. Finally, it is expected that quodons will be created copiously in devices involving swift ions, such as potential fusion reactors.

Multi-class classification of crystal lattice waves

Jānis Bajārs, Filips Kozirevs

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter X, August 25, 2022, 2:00 PM - 3:30 PM

Recently in [1] we proposed data-driven machine learning algorithms for classification and detection of lattice waves in one-dimensional crystal lattice models. Linear and nonlinear kernel Support Vector Machine classifiers (SVCs) [2, 3] were trained to differentiate between linear phonon and nonlinear localized waves, also known as intrinsic localized modes (ILMs) or discrete breathers (DBs), based on locally sampled data of particle displacements, momentum and energy density values. Efficiency of classification algorithms was further improved by two dimensionality reduction techniques, i.e., principal component analysis (PCA) and locally linear embedding (LLE) [2]. Motivation of this work stems from the open and challenging problem of study and detection of localized energy transport by lattice excitations in numerical simulations of muscovite mica crystal models [4, 5, 6]. Such phenomenon is also supported by laboratory experiments [7]. Proposed methods were analyzed and successfully applied to multiple discrete breather simulations to detect localization regions. Machine learning algorithms were able to detect ILMs in crystal lattice simulations. In general, developed methodology extends to any one-dimensional crystal lattice model which supports localized wave solutions. In this work we have extended SVCs to multi-class problem where we are able to differentiate between linear phonon waves, stationary and propagating DBs. We explored dimensionality reduction techniques PCA and LLE and observed that it is not sufficient in multi-class problem to reduce data dimensionality to two dimensions, therefore, classification algorithms such as linear and nonlinear kernel SVCs should be trained in high dimensional spaces. Trained multi-class classifiers in combination with sliding window object detection method are applied to discrete breather collision numerical simulations. Not only the localization regions are detected, but the particular type of localized waves is identified as well.

Jānis Bajārs acknowledges support from PostDocLatvia grant No.1.1.1.2/VIAA/4/20/617.

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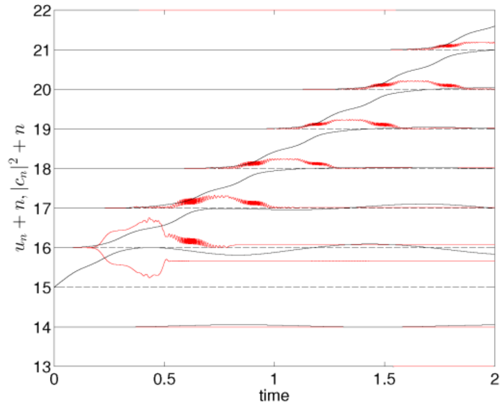
Polarokinks and polarobreathers in a model for silicate layers

Juan Archilla, Janis Bajars, Yusuke Doi, Masayuki Kimura

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter X, August 25, 2022, 2:00 PM - 3:30 PM

It has been observed in fossil tracks and experiments in mica muscovite and other layered silicates that the transport of charge through the cation layers sandwiched between the silicate tetrahedra-octahedra-tetrahedra layers [1].
Lattice kinks or crowdions imply the movement of the cation in the K+ layer and therefore the transport of charge at supersonic speed. Single crowdions and double crowdions with no radiation have been found in [2,3]. The energy of single crowdions is large, about 26 eV and could be a good candidate for primary tracks in muscovite. There are however fainter tracks, called secondary tracks, scattered from the primary tracks that should have much smaller energies of the order of tenths of eV. Moving exact breathers with such energies have also been found in [4]. However, they do not transport charge.
If a K+ ion loses an electron, for example by beta- decay of the nuclei, or other causes, it can be described as the creation of a trapped positive hole. Within an insulator, the probability of the hole to be transferred to another ion is very low but a relatively large vibration enhances enormously the probability of transmission [5]. In this way a travelling anharmonic vibration can trap a hole and move along the lattice.
This charged vibration can be a polarokink, that is a kink or crowdion trapping an extra hole as seen in the figure.



A kink is called a crowdion because it is basically a moving interstitial, which in an ionic crystal implies a moving charge. Therefore, a polarokink transports two units of charge. It should be noted that an electric current, as measured in hyperconductivity experiments, needs this extra charge because electrons have to move through the metal contacts and wires. The anharmonic vibration can also be a breather trapping a hole, that is a polarobreather.
We study the conditions of the transfer integrals for travelling anharmonic vibrations and their properties, analyzing which are more consistent with the experimental results.

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Nonlinear Waves in Fully Nonlinear Mass-in-Mass FPUT Chains

Jonathan Wattis, Reem AlMarashi

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XI, August 25, 2022, 4:30 PM - 6:00 PM

We present and analyse a generalised Fermi-Pasta-Ulam-Tsingou chain in which every node contains a resonator which coupled nonlinearly to the outer shell, and each outer shell is coupled nonlinearly to its two nearest neighbours. The asymptotic analysis results in four cases, depending on the form of nonlinearity of each interaction. Three cases reduce to the nonlinear Schrodinger equation, and one to a form of the Complex Ginzburg-Landau equation. We present numerical simulations of the system, showing breathers, kinks, and breather-kink combinations; we consider both stationary and moving modes. Whilst some of the predicted forms are clearly unstable, many appear to be stable, or at least extremely long-lived.

Nonlinear bandgap transmission in a discrete flat-band lattice

Alain Bertrand Togueu Motcheyo, J. E. Macias-Diaz

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XI, August 25, 2022, 4:30 PM - 6:00 PM

We consider a cross-stitch lattice [1,2] modelled by coupled time-dependent discrete nonlinear Schrödinger (DNLS) equation. The study of the linear equations reveals the presence of the additional frequency which is not a function of the wave vector in the Brillouin zone. By considering one complex wave component proportional to another, we depict the homoclinic connection of the 2D map [3,4] helps to understand the types of the gap solutions present in the lattice. Contrary to the longitudinal dust grain oscillations in dusty plasma crystals [5], the train of bright soliton (see FIG. 1) generated by driving the lattice with a periodic source is carried by a travelling kink

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Nonequilibrium non-Markovian steady states in open quantum many-body systems: Persistent oscillations in Heisenberg quantum spin chains

Regina Finsterhoelzl, Manuel Katzer, Alexander Carmele, Andreas Knorr

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XI, August 25, 2022, 4:30 PM - 6:00 PM

We investigate the effect of a non-Markovian, structured reservoir on an open Heisenberg spin chain by applying coherent time-delayed feedback control to it. The structured reservoir couples frequency-dependent to the spin chain and therefore induces a memory, thus the spin chain interacts partially with its own past. We demonstrate that with this new paradigm of non-Markovian temporal driving scheme, it is possible to generate persistent oscillations within the many-body system and thus induce highly non-trivial states which dynamically store excitation within the chain. These oscillations occur at special points in the stability landscape and persist for different chain lengths and different initial excitations within the chain. We propose a non-invasive partial characterization of the chain by exploiting the fact that the different trapping conditions which arise each relate to specific steady states within the chain.

Standing and traveling discrete breathers in bcc crystals

Yusuke Doi, Akihiro Nakatani

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XII, August 26, 2022, 9:00 AM - 10:00 AM

Discrete breathers excited by nonlinearity and discreteness are expected to be applied as atomic-scale energy localized modes in crystals. In particular, it is expected to understand and apply the phenomena as an energy transport mechanism in the lattice, which is different from phonons. In this study, we investigate the dynamics of discrete breathers in a BCC crystal model using numerical simulations based on molecular dynamics simulations. Two types of standing DB with different spatial symmetries are found by molecular dynamics simulation and the Newton-Raphson method used as temporal evolution. We investigate not only the localized core but also the structure of the surrounding atoms, and investigate the relationship between the spatial symmetry of the crystal structure and the spatial symmetry of the vibrational displacement. A traveling DB, which propagates at a constant velocity through the system, is also found by the Newton-Raphson method. The obtained numerical solution of the traveling DB is demonstrated to propagate stably for a certain period of time, even when used as the initial condition for larger system sizes. Furthermore, the stability and localized energy of standing DBs are evaluated and their relationship with DB mobility is investigated. We will also investigate how to provide a perturbation to generate a mobile DB from a standing DB.

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Nonlinear supratransmission in a magnetically coupled elastic rods arranged in three lines

Masayuki Kimura, Jung-Jin Lee, Alain Bertrand Togueu Motcheyo, Shinji Doi

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XII, August 26, 2022, 9:00 AM - 10:00 AM

Nonlinear supratransmission in lattices is known as a kinetic energy transfer in which moving localized vibrations are carriers [1]. For nonlinear lattices, standing localized vibrations also exist. They are called intrinsic localized modes (ILMs) or discrete breathers (DBs) and have been widely investigated theoretically and experimentally [2].
We focus on moving/standing ILM/DB in magnetically coupled elastic rods arranged straightly which is inspired by the two-dimensionally arranged pendula with permanent magnets [3]. Each elastic rod can move not only along the axis of the array but also perpendicularly to the axis. Two types of standing ILM/DB are numerically identified. One vibrates along the axis and the other mainly vibrates transversally. The former is called longitudinal ILM (L-ILM) and the latter transverse ILM (T-ILM) in this research. It is numerically revealed that the L-ILM loses its stability when the amplitude becomes large, which is similar to the L-ILM in the flexible Fermi-Pasta-Ulam lattice [4]. The instability of L-ILM may affect the stability of moving ILM generated by the sinusoidal excitation at the end of the array. The large amplitude excitation generates moving ILMs, but they decay immediately. To suppress the instability, we added two resonators array to surround the transmitting line of moving ILMs. Although the effect of surrounding arrays is weak, it is observed that the rather large amplitude moving ILM can travel long distances without decay. Interestingly, it is found that the surrounding arrays make the T-ILM stable. We will discuss the effects of the surrounding arrays on both standing and moving ILMs.

Acknowledgments
This work is partially supported by JSPS Kakenhi No. 18K04020 and No. 21K03935.

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Experimental and numerical study on excitation and interaction of nonlinear localized oscillations in a mass-spring chain

Yosuke Watanabe, Yusuke Doi

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XII, August 26, 2022, 9:00 AM - 10:00 AM

Nonlinear localized oscillations excited and propagated in a mass-spring chain are studied. Letting the mass at one end of the chain driven sinusoidally at high frequency and large amplitude, localized oscillations can be excited intermittently near the end and propagated down the chain one after another at a constant speed. This phenomenon is known as supratransmission [R. Khomeriki, et al., Phys. Rev. E 70 (2004) 066626; F. Geniet and J. Leon, Phys. Rev. Lett. 89(13) (2002) 134102]. We have experimentally observed the supratransmission by a mechanical mass-spring chain which emulates the Fermi-Pasta-Ulam (FPU) one of beta type [Y. Watanabe, et al, Phys. Lett. A 382 (2018) 1957-1961]. At one end of the chain the device to drive the end sinusoidally in the direction of the array is attached and at the other end the chain is simply fixed. Keeping driving the end at a high frequency, we can observe that the localized oscillations excited at intervals propagate down the chain one after another and reflect at the fixed end. Our experimental results show that, the higher the driving frequency is, the longer the time intervals of excitations of localized oscillations become. (In the case that driving frequency is higher than threshold, no localized oscillations are excited.) When taken the value of driving frequency near the threshold, it may be possible for us to observe the collisions or interactions between two independent localized oscillations. In this study, we consider the behavior of the collisions and compare the experimental results with the numerical ones.

Modeling of dynamics of nonlinear wave propagation in phononic crystals

Jun Takayanagi

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XIII, August 26, 2022, 10:00 AM - 11:00 AM

Metamaterials are getting greater attention for their property which can be used for wide applications. Among them, one of the most attracting characteristics of metamaterials is existence of band gap. For example, phononic band gap (PnBG) appears in phononic crystals (PnCs), which is a type of artificial structure in which a scatterer made of a hard material is embedded in the base of a soft material. Moreover, new properties have been realized by applying nonlinear dynamics in metamaterials. For example, it has been reported that the PnC can realize switching behavior by combining the PnBG and nonlinear wave propagation. This structure is called switching structure (SS). The SS has a structure in which the PnC scatterers are partially replaced with structures with different property. The switching behavior at which wave does not propagate when the amplitude of the wave is increased at certain frequency, is expected to be applied to logic gates. However, in order to put the SS to practical use, it is necessary to understand the mechanism of this nonlinear behavior. In this study, we construct a dynamics model of PnCs and the SS to understand this nonlinear behavior.

The model consists of mass points and linear springs. To represent the difference in material properties between the background and the scatters, mass of the scatter mass points is multiplied by 10 times and similarly spring constant of the adjacent springs is by 1000 times compared to them of the background. Moreover, nonlinearity is added to the model by changing the mass of each mass point in response to the displacement of the mass point.

We perform frequency response simulations in the model. In this simulation, a forced vibration is applied to the one end of the model to investigate how the wave propagation behavior changes in response to the frequency of forced vibration. The numerical results shows that the vibration propagated only near the natural frequencies of the model. It is also confirmed that a band gap is realized in the model in the frequency range where no natural frequency exists (f = 0.26-0.32 [Hz]). Moreover, Fourier analysis of these results show that the frequency distribution disperses in proportion to the distance from the one end of the model, but that only the frequency components near the natural frequency propagate. And, dispersion curve of this model indicates existence of band gap near this frequency band (f = 0.26-0.32 [Hz]), which shows validity of the model.

Nonequilibrium spintronic transport through Kondo impurities

Anand Manaparambil, Andreas Weichselbaum, Jan von Delft, Ireneusz Weymann

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XIII, August 26, 2022, 10:00 AM - 11:00 AM

Spin and electronic transport through Kondo impurities under equilibrium conditions can be well described using the numerical renormalization group. This method is not directly applicable, though, for describing non-equilibrium transport through such Kondo impurities while treating the correlations exactly. We implement a recently-developed hybrid technique combining the Numerical Renormalization Group (NRG) and time-dependent Density Matrix Renormalization Group (tDMRG) methods in a thermofield quench framework.
In particular, we theoretically investigate the electronic transport through a quantum dot coupled to ferromagnetic leads under finite potential bias conditions. The behavior of the zero-bias conductance peak - exhibited by Kondo impurity systems - has been thoroughly studied against the influence of spin polarization on the leads and other external parameters. We observe a characteristic reduction in the Kondo energy scale when the impurity orbital level is at the particle-hole symmetry point, and a suppression of the zero-bias conductance due to the emergence of an exchange field when the impurity is tuned out of the particle-hole symmetry point. We further analyze the behavior of the split-Kondo peak - formed when exchange field is greater than the Kondo energy scale - against external parameters, such as magnetic field and temperature. Our work provides quantitatively accurate results for nonequilibrium behavior of quantum dot spin valves that may serve as a benchmark for future theoretical and experimental research.

This work was supported by the Polish National Science Centre from funds awarded through the decision No.2017/27/B/ST3/00621.

Interactions of solitons with a localized impurity in Schrödinger lattices with saturable nonlinearity

Joël François Tsoplefack, Jesus Cuevas-Maraver, Faustino Palmero Acebedo, Astero Provata, Dimitri Frantzeskakis

MC39: LONE 2022 - Localized Nonlinear Excitations in Condensed Matter XIII, August 26, 2022, 10:00 AM - 11:00 AM

We study the interactions of moving discrete solitons with a localized impurity in periodic systems described by the discrete nonlinear Schrödinger equation. The localized impurity is modeled by the delta function. Numerical simulations of collisions between moving solitons and the impurity show that the soliton can be transmitted, reflected, trapped or scattered by the imputity during the interaction, depending on the velocity of the incoming soliton and the impurity strength. The trapping of soliton is explained by resonance between the soliton and the nonlinear impurity mode. For different values of the soliton frequency ranging from ω= 0.1 (high amplitude) to ω=0.9 (small amplitude), we elucidate in details as a function of impurity strength and soliton initial velocity, the different regimes of soliton-impurity interaction (pure trapping, pure transmission, pure reflection, reflection and transmission, trapping and transmission, trapping and reflection, and trapping with reflection and transmission). We observe that as the soliton frequency increases towards 0.5, the trapping region becomes larger, and becomes narrower when it increases from 0.5 to 0.9. We determine specific values of impurity strength and soliton initial velocity for which the incoming soliton is split equally into a reflected and transmitted parts (for ω=0.7 and ω=0.9), and for which we observe the phenomenon of "double" trapping and "simple" transmission followed by "simple" trapping and "double" transmission (for ω=0.3).