LONE2023: Localized Nonlinear Excitations in Condensed Matter. Experiments and theory.

Mini-coloquium within CMD30, the 30th Conference of the Condensed Matter Division of the European Physical Association. Milan, Italy, September 4-8, 2023.

Organizers:
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Keywords
Nonlinear localized excitations. Energy and charge transport. Disordered systems

Abstract

Localized excitations appear in different systems in condensed matter as crystals, polymers, and biological systems. The combination of nonlinearity and discreteness produces localized waves known as kinks, solitons, and breathers. When they transport electric charge they are known as quodons, polarons, solectrons, or polarobreathers. They have been obtained mathematically, but also with classical molecular dynamics and ab initio molecular dynamics.

An easy method to produce nonlinear waves is through bombardment with alpha or other particles. Created nonlinear excitations produce the ejection of an atom at the opposite side of a crystal, and hyperconductivity, i.e., and electric current in the absence of an electric field. The possibility of serious negative effects induced by this type of charge transport in tokamak fusion reactors need to be addressed and evaluated.

Spectral theory is an efficient tool for analyzing exact solutions and interpret neutron spectroscopy. Wavelet analysis is useful for detecting transient localization. For nonlinear waves transporting charge the difference in time scales between electrons and atoms brings about the need of developing numerical methods that conserve all the properties of the physical system.

Biological systems are also of particular interest. For example, enzymes catalyze biochemical reactions that are essential to life often through rate-promoting vibrations localized at the active sites that couple to the reaction coordinates, thus increasing the reaction speed by many orders of magnitude.

We need novel theories and mathematical methods to predict properties that can be measured and more experimental proofs of localization. Among relevant topics one may list spectroscopy, interaction with defects and phase transitions, electric currents, carrier density, and production by plasmas and ions. This is the objective of the mini-colloquium.

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Speakers (alphabetical order)

CMD30 FisMat2023 - Submission - View

Abstract title: Spectral properties of exact stationary and moving polarobreathers

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Abstract

We have developed a semiclassical, tight-binding model for the transfer of an electron or hole between ions in a layered silicate which is also an insulator without free states in the conduction and valence bands a large band gap. The transfer probability increases exponentially when ions became closer allowing the coupling of vibrations and electron transfer. We have solved the problem of the large different time scales between electron and ions movement using powerful algorithms that are symmetric, symplectic and conserve the charge probability at each integration step [1], reproducing the physical properties of the system and the analytical properties of the model. We have been able to obtain breathers, that is, localized vibrations that when coupled to a charge are called polarobreathers. They can be stationary with long-life and they can also travel long distances. We obtain approximate ones using specific but simple initial conditions and using them as a seed obtain exact polarobreathers that reproduce their profile after an integer number of sites called the step, extending the theory developed for exact breathers without charge [2,3].The frequency-momentum spectrum of the lattice, the charge probability and the charge amplitude are related but show different frequencies. For the exact polarobreathers there is a fundamental period which is multiple of both the fundamental periods of the three quantities. These quantities have also different steps, that is, the number of sites when a function is repeated. We developed methods to deal with the invariance of the charge amplitude under multiplication by exp(-i mu t), one of them based on the density matrix theory. The results allow for a precise description of exact polarobreathers and advance the possibility for identification in real systems. They can also explain the phenomenon of hyperconductivity observed experimentally in layered silicates, which consists of the transport of charge in absence of an electric field when the crystal is bombarded with alpha particles [4-7].

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Abstract title: Soliton mechanism of the long-range electron transport in donor--acceptor systems mediated by polymers

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Oral presentation/Poster (Author's request): Oral presentation (invited)

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Abstract

Dedicated to 50 years of the Davydov's soliton. 50 years ago A. Davydov and N. Kislukha have published the paper on self-trapping of a molecular excitation in a soliton state in a 1D molecular chain with account of the electron-lattice interaction [1-3]. This work has initiated an intensive research of nonlinear localized modes in LD systems. It was extended to the case of electron self-trapping and used to explain dissipativeless energy and electron transport in biological and solid state systems. Physical systems include donor and acceptor molecules mediated by polypeptides, polymers or other semiconducting molecular chains, and the question if soliton mechanism can work in such complex systems remained to be open. Here the results are reported on the modeling of the long-range electron and energy transfer mediated by Davydov's solitons formed in a molecular one-dimensional chain [4] or in an α-helix three-spine polypeptide chain [5] coupled to donor and acceptor molecules at opposite ends. It is shown that there exists the broad interval of the parameters for which an electron initially located on the donor, can tunnel onto the chain forming a soliton-like state in it, which then travels to the opposite end, where it is captured by the acceptor. It is shown that when the donor and acceptor molecules are coupled to all three spines, the efficiency of the electron transport from donor to acceptor can reach 90%. For polypeptide parameter values this process is proved to be stable at physiological temperatures.These results explain highly efficient long-range donor-accepor electron transport in redox reactions in photosynthesis and cellular respiration in biological systems, and in donor-acceptor systems mediated by various types of long molecular chains, widely used in modern microelectronics and nanotechnologies (see, e.g., [6-8] and references therein). [1] A.S. Davydov, N.I. Kislukha, Phys. Stat. Sol. B **59** (1973) 465.[2] A.S. Davydov, Solitons in Molecular Systems. Dordrecht, Reidel, 1985.[3] A.C.Scott. Phys. Rep. **217** (1992) 1.[4] L. Brizhik, B. Piette, W. Zakrzewski, Phys.Rev. E 90 (2014) 052915[5] L.S. Brizhik, J. Luo, B.M.A.G. Piette, W.J. Zakrzewski, Phys. Rev. E, **100** (2019) 062205.[6]Y. Tan, R. Y.Adhikari, N.S. Malvankar, et al., Small, 12 (33), 4481-4485, (2016).[7] N. L. Ing, M.Y. El-Naggar, A.I. Hochbaum, J. Phys. Chem. B 122, 10403-10423, (2018)[8] Z-F. Yao, J.-Y. Wanga, J. Pei, Chem. Sci., **12** (2021) 1193-1205.

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Abstract title: Hidden Landscapes of Protein Functions

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Oral presentation/Poster (Author's request): Oral presentation (invited)

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Abstract

This presentation explores the emergence of biomolecular functions, such as catalysis and intramolecular communication in proteins, through a wave-based approach. By analyzing the vibrational responses of protein structures to environmental temperature fluctuations, we demonstrate that topological irregularities arising from protein folding lead to anisotropic dissipation of thermal energy by phonons. This process generates a networked entropy flow across distinct domains within the protein. Building on this understanding, we identify functionally significant residues using an in silico method that employs a mathematical tool called the localization landscape. Our computational approach has the potential to significantly advance drug design, therapeutic strategies, and the development of biomimetic materials in the field of solid-state physics.

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Abstract title: Noise-induced sine-Gordon breathers in ac-driven long Josephson junctions: Emergence and detection

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Abstract

We observe the formation of remarkably stable sine-Gordon breathers, for a sufficiently high temperature, in ac-driven long Josephson junctions. Both the breather generation probability and the energy spatial correlations are demonstrated to behave nonmonotonically versus the thermal noise strength, which represents a powerful control parameter. We then discuss the reliability of the approach for different breathing frequencies, as well as the influence of both topology and noise on the full counting statistics of the number, position, and amplitude of the excited breathers. Based on these findings, we show that the breather induces peculiar oscillations into the junction's resistive switching characteristics, i.e., we find a clear experimental signature of the elusive solitonic excitation.Reference: D. De Santis, C. Guarcello, B. Spagnolo, A. Carollo, D. Valenti, Chaos, Solitons and Fractals 170 113382 (2023)

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Abstract title: Thermalization Universality Classes for Weakly Nonintegrable Many-Body Dynamics

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Oral presentation/Poster (Author's request): Oral presentation (invited)

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Abstract

We observe different universality classes in the slowing down of thermalization of many-body dynamical systems upon approaching integrable limits. We identify two fundamentally distinct long-range and short-range classes which stem from the type of nonintegrable perturbations - weak two-body interactions (nonlinearities) versus weak lattice coupling (hopping) [1,2,3]. We study the scaling properties of the full Lyapunov spectrum [4,5]. The long-range class results in a single parameter scaling of the Lyapunov spectrum, with the inverse largest Lyapunov exponent being the only diverging time control parameter and the rescaled spectrum approaching an analytical function [4]. The short-range class results in a dramatic slowing down of thermalization and a rescaled Lyapunov spectrum approaching a non-analytic function. An additional diverging length scale controls the exponential suppression of all Lyapunov exponents relative to the largest one [4].

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Abstract title: Traveling Localized Vibrations Generated by an External Exciter Attached to an Edge of a Mass-spring ladder with Piecewise Linear Coupling

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Abstract

Moving intrinsic localized mode (moving ILM), which is also called moving discrete breather (moving DB), plays a crucial role in energy transfer in a nonlinear regime [1]. Nonlinear supratransmission is one of the nonlinear energy transfer phenomena in which moving ILMs are generated at the edge of a nonlinear mass-spring ladder with a frequency outside the phonon band of the ladder [2,3]. The supratransmission is also experimentally observed in a mechanical system in which masses are coupled by a piecewise linear spring [4,5]. In this study, we numerically investigate where the moving ILMs are generated by an external exciter attached to the mass-spring ladder with piecewise linear coupling in the frequency-amplitude plane of the exciter. As reported in Refs. [4,5], the region where several moving ILMs are individually generated is found outside the phonon band. In addition, traveling localized vibrations which are not separated from each other are observed inside the band. We will discuss the mechanism of how the traveling localized vibrations occur inside the band.**Acknowledgments**This work is supported by JSPS Kakenhi No. 21K03935(MK), No. 17K05577(YW), and No. 23K03582(YW).**References**[1] S. Flach, A.V. Gorbach, Phys. Rep. 467, 1 (2008).
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Abstract title: Localized states in low-dimensional materials and nanostructures

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Abstract

Periodicity and non-interacting particle approximation formed the basis for understanding electron, phonon, and other linear wave excitations in bulk solids. In perfect crystal lattices, Bloch states in allowed energy/frequency bands and forbidden gaps determine basic material properties. General solutions are linear combinations of eigenmodes so that transport properties are mainly determined by the linear spectrum. In spatially periodic systems, the existence of extended eigenmodes implies that initially localized wave packets will generally disperse. However, when electron-phonon, electron-electron and other interactions are included, nonlinearity is introduced, linear superposition breaks down and self-trapping phenomena emerge. For instance, exact spatially localized solutions, the discrete breathers (DBs), may appear with frequencies in the gaps of the linear spectrum, trapping finite amounts of energy. While their general mathematical theory is well developed, DBs physical manifestations and implications in periodic crystals are still under investigation in condensed matter and materials physics, photonics, cold atoms, etc. On the other hand, when periodicity is broken, localized states due to defects and disorder have been studied extensively. A strongly disordered system is characterized by a purely discrete linear spectrum with localized eigenmodes (Anderson localization). Then, initially localized wave packets do not spread and there is no energy diffusion. When nonlinearity is introduced in these systems, mode interactions change the nature of localization. The interplay of disorder and nonlinearity results in non-trivial and complex phenomena. We will present theoretical and computational results on localization and self-trapping in nanostructured, defected, and disordered systems with emphasis on specific quasi-1D and 2D nanostructures which are related to recent developments in the field of materials of atomic thickness, such as graphene and transition metal dichalcogenides.Support by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the “1st Call for H.F.R.I. Research Projects to support Faculty Members & Researchers and the Procurement of High-cost research equipment grant” (project number 1303) is acknowledged.

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Abstract title: Burgers turbulence in the Fermi-Pasta-Ulam-Tsingou model

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Oral presentation/Poster (Author's request): Oral presentation (invited)

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Abstract

We prove analytically and show numerically that the dynamics of the Fermi-Pasta-Ulam-Tsingou chain is characterized by a transient Burgers turbulence regime on a wide range of time and energy scales. This regime is present at long wavelengths and energy per particle small enough that equipartition is not reached on a fast timescale. In this range, we prove that the driving mechanism to thermalization is the formation of a shock that can be predicted using a pair of generalized Burgers equations. We perform a perturbative calculation at small energy per particle, proving that the energy spectrum of the chain decays as a power law. We predict that the exponent of the power-law takes first the value 8/3 at the Burgers shock time, and then reaches a value close to 2 within two shock times. This value of the exponent persists for several shock times before the system eventually relaxes to equipartition. During this wide time window, an exponential cutoff in the spectrum is observed at large wavenumbers, in agreement with previous results. Such a scenario turns out to be universal, i.e. independent of the parameters characterizing the system and of the initial condition, once time is measured in units of the shock time.

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Abstract title: Role of quodons in irradiation of materials

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Oral presentation/Poster (Author's request): Oral presentation (invited)

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Abstract

Quodons are mobile, highly localized, nonlinear excitations created by swift particles colliding with atoms in condensed matter. As they exist and propagate in a charge-neutral environment, there is no practical way for them to be studied individually in situ. However, they can bond with a positive or negative unit of charge, which enables them to be observed and thus studied. To first order, they behave like very stable nano-scale atomic shock-waves that can propagate great distances in any material and are independent of temperature. This is how evidence of their existence was found first in metastable crystals of the insulating mineral muscovite, in which their paths were made visible by triggering precipitation of an impurity. This led to them being interpreted initially as intrinsic localized modes of discrete particles, in particular optical mode discrete breathers. Since they require energetic individual collisions of swift particles with atoms, as opposed to collective excitation, they are created naturally by cosmic rays, radioactivity and high energy physics apparatus.
The ability of quodons to transport charge at near sonic speed over large distances at any temperature suggested use in a hyperconducting cable with an insulating sheath. This prompted the study of quodons in electrically insulating materials such as PTFE and nylon. Irradiation of a sample of PTFE with He ions of up to 5 MeV energy showed hyperconductivity could occur in solid polymers, as indicated in the figure. The near instantaneous drop of current and subsequent rise caused by interrupting irradiation shows the measured current is not due to progressive build-up of an emf in the sample. The fact that quodons can transport charge in absence of an applied emf in an electrical insulator of very high resistivity enabled separation of hyperconduction from conduction currents by use of the triple filter technique. This allowed study of quodon propagation in metals and other condensed materials. It also allowed study of the transmission of quodons across interfaces between the same or different materials. It showed that quodons can spread easily in complex physical devices, but cannot exist under gaseous or vacuum conditions. One consequence is that charge carried by quodons is short-circuited to ground through the insulation in coaxial cables. Special isolation procedures are thus needed for measurement of quodon current in experiments.
These results showed that quodons will be created in any process involving collisions due to scattering of swift particles propagating through any material. They will be produced in any apparatus involving relativistic particles and especially in both nuclear fission and fusion reactors. Their main benign effect in fission reactors is to help anneal radiation damage. In tokamak fusion reactors they will present significant hurdles to achieving commercial electrical generation.

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Abstract title: Breathers in two dimensional triangular Klein-Gordon lattices

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Oral presentation/Poster (Author's request): Oral presentation (invited)

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Abstract

We outline the form of breather modes in a two-dimensional triangular lattice in which each node is coupled linearly to six nearest neighbours and experiences a nonlinear onsite potential. Atoms at nodes are allowed to move in both directions within the plane of the lattice. The resulting system has the form of a Klein-Gordon lattice, for which we find the dispersion relation - which has two surfaces that meet at Dirac points. We extend the asymptotic analysis to find expressions for second order correction terms and the resulting two dimensional nonlinear Schrodinger equation. We obtain ellipticity and focusing criteria required for the existence of fully localised breather modes. We illustrate the dynamics with numerical simulations.

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