ABSTRACTS

PLENARY TALKS

Superstatistical techniques for complex systems with time scale separation

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Many complex driven nonequilibrium systems are effectively described by a superposition of several statistics on different time scales, in short a 'superstatistics'. Superstatistical techniques have been successfully applied to a variety of complex systems, for example turbulence (Lagrangian, Eulerian, environmental), hydroclimatic fluctuations, pattern formation, mathematical finance, traffic delay statistics, random matrix theory, networks, scattering processes in high energy physics, cancer survival statistics, and foreaging animals. In medical and biological applications superstatistics often arises out of the fact that populations are heterogeneous, in this way complexity arises out of the mixing of simple Markov processes at individual level. In this talk I will first give a general overview of the superstatistics concept and its recent applications. I will then explain how to extract the relevant superstatistical parameters out of a given experimentally measured time series. Finally I will show how to formally map superstatistics onto a complicated equilibrium statistical mechanics by means of an exotic effective Hamiltonian.

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Quasi–Stationary Chaotic States in Multidimensional Hamiltonian Systems

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We study numerically statistical distributions of chaotic orbit coordinates, viewed as independent random variables, in weakly chaotic regimes of three multi–dimensional Hamiltonian systems: Two Fermi–Pasta–Ulam (FPU–β) oscillator chains with different boundary conditions and number of particles and a microplasma of identical ions confined in a Penning trap and repelled by mutual Coulomb interactions. For the FPU systems, we show that, when chaos is limited within "small size" phase space regions, statistical distributions are well approximated, for surprisingly long times (typically up to $t \approx 10^6$), by a q–Gaussian ($1 < q < 3$) distribution function and tend to a true Gaussian ($q = 1$) for longer times, as the orbits eventually enter into "large size" chaotic domains of phase space. In the case of the microplasma Hamiltonian, we make use of these q–Gaussian distributions to identify: (a) a low–energy range of "weak chaos", over which the system "melts" and the q–index of the distributions attains a maximum $q \approx 1.8$ returning quickly to the $q = 1$ (Gaussian) value and (b) a wide energy range, over which a "liquid to gas" transition occurs, where q rises again, reaching $q \approx 1.4$ at $E \approx 50$, before returning slowly back to $q = 1$, at higher energies $E > 200$.

Quantum thermometers: Thermalization and ergodicity in many-body quantum systems

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The emergence of canonical ensembles in quantum

statistical mechanics from first principles is one of the key remaining old questions of theoretical physics. Even the definition of the temperature at the nanoscale poses a challenge. Indeed, how precisely the canonical distribution arises from dynamical laws, without a priori statistical assumptions, is still unclear. Our results provide evidence that quantum chaotic systems do thermalize, that is, they exhibit relaxation to an invariant ergodic state.

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Spectral Renormalization Group Theory on Networks

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We set up a renormalization group scheme by expanding an arbitrary scalar field living on the nodes of an arbitrary network, in terms of the eigenvectors of the normalized graph Laplacian [1]. The renormalization tranformation involves, as usual [3] the integration over the more "rapidly varying" components of the field, corresponding to eigenvectors with larger eigenvalues, and then rescaling. The critical exponents depend on the particular graph through the spectral density of the eigenvalues, as is also found for real space renormalization group schemes [2].

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Dynamics of Complex Systems with an emphasis on Criticality and Record Dynamics

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Complex systems consisting of many interacting components often exhibit intermittent irregular dynamics.

The paradigm of Self-Organised Criticality emphasises systems in a stationary state created by the action of a slow external constant driving rate. SOC postulates that the driven system self-organises to a critical state. In the critical state the system is expected to exhibit abrupt releases of energy in the form of macroscopic events termed avalanches. The focus is on the probability distributions of the even sizes, which are presumed to be scale free power laws in the limit of infinite system size. Candidates for SOC are e.g. earthquakes, rain, forest fires and many others.

The scenario of Record Dynamics is concerned with non-stationary and non-critical complex systems undergoing relaxation in order to release a (generalised) internal strain induced at the moment of preparation. The rate of activity decreases as one over time and the distribution of event times follows a Poisson process in logarithmic time. The events sizes can follow any distribution. Systems, which appear to follow the log-Poisson, include spin-glasses, over-damped relaxing particle models, models of long time macroevolution and experiments on dynamics of ant colonies. Log-Poisson relaxation can also be related to onset of synchronisation.

Is there a Climate Network – A Backbone of the Climate System?

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We consider an inverse problem: Is there a backbone-like structure underlying the climate system? For this we propose a method to reconstruct and analyze a complex network from data generated by a spatio-temporal dynamical system. This technique is then applied to reanalysis and model surface air temperature data. Parameters of this network, as betweenness centrality, uncover relations to global circulation patterns in oceans and atmosphere. We especially study the role of hubs and of long range connections, called teleconnections, in the flows of energy and matter in the climate system. The global scale view on climate networks offers promising new perspectives for detecting dynamical structures based on nonlinear physical processes in the climate system.

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Systematic Identification of Order Parameters in Biophysical Systems

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Cooperative couplings between degrees of freedom in biophysical systems lead to effective dimensionalities far less than the $3N$-dimensional coordinate space of the N constituent atoms, suggesting that the underlying dynamics of the system may be characterized by a relatively small number of order parameters. This effective reduction in dimensionality has been framed as a separation of timescales, whereby the fundamental dynamics reside in a "slow subspace" to which the other degrees of freedom are slaved. Geometrically, the slow subspace may be considered a - possibly highly convoluted - low-dimensional hypersurface, termed the "intrinsic manifold", to which the dynamics are effectively constrained. In this work, we apply a nonlinear dimensionality reduction technique known as the *diffusion map* [1] to systematically extract the intrinsic manifolds, and good order parameters with which to parameterize them, for a variety of systems of biophysical relevance.

N-Alkane chains in water are well-studied systems of interest to the biophysical community as models for the role of hydrophobicity in protein folding. We have conducted solvated and ideal-gas phase simulations of C_8, C_{16} and C_{24} n-alkane chains, and applied diffusion maps to the simulation trajectories to extract approximately three-dimensional intrinsic manifolds. In the case of C_8, we find the dihedral angles to be good order parameters with which to describe transitions between local free energy basins. For the longer chains, we extract three global order parameters describing the underlying dynamics: the degree of chain collapse, the location of a bend in the chain and the handedness of the chain helicity. The dynamic relevance of the intrinsic manifolds furnished by the diffusion map approach allowed us to determine the low-free energy collapse pathway for solvated n-alkanes to proceed by a "kink and slide" mechanism.

Over 100ns of replica exchange molecular dynamics simulations of the linearized form of the 21-residue antimicrobial "lasso" peptide MicrocinJ25 (proMccJ25) in explicit solvent were conducted, and diffusion maps applied. We determined two global order parameters for the dynamics, well-correlated with the Glu8 Ψ angle and the identity of the residue at the β-hairpin turn, and identified three distinct folding pathways from the global free energy minimum: hydrophobic collapse, folding into a left-handed lasso, or formation of an "unwrapped lasso". Interestingly, although the peptide spontaneously adopts a left-handed lasso conformation, the native peptide - in which the lasso is covalently "sealed" in place by a post-translational modification enzyme - has a right-handed topology. These results suggest a role for the maturation enzymes, or leader sequence of the peptide precursor, in facilitating the folding process.

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Phase transitions in the presence of quenched disorder

Nicolas Sourlas
Ecole Normale Superieure

I will discuss the validity of perturbative renormalisation group in the presence of quenched disorder.

Similarity between brittle fracture and financial crisis: How can we introduce plasticity in financial world ?

Hideki Takayasu
Sony Computer Science Laboratories and Meiji Institute for Advanced Study of Mathematical Sciences

Concepts and mathematics developed in material science can be applied to finance. In this talk I will focus on occurrence and avoidance of financial crisis in view of brittle fracture and plastic deformation.
Brittle fracture and financial crisis have many features in common:

1. The system looks strong before the occurrence of a breakdown.

2. Potential stress tends to concentrate on a weak point.

3. A breakdown occurs suddenly based on a threshold rule.

4. A breakdown induces successive breakdowns.

5. The failure causes an irreversible damage to the whole system.

In order to get rid of fragility from the financial world, it is necessary to introduce plasticity by any means. In this talk I will introduce a new way of financing without using fixed interest rate by taking into account the statistical properties of business firm growth rates.

The structure and statistical properties of Japanese business firm network

Misako Takayasu
Tokyo Institute of Technology, Japan

Network structure of about 1 million business firms in Japan is studied by analyzing a comprehensive database. It is found that link numbers follow a power law distribution showing that the network is a typical scale-free type. The exponent of the power law of the cumulative distribution is about 1.3 with the mean link number 4.5. Other basic quantities such as PageRanks, degrees of hub and authority, distribution of pair distance are also observed.
We can construct a dynamic model of business firm network by modeling the processes of birth, death and merger of business firms. It is shown that the model converges to a statistically steady state in which most of the network properties are reproduced.

Thermodynamic derivation of entropy of complex systems

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Following a thermodynamical argument - i.e. understanding the consequences of bringing interacting systems in thermal contact - we derive a two-parameter entropy. It is shown to cover practically all interacting and non-interacting statistical systems. The corresponding distribution functions are explicitly presented. Special regions in the two-parameter space correspond to Boltzmann-Gibbs statistics, Tsallis statistics and regions characterized by stretched exponential distribution functions. To our knowledge the proposed method can be seen as a first derivation of generalized entropies from first thermodynamical principles.

Nonadditive entropy and nonextensive statistical mechanics - Recent predictions, verifications and applications

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A plethora of natural, artificial and social systems exist which defy Boltzmann-Gibbs (BG) statistical mechanics in the sense that they do not satisfy the basic requirements for its validity. These are, for classical systems, ergodicity, positive maximal Lyapunov exponent (sufficient but not necessary for ergodicity), Markovian mesoscopic processes, and equivalent ones. Such complex systems can be handled in a variety of manners. However, if we wish to follow a statistical mechanical path, it appears to be necessary the use of nonconventional entropies such as the nonadditive one $S_q \equiv k\frac{1-\sum_i p_i^q}{q-1}$ ($q \in \mathcal{R}$; $S_1 = S_{BG} \equiv -k\sum_i p_i \ln p_i$). Important properties such as thermodynamical extensivity and finite entropy production per unit time can be achieved by tunnig the index q on precise values which reflect the dynamical/geometrical structure of occupancy of the Γ phase space (or Hilbert or Fock spaces, if quantum) of the system or, more precisely, of its nonextensivity universality class. This fact has also implications for the corresponding attractors in the sense of the Central Limit Theorem (q-generalized in [1, 2]). In addition to these conceptual aspects [3, 4], various recent predictions, verifications and applications will be briefly presented as well, in particular the recent ones achieved in the LHC and Brookhaven accelerators [5, 6, 7].

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INVITED TALKS

The functional instability of native DNA

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With the discovery of the double helix structure of DNA, by Watson and Crick in 1953, the topological problem, arising from the need of the double helix to unwind in order to replicate, was recognised as an issue of primary concern. This point was resolved only 25 years later, with the advent of topoisomerases. Meanwhile, the great stability of DNA helix was documented, as a supercoil packed within the nucleosome structure in the chromosomes. At the same time a wide array of functional sites in the DNA topography were discovered, that need to undergo destabilization in order for the major cell functions to be accomplished. Such destabilisable sites are Origins of DNA replication and Promoters -enhancers-silencers of DNA transcription into RNA, that are the sites of actions for general or specific DNA binding proteins. Furthermore, it is currently understood that not only the genes that code for protein, rRNA and tRNA but almost the whole of the genome is transcribed. There is intergenic transcription as well as transcription for the production of a high number of small nuclear RNA molecules that are regulators of gene expres-

sion. This whole complex system poses a challenging task for the recognition of the destabilisable DNA sites that are involved in the regulation of transcription. Additionally, the regulation of transcription is only part of the regulation of gene expression program that specifies the cell type and developmental stage at which a gene is expressed (is allowed to produce the product that is coding for). The gene expression process is closely associated with the nuclear architecture and nuclear scaffold/matrix, through another type of destabilisable DNA site the so -called Scaffold and Matrix Attachement Regions (S/MAR). The functional instability of DNA sites like origins of replications, promoters and other transcription DNA elements and S/MARs often is not entirely a property of the site itself, but it also depends on other sequences along the same DNA molecule. The knowledge of the destabilization potential of these elements is of crucial importance for the experimental design of DNA structures, such as DNA plasmids and artificial chromosomes. Such DNA structures are used for the gene transfer into cells and are required to be able to direct their own DNA functions. The use of such elements will be discussed, within the context of formulating gene transfer vectors for gene therapy strategies.

Non-Hamiltonian Chaos from Nambu Dynamics of Surfaces

Minos Axenides
NCSR Demokritos, Attiki, Greece

We extend the framework of Nambu Mechanics to include dissipation in R3 phase space. We demonstrate that it accomodates the phase space dynamics of low dimensional dissipative systems such as the much studied Lorenz, Roosler as well as many other Strange attractos. In all cases the rotational, volume preserving part of the flow preserves in time a family of two intersecting surfaces, the so called Nambu Hamiltonians. They foliate the entire phase space and are, in turn, deformed in time by Dissipitation which represents their irrotational part of the flow. The latter is given by the gradient of a scalar function . The interplay of the all three surfaces defines the chaotic flow and is responsible for the emergence of the Strange Attractor.

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[2] M. Axenides and E. Floratos, *JHEP*, **0902**:039, (2009).

Self-organization in dissipative optical lattices

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We show that the transition from Gaussian to the q-Gaussian distributions occurring in atomic transport in dissipative optical lattices can be interpreted as self-organization by recourse to a modified version of Klimontovich's S-theorem. As a result, we find that self-organization is possible in the transition regime, only where the second moment is finite. Therefore, the nonadditivity parameter q is confined within the range $1 < q < \frac{5}{3}$, although whole spectrum of q values i.e., $1 < q < 3$, is considered theoretically possible. The range of q values obtained from the modified S-theorem is also confirmed by the experiments carried out by Douglas et al. [1]

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Finding a partner: Effect of gift

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People are seeking for a partner for date. While trying to find a suitable partner, they look for some criteria. Are there any criteria that are indispensable for people? Are these criteria subject to change according to the personal difference of people? Are there differences between men and women? We analysed a web based dating network of 286,786 men and 226,512 women in Turkey. We found that there are gender asymmetries. Men and women have different criteria. Some criteria are crucial for both men and

women; however, some criteria are only valuable for men or women. It is observed that giving gifts turns out to be an important creteria in decision making.

Dilute magnetic semiconductors: combined density functional theory and quantum Monte Carlo approach

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We use the Haldane-Anderson model to discuss the substitution of transition-metal impurities into semiconductors. We study this model with the Hirsch-Fye Quantum Monte Carlo (QMC) technique in the dilute limit. The QMC results show that the occupation of the impurity bound state plays an important role in determining the nature and the range of the magnetic correlations between the impurities [1] in agreement with the Hartree-Fock predictions [2]. In order to make direct comparisons with the experimental data, we combine the Density Functional Theory (DFT) with the QMC technique. In particular, we first use the density-functional theory to calculate the host band structure and the impurity-host hybridization matrix elements, which are input parameters for the Haldane-Anderson model, and then perform the QMC simulations with these realistic model parameters [3]. For the case of (Ga,Mn)As, the DFT+QMC approach leads to an impurity bound state located 100meV above the top of the valence band in agreement with the experimental value of 110meV. In addition, we observe an anisotropic distribution for the local density of states at the impurity-bound state energy, which is consistent with the STM data. Hence, we think that the DFT+QMC approach is a useful tool for performing realistic calculations for the various compounds of dilute magnetic semiconductors.

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Vibrational Behavior of Metal Nanowires under Tensile Stress

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We have investigated the vibrational density of states (VDOS) of ultrathin Cu nanowires with $< 100 >$ and $< 111 >$ axial orientations and considered the effect of axial strain. The VDOS are calculated using a real space Green's function approach with the force constant matrices extracted from interaction potential based on the embedded atom method. Results for the vibrational density of states of a strain-free nanowire show quite distinctive characteristics compared to that of a bulk atom, the most striking feature of which is the existence of high frequency modes above the top of the bulk spectrum. Taking the specific example of the 5×5, H5 types and pure Cu nanowires at their 0K ground state configurations, we show that the existence of high frequency modes above the top of the bulk phonon spectrum is a reflection of the reduced dimensionality of the system rather than being an end effect of contamination or temperature. Through the projection of the total VDOS on local atoms of the wire, we identified the leading contributors to the enhancement of the modes at low and high frequencies: while the anomalous low frequency modes are primarily moderated by corner atoms, the aberrant high frequency modes are dominated largely by center atoms. In contrast to the case of helical nanowires, the existing aberrant high frequency modes shift to higher frequencies upon stretching the nanowire. However, the vibra-

tional behavior at low frequencies remains almost the same with increasing axial strain. We, additionally, find that while the high frequency band above the top of the bulk phonon shifts to higher frequencies, the characteristics at low frequencies remains almost the same upon stretching the nanowire along the axial direction. More interestingly, these characteristics are found to be independent of the axial direction of the wire.

This work has been supported by the Scientific and Technological Research Council of Turkey - TUBITAK under Grant No. 109T105. Computations were carried out through the National Center for High Performance Computing, located at Istanbul Technical University, under Grant no. 20132007.

Quantum Information Devices and the problem of Decoherence. Some results from toy models

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Quantum Information is the manifestation of quantum coherence as this is involved in the creation of entangled quantum states. Entanglement is a resource that can be stored and manipulated with special arrangements of quantum systems, the quantum information devices. But the original quantum property of coherence is very fragile under the influence of environmental perturbations. Thus the loss of coherence in a very short time makes these quantum devices useless. As it is impossible to completely isolate a quantum system from its local or global environment, there is a great effort either to algorithmicly correct random errors, or to engineer the local environment for increasing the decoherence time. Since the problems become graver with the increase of the quantum system (problem of scalability) and the possibility to simulate a big quantum system is fundamentally impossible (Feynman's Thesis), it is necessary to investigate these difficulties with specific toy models that capture the essential problems. In this talk we present some results from few simple models which can represent a quantum device in interaction with local and global environments. These environments are taken as classical or semi-classical. In addition, in some cases we investigate the influence of classical noise which has a surprising and unexpected signature on the behavior of the systems.

Transformation Optics: Bending the light

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Transformation optics is a new field of optical and material science and engineering comprising metamaterials, plasmonics and nanophotonics. It deals with the transformation of permittivity and permeability tensors of a medium due to a desired transformation of the coordinate system, such that the Maxwells equations preserve their form. By the common essence of all wave propagation phenomena, a sibling field has also emerged which is known as the transformation acoustics.

Metamaterials are artificially structured media that can respond with designed permittivity and permeability values at a particular frequency band of the electromagnetic spectrum. Their development eventually opened the way to the field of transformation optics.

This talk aims to provide a general view to the field of transformation optics by presenting several intriguing examples, such as optical cloaking, illusion optics, and superlenses. We also report the first experimental study of a particular electromagnetic cloak structure based on chiral resonant particles.

Phase diagram of the hardcore Bose-Hubbard model on a checkerboard superlattice

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We obtain the complete phase diagram of the hardcore Bose-Hubbard model in the presence of a period-

two superlattice in two and three dimensions. First we acquire the phase boundaries between the superfluid phase and the 'trivial' insulating phases of the model (the completely-empty and completely-filled lattices) analytically. Next, the boundary between the superfluid phase and the half-filled Mott-insulating phase is obtained numerically, using the stochastic series expansion (SSE) algorithm followed by finite-size scaling. We also compare our numerical results against the predictions of several approximation schemes, including two mean-field approaches and a fourth-order strong-coupling expansion (SCE), where we show that the latter method in particular is successful in producing an accurate picture of the phase diagram. Finally, we examine the extent to which several approximation schemes, such as the random phase approximation and the strong-coupling expansion, give an accurate description of the momentum distribution of the bosons inside the insulating phases.

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Anharmonicity, mode-coupling and entropy in a fluctuating native protein

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We develop a general framework for the analysis of residue uctuations that simultaneously incorporates anharmonicity and mode-coupling in a unied formalism. We show that both deviations from the Gaussian model are important for modeling the multidimensional energy landscape of the protein Crambin (1EJG) in the vicinity of its native state. The eect of anharmonicity and mode-coupling on the uctuational entropy is on the order of a few kcal/mol.

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Breather induced anomalous charge diffusion in a DNA model

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We present results on the diffusive motion of a charge propagating along a double stranded DNA, when the charge carrier interacts with the nonlinear stretching dynamics of base-pairs [1]. The coupled charge-lattice system is studied in the framework of the semi-classical dynamical equations [2].

Signatures of anomalous diffusive properties are found at relatively high temperatures. A sublinear diffusion and a plateau appear before the standard long-time diffusion, during the evolution of charge's mean squared displacement, and also a significant degree of heterogeneity is exhibited among individual trajectories [3]. The higher the temperature, the more evident is the anomalous charge's relaxation.

These properties are connected with the existence of vibrational hot-spots (breather or multibreather excitations) in the lattice component of the system, which result in an enhanced confinement of the charge, at the microscopic level [4].

Macroscopic charge transport parameters are strongly affected in this case, as it can be exemplified by the significant suppression of the diffusion coefficient D [3, 5]. The variation of D with temperature follows a stretched exponential law. These results are contrasted with the corresponding ones in the case of a linearized lattice, in the absence of breathers.

Such an anomalous diffusion of a charge coupled to a thermalized lattice may be also relevant in other low-dimensional soft materials with strong anharmonicities, like for example in conducting polymers.

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Met. **141**, 93 (2004).

[5] G. Kalosakas, work in progress.

Wave Propagation in Nonlinear Disordered Chains

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The absence of wave packet diffusion in disordered linear models is well established and Anderson localization in one-dimensional chains is universal. When nonlinearity is introduced, interactions between localized eigenmodes may increase the localization length. Numerical studies in nonlinear disordered models even suggest that this length diverges and that Anderson localization is destroyed as a consequence of nonlinearities. Localization in disordered media originally received considerable attention in condensed matter physics, where nonlinearities may be present due to interactions (such as between electrons and phonons [1]). In recent experiments with nonlinear optical systems and Bose-Einstein condensates, the combined effects of disorder and nonlinearity were observed. Further theoretical and numerical work is required in order to determine the infinite time limit profile of initially localized states in spatially infinite nonlinear disordered chains.

We examine the long time evolution of wave packets in Discrete Nonlinear Schrödinger (DNLS) and related models. For initially localized packets of finite energy injected in isolated systems at some initial time, we present cases where there is absence of diffusion, i.e., localization is not destroyed by nonlinearity. Localized initial solutions in the form of stable intraband or extraband discrete breathers [2] persist for infinite time at zero temperature. When the initial wave packet is not an exact discrete breather solution, we prove that in DNLS models with strong enough nonlinearity, the participation number (a measure of localization) of the wave packet cannot diverge [3]. Besides these cases, where absence of diffusion is rigorously proven, we provide numerical evidence that localization persists in general in isolated systems. Even when nonlinearity induces an increase in second moment and participation number, the latter may not diverge. We describe results for DNLS-like models which are also norm conserving but with purely nonlinear nearest (and next nearest) neighbor interactions, where rigorous results are available at weak nonlinearity. For small enough nonlinearity, we observe non-diffusive quasiperiodic (KAM) solutions, in agreement with theorem predictions, and no spreading of initially localized wave packets. For higher nonlinearity, after an initial chaotic spreading, there is absence of diffusion.

Nonlinear transmission in externally driven systems is also discussed [4]. We study propagation in time-periodically driven disordered nonlinear chains. For frequencies inside the band of linear Anderson modes, we observe three different regimes with increasing driving amplitude: (1) Below threshold, localized quasiperiodic oscillations and no spreading; (2) Close to threshold, initially almost regular oscillations, weak chaos and slow spreading for intermediate times, and finally strong diffusion; (3) Immediate spreading for strong driving. The thresholds are due to bifurcations, obtained as turning-points of the nonlinear response manifold.

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Detecting causality in multivariate time series

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In the analysis of multiple time series the main interest is to identify the inter-dependencies among the different variables or subsystems corresponding

to the time series. Besides the form and strength of inter-dependence, given as cross-correlation, coherence, coupling or synchronization, it is often important to identify its direction, a term often referred to as Granger causality. One should be aware that pair dependencies may be caused by the effect of other variables or systems. Distinguishing direct from indirect causal effects when more than two time series are available is the topic of this paper.

Linear analysis has provided appropriate tools to deal with Granger causality, e.g. improvement of fit with vector autoregressive over autoregressive model for the time domain and directed coherence for the frequency domain. For direct causal effects, the most popular measure is the Partial Directed Coherence (PDC) [1, 2]. Measures for Granger causality have been developed recently based on nonlinear dynamics and information theory, such as the transfer entropy (TE) [3]. We have also proposed very recently a causality measure derived directly from a mixed embedding scheme based on conditional mutual information criterion, which we call mutual information from mixed embedding (MIME) [4]. In this paper, we extend the measures of TE and MIME to be able to identify direct causal effects, and we name the Partial TE (PTE) and Partial MIME (PMIME).

We compare the proposed measures PTE and PMIME to each other and also to the linear counterpart PDC on some known systems, such as vector autoregressive systems and the Henon coupled maps. Further, we apply the three measures on two real-world applications, multi-channel scalp EEG recordings before, during and after epileptic seizure, and world market indices from some representative countries. A main drawback of the nonlinear measures PTE and PMIME is their inability to account for the effect of many other systems (beyond the assumed driving and response system). Also, PTE turns out to be more biased towards detecting direct causal effects (often giving spurious results), while for PMIME this problem can be treated by adjusting appropriately a free parameter. We discuss the performance of the three measures also in view of the results on the real data.

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Effects of Climate Change on Eastern Mediterranean Region with a special focus on Greece and Turkey

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For a physicist, climate change is not a possibility but a fact. The simple reason behind this argument is the fact that the Earth receives an average power of $342 W/m^2$ from the Sun and it only radiates back $341.3 W/m^2$ which leaves us with an excess energy of $0.7 Joules/second/m^2$ and this excess energy inevitably warms up the Earth. Therefore the question is not whether the Earth warms up but it simply is which region of the Earth will warm up more than the others. Unfortunately the answer to that question is not a happy one'for the Greek and Turkish communities as many predictions show significant warming in our area.

In this talk I will be presenting three sets of results. The first set comes from the global coupled atmosphere ocean simulations showing the changes for the whole Earth until 2100 using different scenarios with very low resolution. This set clearly shows that our region warms up much more than the average and the precipitaion also decreases significantly.

The second set consists of the results of European project called PRUDENCE where low resolution regional climate model simulations were performed for the whole European region. The benefit of this project is to be able to observe the results of quite a few different regional models even though they have reasonably low resolution.

Finally I will present the results of the higher

resolution simulations we have performed for the Aegean basin using ICTP's regional climate model RegCM4.0. As it is lately the norm, the model is run using a SRES scenario A1B which is in the middle of the optimistic and pessimistic scenarios. For the global enforcement data we have used EH5OM5 Global dataset of Max Planck Climate Research Center. The results show significant warming and decrease in the summer precipitation in our region.

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Spontaneous Breather Generation in Model Binary Metamaterials

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The last decade, the study of metamaterials, i.e., of artificially structured materials that exhibit electromagnetic properties and functionality unattainable from natural materials, has attracted great attention. A specific class of metamaterials that exhibit significant magnetic properties at Terahertz and optical frequencies is represented by the magnetic metamaterials [1, 2], which are customarily comprised of regular arrays of split-ring resonators. Real-time dynamic control over the effective metamaterial parameters is of great importance for potential applications. That lead to the construction and detailed study of nonlinear metamaterials, which found to be dynamically tunable by varying the input power [3].

The nonlinearity, along with the inherent discreteness of the metamaterials, allows for the excitation of intrinsic localized modes or discrete breathers [4, 5], i.e., spatially localized, time-periodic and stable excitations that may be produced generically in discrete lattices of weakly coupled nonlinear elements. Discrete breathers may appear spontaneously in a lattice either statistically or by a purely deterministic mechanism that relies on a fundamental instability for wave propagation in nonlinear media (modulational instability).

Recently, a novel magnetic metamaterial comprised of two types of split-ring resoantors was investigated theoretically and it was demonstrated that in the nonlinear regime it is well suited for the observation of phase-matched parametric interaction and enhanced second harmonic generation. The binary structure of the split-ring resonator lattice allows for generation of breathers through direct external induction by a frequency-chirped incident field [6, 7, 8]. That method has been applied succesfully for dissipative breather generation in experiments on di-element cantilever arrays [9]. We have generated numerically a variety of high amplitude dissipative breathers by frequency chirping of the driving field in a model nonlinear binary magnetic metamaterial, and we demonstrated their stability that results from a delicate balance between the input power and the intrinsic losses. These breathers may exist either in the bulk or at the surface of the metamaterial, and they modify locally its magnetic response.

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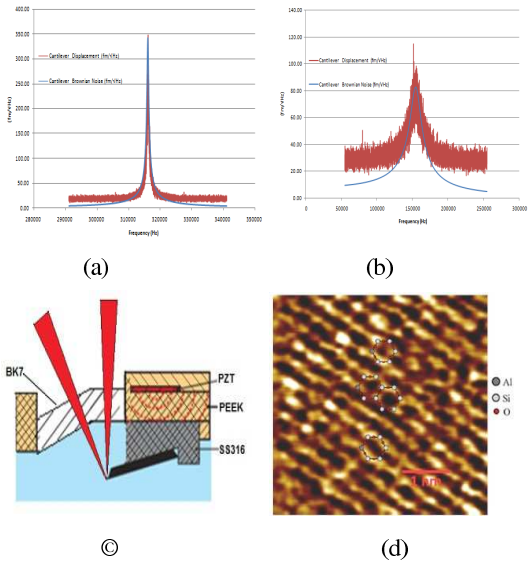

Figure 1: Fig. 1. (a)Thermal Noise Spectrum of the cantilever in air and (b) in pure water. The red lines show experimentally measured values while the blue lines show theoretically calculated values for thermal Brownian motion. (c)Schematics of the cantilever holder. (d)The atomic resolution AFM image of the cleaved clean mica taken in PBS solution.

Atomic Resolution nc-AFM imaging in a closed liquid cell: New potentials in Chemistry and Molecular Biology

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We have designed a non-contact Atomic Force Microscope, which can achieve true atomic resolution in a closed liquid cell, which does not suffer from evaporation of fluids during imaging. Non-contact Atomic Force Microscope (nc-AFM) in liquid environment offers the potential of visualization of individual molecules in real space under physiological environments at atomic resolution opening up very interesting possibilities from chemistry to molecular biology. A High Resolution nc-Atomic Force Microscope(AFM) system from NanoMagnetics Instruments Ltd.[1] is used during the experiments. We added a band-pass filter(BPF) after the quadrant photodetector amplifiers and before the PLL. The frequency shift signal from the Phase Locked Loop(PLL) is fed into the feedback electronics which controls the high voltage signal applied to the custom made piezotube scanner. We have designed a closed liquid cell where we can flow the fluid using a syringe or a peristaltic pump. The AFM cantilever holder was designed as described in [2] to eliminate acoustical resonances. We can obtain resonance curves without spurious acoustic peaks in liquid using a piezoactuator. We have used an RF modulated 635 nm low noise diode laser. RF modulation is effective to reduce the optical feedback noise and the optical interference noise[3]. Deflection noise density of designed system is 20 fm/Hz in air and 25 fm/Hz in liquid as shown in Figure 1 (a) and (b). The observed frequency noise at the PLL output was 1Hzpp in liquid. Force sensitivity of our system is demonstrated by imaging cleaved mica surface in liquid environment as shown in Fig.1.(d) with Df = +50Hz, A=0.9nm, k=32N/m & Q 11

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Probing the optical phonons of graphene by mechanical loading

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Central to most applications involving monolayer graphenes is its mechanical response under various stress states. To date most of the work reported is of theoretical nature and refers to tension and compression loading of model graphenes. In this work, graphene flakes are subjected to uniaxial tension and compression using the polymer cantilever beam technique [1, 2]. The mechanical response is monitored by simultaneous Raman measurements through the

shift of either the G or 2D phonons of graphene using different excitation wavelengths. The G mode at around 1580 cm^{-1} corresponds to the doubly degenerate E_{2g} phonon at the Brillouin-zone center. The 2D peak at about 2680 cm^{-1} (λ=514.5 nm) is the second order of the D peak which originates from the breathing modes of sp^2 rings and requires a defect for its activation. In tension, the embedded flake seems to sustain strains up to 1.3% in a reversible manner,whereas in compression there is an indication of flake buckling over 0.6% strain. The experimental findings are compared and discussed with changes of the electronic and vibrational properties of graphene under strain, using first principles calculations [3].

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Travelling Waves in nonlocal lattice equations

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Existence and bifurcation results of quasi-periodic traveling waves of discrete nonlinear Schrödinger equations with nonlocal interactions and with polynomial type potentials are considered. The approach is based on variational techniques and concentration compactness. Several concrete nonlocal interactions are studied as well.

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Melting of genomic DNA sequences: predictive modeling by nonlinear lattice dynamics

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Over the last twenty years, mesoscopic, nonlinear dynamics-based (Peyrard-Bishop-Dauxois, PBD) modeling has been instrumental in elucidating important qualitative aspects of the cooperative behavior which characterizes the thermal separation of the two DNA strands. Highlights to date include (i) establishing the infinite homopolymer DNA chain as one of the few nonpathological one-dimensional systems which exhibit a true thermodynamic phase transition, (ii) statistical and dynamical modeling of the denaturation bubble involved in the transcription process. Curiously, although this type of minimal, mesoscopic approach is uniquely suited to describe the details of the multistep, cooperative melting process taking place at long genomic sequences, the PBD model has not yet been subjected to this obvious, detailed reality test.

I will present a PBD-based analysis of experimental melting profiles for a number of specific sequences with many thousands of base pairs. The results [1] suggest that it is possible to predict complex melting profiles of long genomic sequences without any adjustable parameters, using only the salt concentration and the sequence data.

The proposed new parametrization of the PBD model - largely based on physically motivated estimates - provides a quantitative understanding of a number of further aspects of DNA structure and/or low-frequency dynamics. Thus, (I) calculated probabilities for single base-pair opening are consistent with the very low values (of the order of 1ppm) obtained from imino proton exchange experiments [2], although (II) extended bubbles may occur with relatively high probabilities at selected sites of genomic sequences, (III) low-frequency transverse optical phonons in model heterogeneous chains are in the range experimentally observed in DNA Raman spectra [3], and (IV) calculated structure factors are in agreement with recent neutron diffraction measurements [4].

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Density functional theory and its applications to contemporary problems in physics

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Since its proposition in 1964 [1] density functional theory has seen a tremendous amount of development both in terms of its theoretical foundations and with recent advances in computational resources also in practical applications. The method, shifting the focus from a wavefunction-based description of the many-particle problem to the particle density, has provided a much more affordable treatment of numerous physical systems. A search in ISI Web of Knowledge reveals some 38000 publications on density functional theory between the years of 2005 and 2010.

Traditionally utilized heavily for atomistic problems such as those in quantum chemistry and solid state physics, other many-particle applications in physics have recently been tackled with density functional theory, uncovering new insight that has been absent in models previously developed.

In my talk, I will first give a brief description of the density functional theory, including its foundations and some practical concerns. I will then give two (or three, time permitting) examples currently under investigation in our group. The example that I will explain most extensively is our density functional treatment of the ultracold dipolar atoms in a harmonic trap which has previously been treated within a variational Thomas-Fermi approach [2]. I will conclude with a survey of similar novel problems tackled using density functional theory in literature and conclude with a future outlook.

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Small Polaron Hopping Transport in 1D Disordered Systems

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The electrical transport properties of disordered materials have been an active research topic for many years. The realization of innovative applications in nanotechnology has especially generated a widespread interest on the transport properties of 1D systems, such as carbon nanotubes, nanowires and conducting molecules, with DNA being placed among the most promising materials.

The presence of disorder, under certain circumstances, induces localization of the carriers and possible formation of small polarons. Hopping is the responsible transport mechanism for the measured conductivity. Triberis et. al. [1] investigated small polaron hopping transport in 1D disordered systems, such as DNA, at high temperatures (h), ignoring the effect of correlations. An analytical expression for the temperature dependence of the electrical conductivity, $\ln \sigma^h \sim T^{-2/3}$, was obtained. The theoretical analysis was based on the Generalized Molecular Crystal Model (GMCM) introduced by Triberis and Friedman [2], appropriate for the study of small polaron transport in disordered systems, the Kubo formula and theoretical percolation arguments.

When the site energies are not the same, the energy of a site affects the incoming as well as the outgoing impedances connected to the given site, and this gives rise to correlations between neighbouring impedances. Recently, Triberis and Dimakogianni [3] showed that the inclusion of correlations (cr) leads to a $\ln \sigma^{h,cr} \sim T^{-1/2}$ law. Their results reproduced satisfactorily the experimental data reported for λ-DNA and for poly(dA)-poly(dT) DNA [4, 5, 6], considering

DNA as a disordered molecular wire. The maximum hopping distances evaluated support the idea of long distance charge migration in DNA.

Triberis and Dimakogianni [7] also examined the interplay of the electric field, F, and the temperature on the small polaron hopping conductivity of 1D systems, ignoring correlations. The analytical expressions obtained were applied to experimental findings concerning charge transport in Polydiacetylene quasi-1D single crystals [8]. It was shown that the electric field and the temperature act competitively upon the behavior of the electrical conductivity. Their effect on the transition from the ohmic to the non-ohmic behavior of the conductivity was revealed.

Most recently, Dimakogianni and Triberis investigated the effect of correlations on the field and temperature dependence of the small polaron hopping conductivity. The inclusion of correlations results in a much stronger dependence of the conductivity on the magnitude of the applied electric field.

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A Monte Carlo Study of the dynamical behavior of cluster assembled magnetic nanostructures

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There is a growing realization of the enormous potential of cluster assembled films in the production of high-performance magnetic materials. Increasingly attention has been focused on the effect of interactions in cluster deposits that can occur between the clusters, the clusters and substrate, and clusters and coating materials [1]. In this context the exchange interaction is of great importance, since the exchange length is significant compared to the cluster diameter and in interacting cluster films, it is the dominant mechanism [2]. This mechanism produces a number of interesting and technically useful effects. We give two examples of systems where the intercluster interactions determine their magnetic behavior.

First we model the growth process and the evolution of the magnetic behavior of Co clusters on Au surfaces in the case of low temperature co-deposition of Co and Au atoms. The magnetic structure is obtained by a Monte Carlo simulation, which includes exchange and magnetostatic intercluster interactions and perpendicular anisotropy for each Co cluster. The dynamic evolution of the magnetic properties is described by our simulations and it is correlated with the interparticle coupling and the annealing conditions. Our results are in very good agreement with experimental findings.

The magnetization dynamics of a dense cluster assembly has also been modeled using the Monte Carlo simulation technique. The role of the internal characteristics of the assembly (inter-cluster interactions, anisotropy axes distribution, particle size distribution, substrate coverage) and the external parameters (temperature, applied field) has been studied. In very dense Fe cluster films, the frustration resulting from the inter-particle exchange interaction and the randomly oriented intra-cluster anisotropy produces a correlated super-spin glass ground state that is magnetically soft. Clearly a faster magnetization reversal is observed with increasing coverage in agreement with the experimental observation and is attributed to the growing size of the clusters of the exchange-coupled nanoparticles that reverse collectively under the applied field.

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Renormalization Group studies of some Non-equilibrium Systems

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Results of position-space Renormalization Group (RG) studies on two different types of non-equilibrium states with steady-state phase transitions will be presented.

The first type corresponds to an Ising model in contact with two heat baths at different temperatures. Systems of this type had been studied earlier in various limits, in different contexts: Of particular interest has been the case with conserved dynamics (exchanges in different directions being driven by different heat baths) and when one of the heat baths is at an infinite temperature[1, 2]. The problem may be treated exactly when the exchange rate related to the infinite temperature bath is much faster than that for the finite temperature bath[1]. If these rates are equal, Monte Carlo studies indicate that the steady-state phase transition occurs when temperature of the finite temperature bath is at a much *higher* value[2] than the equilibrium phase transition temperature! Using the position-space RG, we determine the global phase transition behavior of this system for arbitrary temperatures of the heat baths and when the driving exchange rates have arbitrary speeds[3].

The second type of non-equilibrium system to be discussed is the "asymmetric exclusion process" (ASEP), which models one-dimensional classical transport systems in which particles can move only in one direction, and only into neighboring vacant sites. The system displays a number of steady-state phase transitions depending on the particle injection and absorption rates at the boundaries. The problem involving only one type of particle has been solved exactly[4], and a number of successful RG studies[7, 8] have been reported. We are analyzing a version of this system with two different types of particles moving in opposite directions[5, 6], using Monte Carlo, mean-field, and RG. An interesting feature of this model is the appearance of broken symmetry, when the transport properties associated with the two types of particles are the same.

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Observation of network formation, fractal nature, universality, internal morphology of the polymer networks: theory and experiment

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A new approach for in situ monitoring of the monomer conversion based on the chemical interaction of a fluoroprobe with polymer chains during the polymerization has been developed [1]. It is proved that the change in the emission spectra of the fluoroprobe during polymerization and gelation is used for *in situ* monitoring of the monomer conversion with great sensitivity [2]. Then, real-time fluores-

cence measurements have been developed for measuring the fractal dimension d_f and critical exponents γ and β simultaneously during the sol-gel transition of acrylamide hydrogels.[3] We observed that d_f passes through a minimum value of 2.5 at the percolation threshold and crossover to 3 above it. The exponents γ and β, measured at the threshold were found to be around 1.8 and 0.45, respectively. All parameters agree with percolation results. In addition a new method is developed for measuring the density distribution and the weight fraction of "the frozen blob clusters" in heterogeneous hydrogels via direct current measurements [4]. It is proved that the current density decreases with time as a series of exponentials where the exponents and the multipliers measure the density and the weight fraction of the corresponding blob generation, respectively. The number of terms in the series that fit best with the experimental data indicates the number of generations of the blobs [5]. This seems like a decomposition of Kohlrausch's stretched exponential function, which gives a bird's-eye view of the internal morphology of a heterogeneous medium.

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On the nonlinear response of a particle interacting with fermions in a 1D lattice

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By the Bethe ansatz method we study the energy dispersion of a particle interacting by a local interaction with fermions (or hard core bosons) of equal mass in a one dimensional lattice. We focus on the period of the Bloch oscillations which turns out to be related to the Fermi wavevector of the Fermi sea and in particular on how this dispersion emerges as a collective effect in the thermodynamic limit. We also discuss the adiabatic coherent collective response of the system to an applied field.

CONTRIBUTED TALKS

Polymer network *pn* junctions with ionic charge carriers

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In this work, new kind of pn junctions with ionic charge carriers were created via polymeric hydrogels. The polymer pn junctions were synthesized in two different ways. In the first way, p and n type doped polyacrylamide hydrogels were synthesized on the top of the other. The dopant molecules with positive and negative counter ions were bound chemically the polymer network during the synthesizing of these gels. In the second way, the pregel solution was prepared so as to include the dopant having both negative and positive counter ions together. This pregel solution was synthesized under an electrical field. In this case positively and negatively charged dopant molecules drift to opposite sides of the gel due to the external electrical field applied on the solution during the polymerization. The charged molecules bind randomly to the ends of the polymer strands and the cross link points of the network [1, 2]. The counter ions create the current under applied voltage when the gels were swollen in pure water that causes the counter ions to be free to move. The mobility of the counter ions of the dopants increases upon swelling of the gel and contribute to the current passing through the gel. The bonding kinetics

of the charged molecules to the network was modeled and observed by the fluorescence measurements [3]. We demonstrate that these two junctions rectify considerably the electric current [4]. We have shown that some of the junction characteristics like doping concentration; threshold voltage etc. can be changed easily.

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Strain Tunable Band Gaps of Carbon Nanotubes

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The electronic energy band gap is a basic property of all semiconductors since it is responsible for the electrical transport and optical properties. Control of the size of the electronic energy band gap is important in optimizing the electronic devices. Single-walled Carbon Nanotubes (SWCNTs) represent a new class of electronic materials where the electronic properties depend upon their size and symmetry. In this talk, I will show that the mechanical deformations such as the application of tensile strain can induce changes in the density of states, modifying the size of the energy band gaps of SWCNTs. Energetics of SWCNTs are obtained using a parallel, Order N, Tight Binding Molecular Dynamic (O(N) TBMD) simulation code designed by Dereli et. al [1, 2, 3]. This code is used in SWCNTs simulations successfully and the details of the technique and the references can be followed in [4, 5, 6]. O(N) TBMD calculates the band structure energy in real space and makes the approximation that only the local environment contributes to the bonding, and hence the band energy of each atom. In this case, the run time would be linearly scaled with respect to the number of atoms [7, 8, 9, 10] . We simulated various semiconducting SWCNTs under compressive and tensile strain values. The zigzag (n,0) SWCNTs are generally semiconducting and they are quasi-metallic only when n is a multiple of 3. Applications of positive and negative strains open up the band gap causing metal - semiconductor transitions in quasi-metallic zigzag SWCNTs. On the other hand, our studies show that for the (n,0) semiconducting nanotubes, this behavior is strongly dependent on whether n mod3 is equal to 1 or 2. In semiconducting (n,0) nanotubes when n mod3 is equal to 1, compressive strain closes the band gap whereas the tensile strain opens it up. For the n mod3 equals to 2 type nanotubes, band gap closes for tensile strain and opens up for compressive strain. These results are extremely important for CNT-based electronics since one gains a mechanical control of conductance.

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Fractal Analysis of Human Brain Diffusion Tensor Images in the 2-D and 3-D Space

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One of the most difficult problems today is to understand the structure and the functionality of the brain. A lot of biophysical methods have been proposed and applied in modern medicine, but the brain still remains an open problem. One of the currently active methods in today's research is the Diffusion Tensor Imaging, a method used to define the structure of the brain, by calculating the direction of neurons, based on the movement of water molecules. Using this method it is possible to trace the general direction of the neuron axons, and thus the physical structure of the brain.

On top of the DTI methods, we were able to estimate the fractal dimension D_f of the brain as a complex structure. The methods used were box counting, lacunarity analysis, correlation dimension and mass dimension. Two types of data sets have been used; (a) a 2-D projection of a 3-D tractography based on a specific areas of interest and (b) a 3-D representation of the neuron tracts emanating from the whole human brain area.

The calculated fractal dimension for the 2-D projection was found to be $D_f \simeq 1.6$ for small areas of interest, and for larger areas of interest seems to occupy the whole 2-D space. In the 3-D space the value of D_f was again constant, varying from 1.5 in the small scales, up to 3 in medium and large scales, thus reflecting the local topology of the neurons. The results in both cases are compatible; when using small areas of interest in the 2-D method, the value of D_f is roughly equal to the D_f of the 3-D approach in the small scales, while both areas in these two approaches have approximately the same size. In large scales both approaches demonstrate that the human brain occupies the whole area, and thus its D_f tends to be equal to the embedded space.

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Coherent oscillations in ensembles of discrete two-state excitable units with global delay coupling

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A two-state excitable unit is considered as an abstract modification for an ion chanel of a neuron. Each state is characterized by a different waiting time density function. This approach allows for a renewal process description of the system dynamics. Exact formulas for the interspike interval distribution and spectral power density are found. At the limit of an infinity ensemble of globally coupled units the mean-field equations for the populations of the two states are derived. Depending on the coupling strength and on the noise intensity the ensemble undergoes saddle-node bifurcations and demonstrates bistability, while a pitchfork bifurcation emerges on a critical point. The ensemble undergoes Hopf bifurcations and coherent oscillations emerge, in the onset of firing events, only in the case that global coupling affect the system with a certain time delay. The stochastic simulations of large ensembles in both cases are in good agreement with the analytical approach.

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Analysis of Metastable States in the Infinite-Range-Interaction Inertial Heisenberg Ferromagnet

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Hamiltonian systems composed by a large number of microscopic elements – interacting through long-range couplings – may pose difficulties in the applicability of the Boltzmann-Gibbs (BG) statistical-mechanics formalism. These types of systems may present a non-extensive behavior in some of its thermodynamic properties, a zero maximum Lyapunov exponent, and breakdown of ergodicity, which represent essential conditions within the standard BG formalism. Herein we discuss a simple model that exhibits such characteristics, i.e., the infinite-range-interaction inertial classical Heisenberg ferromagnet. This model consists in a modification of the well-known Heisenberg model, where the spins are replaced by classical rotators, defined by the Hamiltonian,

$$H = K + V = \frac{1}{2}\sum_{i=1}^{N}\sum_{\mu=1}^{3} L_{i\mu}^2 + \frac{1}{2N}\sum_{i,j=1}^{N}(1 - \vec{S}_i.\vec{S}_j) \ , \quad (1)$$

where the index μ ($\mu = 1, 2, 3$) denotes Cartesian components and $L_{i\mu}$ represents the μ-component of the angular momentum (or the rotational velocity, since we are assuming unit inertial moments) of rotator i. The usual canonical-ensemble mean-field solution of the inertial classical Heisenberg ferromagnet is briefly reviewed, showing the well-known second-order phase transition. This model is studied numerically within the microcanonical ensemble, through molecular dynamics. The time evolution of the kinetic temperature indicates that certain basins of attraction exist for the initial conditions, for which the system evolves into a metastable state, before attaining the terminal thermal equilibrium. Some properties of these metastable states are studied and are shown to exhibit curious behavior: (i) Different initial conditions may lead to distinct metastable states; (ii) They are characterized by durations that diverge as $N \to \infty$, implying that the system should remain forever in such states in the thermodynamic limit; (iii) The maximum Lyapunov exponent decreases with N like $\lambda_{\max} \sim N^{-\kappa}$ ($\kappa > 0$); (iv) The angular-velocity distributions computed from time intervals over a single sample, or from averages over samples at a fixed time (i.e., ensemble averages), may present very different behavior; (v) For some initial conditions, the time-averaged angular-velocity distributions are characterized by long tails.

Steered Molecular Dynamics simulation to study elasticity and rupture of a Contactin protein

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To determine mechanism of injury and the consequent failure, the nature of load transfer to cells and their deformation phenomena as well as their material characteristics and mechanical behavior must be understood. Tissue damage such as Diffuse Axon Injury is directly related to cell injury which can be related to the mechanical failure of the cell under extreme external loading or rapid kinematic motion. Molecular Dynamics simulation has been implemented here to study the force-displacement relation and debonding of adhesion molecule between axon and ECM. This molecule is formed of contactin protein, Caspr, NF155 and Necl-1. Here it has been demonstrated how a contacting protein responds to constant forces and how the complex unfolds under dynamic loading. The traction-separation curve, as the constitutive material behavior of the interface, was extracted from MD simulation. Current experimental facilities have been restricted by considerations of infinitesimal size, geometry and biochemical interaction of adhesion. However, Atomic Force Microscopy and optical tweezer experiments measure the extensions of proteins as a function of applied force. Additionally a quantitative and predictive modeling is useful to simulate and study functions of proteins. Recently molecular dynamics approach has been increasingly used as a pow-

erful mean of investigating biomolecular dynamics. In particular, Steered Molecular Dynamics (SMD) is a novel approach to the study of the dynamics of binding/unbinding events in biomolecular systems and of their elastic properties. Using a parallel processing system with 8 nodes, the SMD approach was utilized to apply force on contactin protein and study how it behaves under loading and to evaluate force-displacement relation. The structure of contactin protein was used for simulation from Protein Data Bank (PDB ID 3JXA Ig1-4 fragment). At the first, after removing one chain and generating missed atoms, the energy was minimized for 10,000 cycles. Then the C atom of N-terminus was kept to be fixed and by applying a constant force to the central mass along the direction connecting the initial positions of N-terminus and central mass the atomic coordinates of the whole system were recorded. The elongation of molecule was defined as the increase of the end-to-end distance between the termini from that of the native fold. Such elongation was monitored along with the applied force. The force-displacement diagram was outlined. A dynamic force has also been applied with a constant velocity to show the unfolding behavior of protein to analyze interface separation between cell-ECM. The derived force-displacement relation shows the stiffening response of protein under constant applying force and also the constitutive properties of the interface between cell and ECM that can be used in the modeling of upper scale in Cohesive Zone Method to extract the multiscale modeling of white matter of the brain tissue. This research is the developing stage of a research concerning a proper multiscale modeling of the brain tissue to investigate cellular adhesion effects.

Hierarchical multifractal representation of symbolic sequences and application to human DNA

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The 2-D Density Correlation Matrix (DCM) method is described for symbolic sequences of arbitrary size, based on segments of finite size. Viewed as a surface with random like local heights, this DCM can be characterised by its MultiFractal Spectrum (MFS) which indicates the presence of correlations in the corresponding symbolic sequences. This method is applied to symbolic DNA sequences in entire human chromosomes, reconstructed genomic sequences and artificial random sequences. It is shown that all human chromosomes have common characteristics in their MFS and deviate substantially from random and uncorrelated sequences of the same size. The correlations are shown to be crucial for the form of the multifractal spectra; surrogate shuffled chromosomes present random-like spectra, distinctly different from the actual chromosomes.
Hierarchical reconstruction of 2-D DCMs is further undertaken, based on superposition of tensor products and their MFS are analytically obtained. It is shown that retaining pair correlations when constructing the DCM via hierarchical superpositions, leads to a better representation of the genomic multifractal spectra. The selective presence of characteristic functional units of small sizes (such as the CG/GC combinations) is held responsible for the observed correlations and for the corresponding deviations in the spectra. Retaining higher order correlations in the construction of the tensor products is a way to approach closer the MFS of the actual genomic sequences. This hierarchical approach is generic and is applicable to correlated symbolic sequences in general.

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Scale invariant probabilistic model having two dimensional $q-$Gaussians as $N \to \infty$ limiting distribution

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It has been recently introduced in [**?**] and further generalized in [2] a family of one dimensional scale-invariant probabilistic models characterized by a real number $\nu > 0$ having one dimensional $q-$Gaussians as $N \to \infty$ limiting distributions based on the so called Leibniz triangle [3], and on the Pascal triangle. The model consisted of a set of N *equal, long-range-correlated binary* random variables —corresponding to the binomial distribution in the uncorrelated case— in which scale-invariant correlations were introduced.
In this contribution we generalize the model by allowing the N discrete random variables to take on three different values —hence the trinomial distribution is obtained in the uncorrelated limit. In addition, we introduce the so called Pascal pyramid, as well as what we may call the *Leibniz pyramid*, given by

$$r^{(1)}_{N,n,m} = \frac{2}{(N+2)(N+1)Nn\,,m} \tag{2}$$

where n, m and N are positive integers with $0 \leq n + m \leq N$, and $Nn\,,m$ are the trinomial coefficients.
By properly rescaling certain subpyramids of the Leibniz pyramid tetraedroLeibniz we get a family of pyramids characterized by a real number $\nu \geq 1$, given by

$$r^{(\nu)}_{N,n,m} = \frac{B(n+\nu, m+\nu)B(n+m+2\nu, N-n-m+\nu)}{B(\nu,\nu)B(\nu,2\nu)} \tag{3}$$

which follow the *generalized Leibniz rule*

$$r^{(\nu)}_{N,n,m} + r^{(\nu)}_{N,n+1,m-1} + r^{(\nu)}_{N,n,m-1} = r^{(\nu)}_{N-1,n,m-1} \tag{4}$$

responsible for the scale-invariant character of the correlations; by $B(x,y)$ we note the Beta function. The actual probabilities of the model are given by

$$P^{(\nu)}_{N,n,m} = Nn\,,m r^{(\nu)}_{N,n,m}. \tag{5}$$

The main result of our contribution states that under an appropiate change of variables, the limiting $N \to \infty$ probability distribution of the model is a two-dimensional $q-$Gaussian with a value of q given by

$$q_\nu = \frac{\nu - 2}{\nu - 1}. \tag{6}$$

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Time–Evolving Statistics of Chaotic Orbits of Conservative Maps in the Context of Central Limit Theorem

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The existence of a central limit theory for deterministic variables has been known for some time [1]. More recently, this theory has been the focus of attention from a statistical mechanics viewpoint, aiming to determine the probability density function (pdf) of systems characterized by non-additive entropy S_q [2, 3]. In the past, this direction has been pursued using the distribution of the sum of deterministic variables for some special kind of correlation [4], or even for systems evolving in metastable states [5].
In the present work, we study numerically the pdf of sums of $N \to \infty$ iterates of the conservative (area-preserving) 2–dimensional perturbed Mc Millan map [6], which may be interpreted as describing the effect

of a simple linear focusing system supplemented by a periodic sequence of thin nonlinear lenses:

$$x_{n+1} = y_n, \qquad y_{n+1} = -x_n + 2\mu \frac{y_n}{1+y_n^2} + \epsilon y_n \quad (7)$$

where ϵ, μ are real parameters. In the spirit of central limit theory, we have analyzed the pdf of shifted and normalized sums of the x-component of (7) in "thin" chaotic layers of the x, y phase plane and discovered that they exhibit a very interesting time evolution, for a wide range of parameters (ϵ, μ): In particular, they appear to exhibit "generically" *three stages*, passing from a *q-Gaussian*, to a *triangular* shape and finally to the well–known *Gaussian* form. These stages accompany a slow diffusion process through which the orbits move successively to wider chaotic domains, where the dynamics is more uniformly ergodic and Boltzmann–Gibbs statistics is expected to prevail. Preliminary results by us on a 4–dimensional volume–preserving map, as well as by other researchers on multi–dimensional Hamiltonian systems [7] show similar time–evolving statistics for chaotic orbits diffusing slowly into regimes of more uniformly random dynamics.

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On the 'glassy' transition and fragility of the ferromagnetic plaquette Ising model

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The three dimensional ferromagnetic plaquette Ising model (FPIM) is believed to have a first order phase transition at $T_c \simeq 3.60$ screened by strong metastability leading to a so-called "glassy transition" at $T \simeq 3.40$ when subjected to slow cooling [1,2]. By computing the configurational entropy $S_c \equiv S(\text{liquid}) - \text{S(crystal)}$ in the supercooled temperature range via thermodynamic integration of the internal energy results, we determine the Kauzmann temperature $T_K \simeq 3.18$, defined as that temperature where the extrapolated configurational entropy $S_c(T)$ vanishes. By finding ways to estimate the equilibration time of the supercooled liquid and the nucleation time of the stable crystal droplets, it is shown that $T \simeq 3.4$ is indeed the limit of stability or the effective spinodal temperature $T_{\rm sp}$ at which the two time scales associated with the quasiequilibration of the supercooled liquid, $\tau_{\rm eq}$, and the nucleation of the stable crystal droplets, $\tau_{\rm nuc}$, cross one another, with the former rising above the latter such that the supercooled liquid state becomes physically irrelevant below $T_{\rm sp} \simeq 3.40$ and the impending entropy crisis at $T_K \simeq 3.18$ ($< T_{\rm sp}$) is thus avoided [3]. Hence, what is sometimes called "glassy temperature," is really a kinetic spinodal temperature below which fast nucleation of the mismatched crystal droplets is followed by a glacially slow crystal growth [4]. The Adam-Gibbs relation for the structural relaxation time $\tau = \tau_0 \exp(C/TS_c)$, is found to be valid in the supercooled temperature regime. Fragility is measured, and the rapidity with which the liquid's dynamic properties (such as the viscosity) change as the polycrystalline state is approached is compared between FPIM and another homogeneous glassy model known as the Coupled two-level system (CTLS). The results reveal that FPIM is more fragile than the other.

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dHAN Model of a Neural Network in the Light of Experimental Neuroscience

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A model of dense homogeneous associative network (dHAN) of neurons has recently attracted attention due to its unique properties [1, 2]. This model shows several emerging features. It is able to recognize external patterns in noisy background, to focus attention autonomously and to represent hierarchical memory with an internal structure. We have studied various properties of this model in details. In particular, we have focused our attention on two different set of experiments in empirical neuroscience. On one hand, neural culture samples of cerebral cortex of wistar rat which has illustrated dependency of bursting frequency during synchronous firing on network connectivity [3] and on the other hand, an experiment on prefrontal and occupational cortex slices of ferret which has demonstrated a neural system showing collective oscillations that can be forced into an upstate by injecting a positive electric pulse. This state could afterward be terminated by a second pulse of identical polarity, but with specific dependency on pulse intensity and delay to the first one [4, 5]. Here, we present our results for the general properties of this model, and discuss in particular, its success in reproducing recent experimental results.

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Discrete nonlinear Schrdinger equation dynamics in complex networks

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We investigate dynamical aspects of the discrete nonlinear Schrdinger equation (DNLS) in finite lattices. We start from a periodic chain with nearest neighbor interactions and form a small world network by inserting randomly links connecting distant pairs of sites across the lattice. We use a localized initial condition and focus on the time averaged probability of occupation of the initial site as a function of the degree of complexity of the lattice and nonlinearity. For defocusing nonlinearity we find that self-trapping occurs at increasingly larger values of the nonlinearity parameter as the lattice connectivity increases while close to the fully coupled network localization becomes more preferred. For nonlinearity values above a certain threshold we find localization when the number of long distant bonds is small followed by delocalization and enhanced transport at intermediate bond numbers while close to the fully connected limit localization reappears. We present exact time dependent solutions for the fully coupled lattice with arbitrary numbers of sites.

Memory Associativity in a Model for Conscious and Unconscious Mental Processes

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We have modeled conscious and unconscious mental processes in neurosis, by neural network mechanisms, whereby neurotic behavior is described as an associative memory process. Modules corresponding to sensorial and symbolic memories interact, representing unconscious and conscious mental functioning. We proposed an algorithm, based on known microscopic neuronal mechanisms that control synaptic plasticity, which self-organizes the complex memory network to a hierarchical, clustered structure. Memory access was first modeled by a Boltzmann machine (BM). The power-law behavior for the node degree distributions of the topologies of the networks generated by our algorithm suggests that memory dynamics and associativity may not be well described by Boltzmann-Gibbs (BG) statistical mechanics. We thus modeled memory access dynamics by a generalization of the BM called Generalized Simulated Annealing (GSA), derived from the nonextensive formalism. We will show some properties of these memory retrieval mechanisms, with simulation experiments that measure associativity capabilities in our networks.

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POSTERS

Probability densities for the sums of iterates of the sine-circle map in the vicinity of the quasi-periodic edge of chaos

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We investigate the probability density of rescaled sum of iterates of sine-circle map within quasi-periodic route to chaos. When the dynamical system is strongly mixing (i.e., ergodic), standard Central Limit Theorem (CLT) is expected to be valid, but at the edge of chaos where iterates have strong correlations, the standard CLT is not necessarily to be valid anymore. We discuss here the main characteristics of the probability densities for the sums of iterates of deterministic dynamical systems which exhibit quasi-periodic route to chaos. At the golden-mean onset of chaos for the sine-circle map, we numerically verify that the probability density appears to converge to a q-Gaussian with $q < 1$ as the golden mean value is approached.

Weak chaos and the "melting transition" in a confined microplasma system. Connection with the q-entropy

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We present results demonstrating the occurrence of changes in the collective dynamics of a Hamiltonian system which describes a confined microplasma characterized by long–range Coulomb interactions. In its lower energy regime, we first detect macroscopically, the transition from a "crystalline–like" to a "liquid–like" behavior, which we call the "melting transition". We then proceed to study this transition using a microscopic chaos indicator called the *Smaller Alignment Index* (SALI), which utilizes two deviation vectors in the tangent dynamics of the flow and is nearly constant for ordered (quasi–periodic) orbits, while it decays exponentially to zero for chaotic orbits as $\exp(-(\lambda_1 - \lambda_2)t)$, where $\lambda_1 > \lambda_2 > 0$ are the two largest Lyapunov exponents. During the "melting phase", SALI exhibits a peculiar, stair–like decay to zero, reminiscent of "sticky" orbits of Hamiltonian systems near the boundaries of resonance islands. This alerts us to the importance of the $\Delta\lambda = \lambda_1 - \lambda_2$ variations in that regime and helps us identify the energy range over which "melting" occurs as a multi–stage diffusion process through weakly chaotic layers in the phase space of the microplasma. Additional evidence supporting further above findings is given by examining the $GALI_k$ indices, which generalize SALI ($=GALI_2$) to the case of $k > 2$ deviation vectors and depend on the complete spectrum of Lyapunov exponents of the tangent flow about the reference orbit. Finally, we report on some recently obtained results providing strong evidence of a connection of the "melting transition" of such a system with the characterization of its weakly chaotic regime furnished by the Tsallis' distribution.

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Simulation of traffic flow at intersection with traffic responsive signalization

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Modelling the dynamics of vehicular traffic flow by cellular automata has constituted the subject of intensive research by statistical physics during the past years [1, 2, 3]. *City traffic* was an early simulation target for statistical physicists [4, 5]. Evidently the optimisation of traffic flow at a single intersection is a preliminary but crucial step to achieve the ultimate task of global optimisation in city networks [6]. We have developed a Nagel-Schreckenberg for describing of vehicular traffic flow at a single intersection[7]. A set of traffic lights operating either in fixed-time or traffic adaptive scheme controls the traffic flow. Closed boundary condition is applied to the streets each of which conduct a uni-directional flow. Extensive Monte Carlo simulations are carried out to find the model characteristics. In particular, we investigate the dependence of the flows on the signalisation parameters. Our findings show hindrance of cars upon reaching the red light gives rise to formation of plateau regions in the fundamental diagrams. This is reminiscent of the conventional role of a single impurity in the one dimensional out of equilibrium systems. The existence of wide plateau region in the total system current shows the robustness of the controlling scheme to the density fluctuations. The overall throughput from the intersection shows a significant dependence on the cycle time in the fixed time scheme and on the queue cut-off length in the responsive scheme.

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Analysis of return distributions in the coherent noise model

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The return distributions of the coherent noise model are studied for the system size independent case. It is shown that, in this case, these distributions are in the shape of q-Gaussians, which are the standard distributions obtained in nonextensive statistical mechanics. Moreover, an exact relation connecting the exponent τ of avalanche size distribution and the q value of appropriate q-Gaussian has been obtained as $q = (\tau + 2)/\tau$. Making use of this relation one can easily determine the q parameter values of the appropriate q-Gaussians *a priori* from one of the well-known exponents of the system. Since the coherent noise model has the advantage of producing different τ values by varying a model parameter σ, clear numerical evidences on the validity of the proposed relation have been achieved for different cases. Finally, the effect of the system size has also been analyzed and an analytical expression has been proposed, which is corroborated by the numerical results.

Monte Carlo Simulation of confined hard ellipse-fluid

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The structural and thermodynamic properties of a confined hard-ellipse fluid are studied using Mont Carlo simulation. The angular, average number densities and order parameters of hard ellipses confined between hard parallel walls are obtained for various bulk densities, aspect ratios and wall separations. The results show that the effect of the existence of the wall on the molecular fluid structure, either on their directions or their locations, with respect to the bulk, specially close to the walls, is significant. For this system the pressure is also obtained and it is shown that the average density at the wall is proportional to the pressure, $\beta P =< \rho_w >$. Our simulation results show the order parameters depend on the number of the particles in the box unless it exceed a thousand.

Multiple-transit paths and density correlation functions in PASEP

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We consider the partially asymmetric simple exclusion process (PASEP) when its steady-state probability distribution function can be written in terms of a linear superposition of product measures with a finite number of shocks [1]. In this case the PASEP can be mapped into an equilibrium walk model, defined on a diagonally rotated square lattice, in which each path of the walk model has several transits with the horizontal axis [2, 3]. We particularly show that the multiple-point density correlation function in the PASEP is related to the probability that a path has multiple contacts with the horizontal axis from the above or below.

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Discrete-time analysis of traveling wave solutions and steady-state of PASEP with open

boundaries

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We consider the dynamics of a single shock in Partially Asymmetric Simple Exclusion Process (PASEP) on a finite lattice with open boundaries under sublattice-parallel updating scheme. We then construct the steady-state of the system by considering a linear superposition of these shocks. It is shown that this steady-state can be also written in terms of a product of four non-commuting matrices. The main result obtained is that these matrices have exactly the general structure of the matrices first introduced in [1] when the steady-state of a one-dimensional driven-diffusive system can be written as a linear superposition of product shock measures. It is easy now to explain the two-dimensional matrix representation of the PASEP with parallel dynamics introduced in [2].

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Comparison of kinetic and potential energy in annealing process of 2-D and 3-D atomic grid of Krypton by molecular dynamic simulation

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In this study we are dealing with 2-D and 3-D molecular modeling of krypton. A 2-D krypton grid of 20 atoms was produced and settled in a water box. By single point calculations the energy and energy gradient were obtained and the system was optimized by Polak-Ribiere algorithm. In the next step the simulated system was annealed for gaining lower energy minimum, and at last the kinetic and potential energy and temperature diagrams were plotted versus time. Same work as previous was done on the 3-D grid of 100 atoms and the results were compared together. The results show that the energy level depends significantly on the number of atoms and the melting temperatures are different in either case.

Measurement of radon gas in coal mine in the province Corum

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Existence of natural and half-life radio-active sources on earth and their decay products in the environments such soil, rocks, building materials, food, water and air is basic reason for radiation that people exposed to. Due to the fact that these radio-active sources are disproportionate in the environment, and doses people exposed to as a result of inner and outer radio-activation largely differ in accordance with daily routines. Radon is the only radio-active gas appearing as a result of uranium decay and existing in the nature. Because the source of Radon is uranium and uranium's disproportion in the nature, it is necessary to determine its average value in the soil. Annual concentration ratios determined by Turkish Atomic Energy Authority (TAEK) is 400 Bq/m3 at homes and 1000 Bq/m3 at workplaces on average in Turkey. In this study, Radon gas was measured at coal mines located in the province, ORUM. Thirty-three passive Radon detector (Cr-39) were placed in different points and depths of the mine. These detectors were left at these places for approximately sixty days and analysed in an isolated environment at the end of that period. Average Radon concentration activity was measured as 285,89 Bq/m3. As a consequence, it was observed that the results found are considerably below the values determined by TAEK.

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Index