Monday, 7

Introduction: The soliton concept and the new world of computational/experimental nonlinear science and beyond

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I plan to survey features of solitons as an overview of the extraordinary ubiquity of the soliton concept with particular emphasis on the passage from the study of waves in fluid physics to new avenues of research in electron transport phenomena in solid state physics.

Solitons and solectrons and the mechanical control of electrons (electron surfing)

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The concept “solectron” which is surveyed here, is much younger than the soliton concept. It has been developed in the first years of this century in the group of Manuel G. Velarde in Madrid and had from the very beginning its roots in the idea that electrons and currents may be enhanced by interaction with solitonic excitations. Starting with solitonic excitations on dissipative active rings, the investigations went to thermally excited solitons in solids and in polymer-like lattices including their interaction with added conduction electrons. We shall show how currents may be enhanced in driven active as well as in passive thermally excited lattices by interaction with the solitonic excitations. The early studies of one-dimensional lattices (lattice rings) were in last years extended to two-dimensional systems (surface lattices including graphene-type systems).

Electrons in Molecules: Solitons and polarons in dopable conducting polymers

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Theoretical studies performed by the group of MG Velarde et al from 2006 have shown that a 1-dimensional array of N sites coupled by a non-linear potential and able to accept oneelementary charge (“N sites-1 e^-“ problem) can be the siege of deformations propagating with shape conservation (solitons) and even the association of an electron and a moving deformation (solectron). The question addressed here is what kind of

molecular system could present this behavior. A simple idea would be to consider chains of a (dopable) conducting polymer such as polyacetylene. However such a chain has a "dirty" structure, and more annoying, it is a "N sites-(N+1) e^-" system which is subject to Peierls distortion, and for which the distortion associated with the Solectron is different from the one predicted by the above theory.

By contrast, polydiacetylene (PDA) is a "cleaner" material due to its crystallinity, purity and independence from a doping process. Moreover, earlier results by the E G Wilson group strongly suggest that solectrons could be generated in this material. However, in order to get back to the "N sites-1 e^-" problem, the price to pay is to consider a site as made of not only one atom but a C_4H_2 chemical moiety. It is then necessary to add at least one internal degree of freedom on each site, describing the geometrical consequence of the addition or removal of one electron. In the language of Solid State Physics, this corresponds to the coexistence of two electron-photon coupling mechanisms: an intersite coupling (Peierls) and an intrasite one (Holstein). This model will be discussed and compared with similar models in literature, in particular the earlier theoretical treatment of Wilson et al, with the aim of arriving at realistic values of the parameters.

Solitons and solectrons: Computer simulations

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Methods of computer simulations based on numerical integration of classical motion equations and stochastic differential equations of the Langevin type in combination with the quantum Schrodinger equation are considered in problems on localized nonlinear excitations in both one-dimensional (1d) and two-dimensional (2d) lattices of anharmonically interacting particles. Also methodologies for treatment of results of computer simulations (computer experiments) and procedures to calculate different characteristics of processes studied will be discussed.

First, peculiarities of numerical solutions of motion equations by the Runge-Kutta 4-th order algorithm as applied to a chain of particles bound to each other by the Morse forces will be analysed to study characteristics of supersonic solitons. Numerical solutions of the Langevin equations will be analysed to investigate the dynamics of a Morse chain under heating.

Procedures to solve equations of motion and the Schrodinger equation in different 2d lattices (triangular lattice, quadratic lattice, hexagonal lattice, combined lattices like in cuprates) will be presented. The evolution of characteristics of quasi-one-dimensional solitons, plane-wave solitons, horse-shoe like solitons and lump solitons will be analysed.

Problems of transport of charged particles by solitons (solectrons) in both 1d and 2d lattices are observed (computer experiments) and numerical methods to treat them will be suggested. In particular, the problem about control of direction of electron surfing on solitons along the crystallographic axes of 2d lattices via excitation of other (controlling) quasi-1d solitons will be considered.

Bisolitons and bisolectrons

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It has been shown that in a relatively soft molecular lattice two extra electrons (holes) with antiparallel spins form a bound bisoliton state at intermediate values of electron-lattice coupling, when the adiabatic approximation is valid [1,2]. Such a state corresponds to two elelctrons self-trapped in a single potential well formed by the lattice deformation. If the potential energy of the inter-site interactions in the lattice is harmonic, bisolitons are stable at velocities less than the velocity of the sound in the chain. With bisoliton velocity increasing the bisoliton energy increases, it becomes more and more narrow, respectively, the deformation of the lattice becomes stronger and the harmonic approximation in the description of lattice vibrations ceases to be valid. We shall show that the lattice anharmonicity stabilizes bisolitons and results in the formation of bound bisolectron states [3-4] which is stable in the whole range of sonic and supersonic velocities. Such a bisolectron propagates along the chain practically without energy dissipation and is an ideal charge carrier in quasi-one-dimensional molecular systems with moderately strong electron-lattice coupling [5, 6]. Bisolitons and bisolectrons are expected to play a signficant role in the charge transport in redox processes in living organisms during respiration or photosynthesis. They seem to exist and be responsible for the relatively high electroconductivity of some conducting polymers and other low-dimensional systems. They can also be formed in organic superconductors and high-temperature superconducting materials which possess highly anisotropic physical properties.

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Solitons and "discrete breathers" (intrinsic localized modes in crystals)

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In a pedagogical manner the concepts of such nonlinear excitations in crystals as ***discrete breather*** (DB, otherwise ILM) [1] and ***crowdion*** will be introduced and conditions of their existence and stability will be discussed. DB is a group of atoms in a defect-free crystal, performing oscillations of large amplitude [2]. Theoretically, in the absence of thermal vibrations and other perturbations, DB does not radiate energy and can last forever. This occurs because DB frequency is outside the range of small-amplitude vibrations of the crystal lattice. In the real world lifetime of DB is finite, but it can be hundreds or thousands of oscillation periods. DB arises in crystals due to thermal fluctuations, by irradiation or by exposure to high-frequency external fields. DB accumulates energy of about 1 eV, can be mobile, transferring this energy over long distances. Crowdion is an interstitial atom which can also move along the close-packed atomic row but with a supersonic speed. Basic properties of DB and crowdions in crystals of different nature will be presented. Based on the analysis of the available theoretical and experimental data, contribution of DB and crowdions to energy and mass transfer in crystals will be discussed. It will be shown that, very likely, DB and crowdions are responsible, at least partly, for such well-known and

poorly understood effects as electro-plasticity, relaxation of metal structure after severe plastic deformation by a pulsed electrical current, reduction of the yield strength of the metal by electron beam irradiation, etc. Arguments in favor of the fact that the role of DB and crowdions is enhanced under conditions far from thermodynamic equilibrium will be presented. The presentation will be ccompleted with a list of open problems and directions for further theoretical and experimental studies on DB (ILM) and crowdions in crystals.

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Solitones, respiradores discretos y resaltos en cristales iónicos

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Recientemente las excitaciones no lineales localizadas que dejan huellas fósiles en capas de silicatos laminares [1] han recibido renovada atención, debido a que se ha observado que las marcas oscuras son producidas por cargas positivas y que igualmente el transporte de carga negativa localizada también puede ser detectado [2,3] . Este descubrimiento abre el camino a la comprensión de un mecanismo para el transporte de carga intermedio entre la conductividad óhmica y la superconductividad, llamado híper-conductividad, del cual también hay evidencia experimental desde hace tiempo en polímeros [4]. El interés no es sólo experimental y teórico sino también debido a sus potenciales aplicaciones en ingeniería [5]. El hecho de que las excitaciones no lineales transporten carga permite el trabajo experimental tratando de detectar cambios significativos en la extremadamente baja conductividad de la mica moscovita cuando las vibraciones no lineales localizadas son excitadas mediante irradiación de iones.

Expondremos en primer lugar el estado actual de la investigación teórica y experimental. En segundo lugar, presentaremos modelos sencillos pero realistas de las capas de silicato en las que aparecen excitaciones localizadas, calculando sus energías y estabilidad. Estas pueden ser tanto resaltos (kinks) como respiradores (DB, breathers) [6], que se puede intentar relacionar con las diferentes marcas observadas y con el transporte de carga.

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Tuesday, 8

Experiments with solitons and intrinsic localized modes

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Solitons have been predicted and observed in almost all scientific disciplines. In some systems, however, the experimental demonstration of solitons is challenging, and in spite of the theoretical studies supporting the existence of solitons, they are still hard to observe. The detection task may be impossible when the system is too complex, its dimensions are too small, or the theoretical understanding about the system is still incomplete. In such cases, analogue models may help in the quest for solitons. We shall introduce the concept of analogue and toy models in physics, and how they can be used to understand the dynamics of more complex systems. Two examples will be discussed. First, the dynamics of a gas micro-bubble cavitating in an ultrasonic field will be discussed. A macro-mechanical analogue of bubbles is then proposed, where solitons of different types emerge easily and their properties can be studied in detail. The analogy with real gas micro-bubles is demonstrated by different approaches. The second example is a system of charged particles interacting by repulsive forces, which is the basic model of crystalline

matter in solid state physics. A toy model based on an array of macroscopic magnets will be used to discuss the existence of propagating solitary perturbations such as kinks and crowdions.

Nano-soliton-assisted electron transport (electron surfing) and a novel ballistic-like field effect transistor (SFET) with extremely low heat dissipation

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A ballistic solectron, comprising a lattice soliton with an associated electron, was discovered, (accidentally), by Donovan and Wilson in 1981 [1]. They found, by experiment, a photocarrier to travel at a velocity close to the sound velocity, when pulled by an electric field. However, the velocity was independent of field, even over 4 decades of field. Moreover, at the lowest field, the velocity was greater than what would be found in any semiconductor at the same field. (In conventional semiconductor language, the low field mobility was ultra-high, > 20 $m^2\ s^{-1}\ V^{-1}$). The carrier had thus a low dissipation of energy to the lattice. The carrier was ballistic. This Solectron was found on the backbone of a polydiacetylene (PDA) crystal. The backbone is made of π conjugated carbon chains. The chains are long, straight and parallel for macroscopic distances. The lowest electronic excitations belong to the backbone chains. The chains are separated by a (electronically) large distance (0.7 nm). Thus they form ideal one dimensional semiconductors. Optical absorption above the band gap (2.4 eV) created electron and hole photo-carriers. It is the ideal one dimensionality which leads to the extraordinary transport properties found.

A model of the Solectron was presented [2] which described the motion as that of an electron trapped within the lattice distortion that it has created, the whole moving together. An estimate of the energy loss to the lattice of a moving solectron was found to be ultra-small; insufficient to prevent the solectron increasing its energy (but not its velocity) at the smallest fields used (10^2 V/m). It was concluded this was the beginnings of an explanation of the experimental results. A further model of the solectron has been presented in 2014 by the group of Velarde (Velarde, Chetverikov, Ebeling, Wilson, and Donovan [3]). It is important that a solectron of thermal energies kT (25 meV) already has a velocity approaching that of sound [2].

It is natural to consider if a device can be created which uses the solectron transport properties. A solectron Field Effect (SFET) has been proposed by Velarde and Wilson [4]. Consider source (S) and drain (D) conducting electrodes evaporated onto the surface of a PDA crystal. Consider, further, that the work functions of the S and D allow either electron or hole injection into the PDA in thermal equilibrium. Then it is anticipated that thermal solectrons, of either electron or hole character, are launched, with velocity approaching the sound velocity, along the chains from beneath the electrodes, in thermal equilibrium, in the absence of any applied fields. (Space charge then returns the carriers to their origin). The SFET is created when an insulator, thickness d, and a conducting gate electrode (G) are evaporated. The gate voltage V_G then controls the charge, and hence the S to D current, I_{SD} in the channel between S and D.

The potential advantage over the conventional silicon FET is twofold. First, the SFET can work at very low power supply voltages V_0, $V_0 = kT/e$ = 25 mV. Nevertheless, the response time can be fast. This reflects the ballistic properties of the solectron. Secondly, the gate insulator thickness, d, can by large. This reduces the gate to channel capacitance C, which is proportional to (1/d). In contrast, in the silicon FET the gate insulator thickness has to be small in order to control the carrier density in the channel. Both these factors are important when considering the energy cost of switching bits in the inverters of computer chips, for the energy cost per bit is $C \times (V_0)^2$. Possible energy consumption reductions of several orders of magnitude in a proposed SFET chip compared to present silicon microprocessor chips, while retaining the operating speed, will be described.

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Action potentials as solitons in neuro-dynamics

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Mathematical formulation of biological processes is a major scientific challenge that should be met in order to design biologically inspired machines. In the context of the nervous system, three main processes are currently tackled for modelling: neurotransmitter release at the synapse, signal transmission within the neuron and signal integration by neural circuits. While the first challenge has been met with reasonable success, the second and third ones have not. The concept of soliton offers some hope to formulate the transmission of action potentials along the neuron in mathematical terms. Some features, however, need to be incorporated in the formulation of solitons before the concept can be applied to model action potential dynamics. Briefly summarized, these are: 1) Action potentials at bifurcation points, 2) Abrupt extinction of action potentials, 3) Bursting versus tonic action potential firing regimes, and 4) Component heterogeneities and fluidity changes along the neuron plasma membrane. We will review these basic features of neuron physiology and the current status of the attempts to accommodate them into the formulation of solitons/soliton-like.

Modos solitónicos simulando la marcha de insectos (hexápodos)

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Mostraremos la relación que tienen dos conceptos en principio distintos: La propagación de solitones por un anillo de osciladores y la locomoción animal, en particular la de insectos (hexápodos). Para ello introducimos los conceptos básicos de solitones en una red/anillo de Toda y añadimos un sistema de bombeo-disipación de energía tipo Rayleigh, de forma que aquellos se mantengan aún con disipación.

Se analizarán los modos de caminar de los cuadrúpedos y hexápodos y su red de nodos neuronales responsables de los modos de caminar, CPG de su sigla en inglés: Central Pattern Generators. Comparando los nodos neuronales con los solitones de la red de Toda podremos definir el movimiento de un robot hexápodo basado en la propagación de esos solitones.

En un paso más, las propias patas y motores de las mismas podrían actuar como osciladores del anillo de Toda generando ellas mismas los modos de caminar adecuados, es decir las patas forman parte del CPG. Estamos ahora en el caso de “inteligencia” distribuida donde los movimientos no son almacenados en la memoria de algún ordenador central (o cerebro superior), sino que son las propias patas, bajo las leyes de Newton, las que generan los movimientos. En esta última fase, la generación del modo de caminar se hace con la intervención del entorno a través de la pata del robot.

Ondas y solitones gravitatorios: predicciones

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Los solitones son soluciones de ciertas ecuaciones de onda no lineales que se comportan en algunos aspectos como partículas extensas. En el año 1967 Gardner, Greene, Kruskal y Miura introducen una técnica conocida como “Inverse Scattering “para resolver dichas ecuaciones. En el año 1978 Belinski y Zakharov extendieron dicha técnica a la solución de las ecuaciones no lineales de Einstein para el campo gravitatorio, bajo ciertas restricciones. A partir de ahí se encontraron un gran número de soluciones exactas que se denominan genéricamente solitones gravitatorios. Algunas de estas soluciones describen perturbaciones en fondos cosmológicos, otras representan ondas gravitatorias cilíndricas, algunas describen ondas gravitatorias planas y su interacción no lineal, destacan también las soluciones de Schwarzschild y Kerr que describen los agujeros negros más generales que se pueden formar por colapso gravitatorio. Presentaré estos temas junto con un repaso a las principales características de la teoría de la gravitación de Einstein, empezando con el principio de equivalencia.

Gravitational waves and solitons: Detection

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Solitons were introduced by Zabusky and Kruskal in 1965. Kruskal has also made important contributions to gravitational physics. First, the behavior of the event horizon of a black hole was best understood after the introduction of Kruskal and Szekeres coordinates in 1960. Second, the robustness of the black hole formation by the collapse of a star was best understood by using asymptotic techniques to account for the generation of gravitational waves by quasinormal modes based, in part, on the asymptotology introduced by Kruskal in 1962. And third, black holes are 2-soliton solutions of the Einstein equations in vacuum, as discovered by Belinski and Zakharov in 1978. They extended the so-called inverse scattering method of Gardner, Greene, Kruskal and Miura (1968-1974) and the dressing operator method of Zakharov and Shabat (1972). Both mathematical

methods were introduced to understand the robustness of solitons under mutual interactions and perturbations.
The scientific breakthrough of 2016 is the direct detection of the gravitational waves produced in the fusion of two black holes into a fast-rotating black hole thanks to both detectors of the Laser Interferometer Gravitational-Wave Observatory (LIGO). Gravitational waves are linear phenomena, however, the cylindrical gravitational waves introduced by Einstein and Rosen (1936-1938) are soliton solutions as discovered by Belinski and Zakharov. Moreover, the fusion of black holes can be understood as the pairwise interaction between gravitational 2-soliton solutions. In fact, the exact solutions for the interaction of N black holes can be written as a 2N-soliton solution. In contrast to the standard elastic interaction between solitons, the interaction between gravitational solitons can result in their coalescence, with the generation of quasinormal modes and the corresponding emission of gravitational waves. Surprisingly, by means of the black hole fusion, gravitational waves are a linear phenomena intrinsically related to soliton theory.