Statistical properties of 1D time-dependent Hamilton systems

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I shall discuss studies of general nonlinear time-dependent 1D Hamiltonian systems. I shall present the general Papamikos-Robnik (PR) conjecture for parametrically kicked Hamilton systems, which says that for such systems the adiabatic invariant (the action) for an initial microcanonical ensemble at the mean final energy always increases under a parametric kick. I shall also present the ABR property, which is a local property, and many examples of the validity of this property which is almost always satisfied, but can be broken in not sufficiently smooth potentials or in cases where we are in the energy range close to a separatrix in the phase space. The general conjecture, using analytical and numerical computations, is shown to hold true for important systems like homogeneous power law potentials, pendulum, Kepler system, Morse potential, Pöschl-Teller I and II potentials, cosh potential, quadratic-linear potential, quadratic-quartic potential, while in three cases we demonstrate the absence of the ABR property: Linear oscillator enclosed in a box, sextic potential and quartic double well potential. In the second part of the talk I shall present the results of other kinds of time-dependent systems, assuming microcanonical ensemble of initial conditions, namely the cases of almost adiabatic (almost infinitely slow) variation, the case of unlimited linear driving of homogeneous power law potentials, where the nonlinear WKB-like method developed by Papamikos and Robnik (2012) can be applied, and analytic results on the statistical properties can be obtained. Finally, I shall discuss the cases of periodic driving.

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Superprevodnost in magnetizem v bližini prehoda kovina-izolator

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Prehode kovina-izolator lahko v splošnem razdelimo v dve kategoriji: v prvi se izolatorsko stanje pojavi kot posledica neke strukturne spremembe, ki odpre energijsko režo med valenčnim in prevodnim pasom, v drugi pa je izvor prehoda povsem elektronski. To drugo kategorijo prehodov znova lahko razdelimo v dve podkategoriji: v prvo sodijo materiali, kjer je prehod posledica močnih elektronskih korelacij (t.i. Mottov prehod), v drugi pa je posledica nereda (t.i. Andersonov prehod).

V tem prispevku bom obravnaval obanašanje različnih elektronskih stanj v bližini takih prehodov. Najprej se bom posvetil Mottovem prehodu v fulerenskih soleh, kjer smo preko meritev z jedrsko magnetno resonanco pod visokimi pritiski spremljali kako (antiferomagnetno) Mottovo-izolatorsko stanje zamenja superprevodnost s številnimi nenavadnimi lastnostmi [1]. V nadaljevanju pa bomo obravnavali vlogo nereda v Ti(O,N) nanožičkah, ki se neposredno odraža v transportnih lastnostih tako v normalni kot tudi v superprevodni fazi [2].

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Superconductivity and magnetism in the vicinity of metal-to-insulator transition

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Generally, metal-to-insulator transitions (MIT) can be divided into two categories. In the first category, the structural phase transition leads to a splitting of the electronic conduction band and hence to MIT. In the second category the transition is purely electronic in origin and can be again divided into two subcategories: one in which the transition is triggered by electronic correlations (i.e. Mott transition) and one in which it is triggered by disorder (i.e. Anderson transition).

In this contribution the behavior of competing electronic states in the vicinity of such transitions will be reviewed. In particular we will describe Mott transition in fulleride salts, where we have shown through comprehensive nuclear magnetic resonance measurements under high hydrostatic conditions that (antiferromagnetic) Mott insulating states is replaced by an unconventional superconductivity [1]. In the last part of the talk we will discuss the role of disorder in Ti(O,N) nanowires and how such disorder affects their transport properties in the normal and superconducting state [2].

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Metoda končnih elementov za teoretsko fiziko

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Predstavil bom nekaj izmed trenutnih zmogljivosti metode končnih elementov (FEM) za teoretsko fiziko.
S primerno vklopitvijo mrežne adaptivnosti v nelinearno minimizacijsko shemo lahko dosežemo v naprej nastavljeno napako. To smo uporabili pri minimizaciji Landau-de Gennes-ovega funkcionala proste energije in testirali na sistemih nematskih koloidov, a podobno je možno tudi za druge funkcionale iz teoretske fizike, kot npr. Ginzburg-Landau za superprevodnost, ali Gross-Pitajevskij za Bose-Einsteinove kondenzate.
Problem kako konkretno upoštevati brezdivergenčni pogoj za električna/magnetna polja v elektromagnetizmu ni bil zadovoljivo rešen kar nekaj let. Nédélec-ov tip končnega elementa je bil razvit nalašč za ta problem. Kratka koda, napisana v FreeFem++, točno izračuna lastne elektromagnetne načine v resonatorju napolnjenim z nehomogeno anizotropičnim materialom (nematski tekoči kristali).

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The finite element method for theoretical physics

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I will present some of the actual possibilities of the finite element method (FEM) for theoretical physics.
Mesh adaptivity, coupled to a nonlinear minimization scheme, can be used to reach an a priori fixed error threshold. This has been applied within the minimization of the Landau-de Gennes free energy functional for nematic liquid cystals, and tested on systems of nematic colloids, but similar functionals from theoretical physics, like the Ginzburg-Landau for superconductivity, or the Gross-Pitajevskij for Bose-Einstein condensates, apply as well.
How to impose the divergence-free condition for electric/magnetic fields in electromagnetism has not been satisfactorily solved/clarified for a couple of decades. The Nédélec type of finite element has been developed on porpouse to solve this particular problem. A short code in FreeFem++ correctly computes EM eigen modes in a resonator filled with nonhomogeneously anisotropic material (nematic).

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Difuzija hitrosti adiabatskega biljardnega plina

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Obravnaval bom dinamiko porazdelitve hitrosti idealnega neinteragirajočega plina ujetega v časovno odvisnem oscilirajočem biljardu. Pokazal bom, da povprečna hitrost plina narašča eksponentno hitro v času, v kolikor je dinamika delca v statičnih biljardih, ki konstituirajo časovo odvisni biljard, mešanega tipa. To je precej drugače kot v plinu trdih kroglic, katerega porazdelitev hitrosti je opisana z Maxwell - Boltzmannovo porazdelitvijo in katerega povprečna hitrost je v adiabatski limiti omejena z adiabatsko invarianto. Pokazal bom, da Maxwell-Boltzmannova porazdelitev ne opiše porazdelitve hitrosti niti v primeru, ko je dinamika delca v biljardu popolnoma kaotična. Konstruiral bom Fokker-Planckovo enačbo za porazdelitev hitrosti in izpeljal njeno fundamentalno in asimptotsko rešitev, ter pokazal odlično ujemanje z numeričnimi rezultati.

Velocity diffusion in adiabatic billiard gas

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I will discuss the evolution of the distribution of velocities of the ideal noninteracting gas in a time-dependent oscillatory billiard. I will show that the average velocity of the gas increases exponentially fast in time if the particle dynamics in a corresponding static billiards of a time-dependent billiard is of the mixed type. This is very different from the gas of hard-balls whose velocity distribution is described by the Maxwell-Boltzmann distribution and whose average velocity is constrained by the adiabatic invariant in the adiabatic limit. I will show that the Maxwell-Boltzmann distribution does not apply even in a fully chaotic time-dependent billiards. I shall construct a Fokker-Planck equation for the velocity distribution in a fully chaotic time-dependent billiard and derive its fundamental and asymptotic solutions, and show that they are in perfect agreement with numerical results.

How to make your own entropy formula?

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The good old exponential formula for the thermodynamical statistical weight factor at a given temperature, $\exp(-E/T)$, is valid only in the presence of huge (infinite) reservoirs in the background, keeping a sharp value for the subsystem's temperature. In high energy accelerator physics experiments typical reservoirs are small, they consist of a dozen or several hundreds to thousands of particles. The one particle energy spectra therefore are not exponential, even if treated statistically. We present statistical hadronization at a fixed total energy but varying particle number: the resulting picture of n-dimensional phase space volumina averaged over a distribution of n provides a cut power-law distribution of the one-particle energy. This generalizes the canonical exponential factor and includes it in the limit when n is Poisson distributed. Based on this experience we obtain the cut power-law statistical factor with general reservoir model equation of state, i.e. entropy – energy relation, S(E), and identify the famous q-factor of non-extensive thermodynamics. Deviations from the Gibbs–exponential are due to finite reservoir size and induced fluctuations in the thermodynamical beta parameter, $\beta = S'(E)$. For Gaussian "normal" fluctuations the Gibbs–exponential is reconstructed. In the general case, however $q \neq 1$, and the entropy is not additive even for ideal systems. We propose to use instead a function of it, $K(S)$, which composes additively between subsystems. From this requirement a prescriptive differential equation emerges for $K(S)$, whose solution pinpoints a certain entropy – probability formula. This fundates the recipe for making your own entropy formula.

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Relaksacijka dinamika več-delčnih sistemov

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Predstavil bom fundamentalno študijo ene in dveh vrzeli v t-J-Holsteinovem modelu pod vplivom zunanjega električnega polja. Ob upoštevanju kvantno mehanske narave problema sledimo časovnemu razvoju sistema začenši z osnovnim stanjem ko vključimo električno polje ob času nič ter vse do stacionarnega stanja. V primeru ene vrzeli opazimo adiabatski režim, kateremu sledi režim linearne $I - V$ karakteristike pri vmesnih električnih poljih [1,2,3]. Pri visokih poljih se sistem nahaja v režimu negativne diferencialne upornosti. Nadalje bom obravnaval tudi relaksacijo koreliranega sistema po vzbuditvi s kratkim električnim pulzom. Pokazal bom, da lahko foto vzbujeni nosilec naboja odda cca 1 eV energije spinskim ekscitacijam v času reda velikosti nekaj fs [4]. V zaključku bom obravnaval relaksacijko dinamiko v primeru sklopitve s spinskimi ter mrežnimi prostostnimi stopnjami [5].

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Relaxation dynamics of many-body systems

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I will present a fundamental study of one and two holes in the two dimensional t-J-Holstein model driven by the electric field. Taking fully into account quantum effects we follow the time-evolution of systems from their ground state as the electric field is switched on at $t = 0$, until they reach a steady state. In the single hole case adiabatic regime is observed followed by the positive differential resistivity at moderate fields where carrier mobility is determined [1,2,3]. At large field the system enters negative differential resistivity regime where current remains finite, proportional to $1/F$. I will also show that an ultrafast relaxation on the time-scale of 10 fs occurs due to inelastic scattering of a photo-excited carrier on spin excitations [4]. Finally, I will present relaxation dynamics of a carrier coupled to spin and lattice degrees of freedom [5].

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Geometrijski gradniki topološke mehke snovi

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Topološko zanimive teme, kot so stabilizacija defektov in solitonov, spletanje in vozlanje značilnih struktur, ter samourejevanje snovi, so uspešno raziskovalno področje v različnih panogah fizike. Med primere spadajo sinteza zavozlanih molekul [1], raziskave topologije v DNK in drugih polimerih [2], ter spletene strukture v ureditvenih poljih svetlobe [3], feromagnetov in različnih faz mehke snovi.

Vzorčni primer snovi, ki omogoča topološko stabilizirane strukture, so nematski tekoči kristali. Zaradi obstoja točkastih in linijskih defektov, močnega odziva na optično in električno polje, ter enostavnosti opazovanja pod mikroskopom, so idealni za demonstracijo teorije vozlov in interakcij med defekti v eksperimentalni postavitvi. Predstavil bom teoretične zakone spletanja in vozlanja nematskih defektov, ki uvedejo topološke invariante in pojasnijo strukture, videne v eksperimentih [4]. Prikazal bom obnašanje in nadzor spletanja defektov na 2D in 3D mrežah koloidnih delcev v tekočekristalnem mediju [5,6], ter v kapljicah kiralnega nematika [7]. Primeri se razlikujejo po geometriji prostora, ki ga zapolnjuje tekoči kristal, in po simetrijskih lastnostih samega tekočega kristala. Predstavil bom temeljne geometrijske gradnike, ki sestavljajo splete defektov v posameznih primerih.

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Geometric building blocks in topological soft matter

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Topological topics, such as stabilization of solitons and defects, knotting and linking of representative structures and self-assembly are targets of active development in different fields. Among them are targeted synthesis of knotted molecules [1], research of topological states in DNK and other polymers [2], and textures in ordering fields in light [3], ferromagnets and various soft materials.

Nematic liquid crystals are a typical medium that supports topologically stabilized structures. The existence of point and line defects, strong response to optical and electric fields, and easy observation under the microscope, make them ideal for demonstraction of knot theory and defect interaction in experimental environment. I present theoretical laws of linking and knotting of nematic defects, introduce topological invariants and explain structures seen in experiments [4]. I demonstrate the behaviour of knotted defects in 2D and 3D colloidal grids in LC medium [5,6] and chiral LC droplets [7]. The cases differ in geometry of the space occupied by the liquid crystal and in symmetry properties of the liquid crystalline structure itself. I review the basic geometric building blocks of defect networks in each of the cases.

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Lokalna integrabilnost in linearizabilnost $(1:-1:-1)$ resonantnega kvadratičnega sistema

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Raziskovali smo kompletno integrabilnost in linearizabilnost tri-dimenzionalnega sistema oblike

$$\begin{aligned}\dot{x} &= x + a_{12}xy + a_{13}xz + a_{23}yz\\ \dot{y} &= -y + b_{12}xy + b_{13}xz + b_{23}yz\\ \dot{z} &= -z + c_{12}xy + c_{13}xz + c_{23}yz.\end{aligned}$$

Pridobljeni so bili potrebni in zadostni pogoji obstoja dveh neodvisnih analitičnih integralov. Potrebni pogoji so bili izračunani z uporabo algoritmov računske komutativne algebre. Za dokaz integrabilnosti in linearizabilnosti je bila uporabljena Darboux-jeva metoda ter teorija normalnih form. Nekateri Darboux-jevi faktorji potrebni za linearizabilnost sistema so bili pridobljeni iz prvih integralov sistema. Obravnavali smo tudi problem obstoja enega analitičnega prvega integrala.

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Local integrability and linearizability of a $(1:-1:-1)$ resonant quadratic system

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We study the complete integrability and linearizability of a three dimensional system of the form

$$\begin{aligned}\dot{x} &= x + a_{12}xy + a_{13}xz + a_{23}yz\\ \dot{y} &= -y + b_{12}xy + b_{13}xz + b_{23}yz\\ \dot{z} &= -z + c_{12}xy + c_{13}xz + c_{23}yz.\end{aligned}$$

Necessary and sufficient conditions for existence of two functionally independent analytic integrals in the family are obtained. The necessary conditions are derived using algorithms of computational commutative algebra. To prove integrability and linearizability we used the method of Darboux and the normal form theory. Some Darboux factors used for linearizability are obtained from first integrals of systems. The problem of existence of only one analytic first integral is discussed as well.

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Collisions of planetesimals and the formation of planets

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Since the last 20 years many planets (approx. 1850 up to now) around other stars were detected either from the ground or by space missions. More than 500 planetary systems with more than one discovered planet are known; for planets being habitable many conditions need to be fulfilled: e.g. the spectral type and age of the hosting star, the location in our galaxy and also the orbit of a planet and its physical nature. Different estimates lead to quite different results especially for planet which host in fact life. In this respect we show the results of collision computations with the aid of Smooth Particle Hydrodynamic (SPH) codes and discuss also in short the role of the tides acting on these bodies.

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Leptokvarki v fiziki okusov in hadronskih trkalnikov

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Leptoquarki interagirajo s kvarki in leptoni in so običajno prisotni v teorijah poenotenja osnovnih interakcij. V teh teorijah, praviloma, imajo mase blizu mase v skale GUT. Vendar, pa v nekaterih teorijah poenotenja imajo lahko skalarni leptokvarki mase reda velikosti 1 TeV. Takšna stanja so lahko prisotna v procesih na nizkih energijah. Obenem, jih lahko opazijo na hadronskih trkalnikih. Naš študij je posvečen raziskavi lahkih leptoquarkov, kateri ne morejo destabilizirati proton. Takšni "nenevarni" leptokvarki lahko imajo relativno velike sklopitve s fermioni standardnega modela. Obravnavamo vpliv teh sklopitev na mehanizme produkcije leptokvarkov na LHC in ugotavljamo, da je za produkcijo leptokvarkov v teh primerih zelo pomemben prispevek t-kanala.

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Scalar Leptoquarks in Flavor and Collider Physics

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Leptoquarks interact with quarks and leptons and they are usually present in theories which unify fundamental interactions. In these theories they naturally have a mass close to the GUT scale. However, in some of unification approaches scalar leptoquarks might have masses of the order 1 TeV. Such are states might modify processes at the low-energies. At the same time they can be seen at Large hadronic collider directly. These light leptoquark states should not mediate proton decay at the tree level. Our analysis is devoted to the light leptoquarks which do not destabilise proton. These "non-dangerous" scalar leptoquarks might have sizeable couplings to the Standard Model fermions. We discuss leptoquark production mechanisms at LHC and demonstrate the importance of inclusion of a t-channel pair production.

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Hopfove bifurkacije v sistemih NDE

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Najprej bom razložila Hopfovo (ali Andronov-Hopfovo) bifurkacijo za ravninske sisteme. Opisala bom limitne cikle na centralni mnogoterosti in degenerirane Hopfove (Bautinove) bifurkacije. Nato bom predstavila enega izmed najbolj znanih problemov kvalitativne teorije navadnih diferencialnih enačb - Hilbertov 16. problem o številu limitnih ciklov dvo-dimenzionalnih sistemov

$$\dot{x} = P_n(x, y), \quad \dot{y} = Q_n(x, y)$$

(n je maksimalna stopnja polinomov na desni strani sistema). Bistven del problema je problem ocenitve maksimalnega število limitnih ciklov, ki bifurcirajo iz singularne točke tipa center ali fokus pod vplivom majhnih motenj koeficientov sistema, t.j. problem cikličnosti. Ključna značilnost našega pristopa je, da je v primeru elementarne singularne točke problem cikličnosti reduciran na algebraični problem iskanja baze določenega polinomskega ideala. Ta pristop nato uporabimo za problem cikličnosti poddružine kubičnih sistemov.

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Hopf bifurcations in systems of ODE's

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First, I will discuss a Hopf (or Andronov-Hopf) bifurcation for planar systems. I will describe also limit cycles on the center manifold and degenerate Hopf (Bautin) bifurcations. Then, I will present one of the most famous problems in qualitative theory of ordinary differential equations - Hilbert's sixteenth problem on the number of limit cycles of two dimensional polynomial systems

$$\dot{x} = P_n(x, y), \quad \dot{y} = Q_n(x, y)$$

(n is the maximum degree of the polynomials on the right-hand side of the system). An essential part of the problem is the problem of estimating of the maximum number of limit cycles which can bifurcate from a singular point of center or focus type under small perturbations of coefficients of the system, the so-called cyclicity problem. The key feature of our approach is that in the case of an elementary singular point the problem of cyclicity is reduced to the algebraic problem of searching for a basis of a certain polynomial ideal. We apply this approach for solving the cyclicity problem for a subfamily of cubic systems.

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Uporaba pristopov s področja kompleksnih sistemov za preučevanje funkcionalne in strukturne organiziranosti sincicija celic beta

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Metodologija s področja kompleksnih sistemov se dandanes vse pogosteje uporablja za preučevanje in razumevanje organizacijskih ter funkcionalnih principov bioloških sistemov, in to na najrazličnejših skalah [1]. V naši študiji se osredotočimo na kolektivno dinamiko celic beta v Langerhansovih otočkih trebušne slinavke, ki vodi do izločanja inzulina. Na osnovi korelacij med izmerjenimi časovnimi vrstami znotrajceličnih kalcijevih signalov, pridobljenih s konfokalnim mikroskopom, smo izgradili funkcionalno mrežo celic beta, s katero okarakteriziramo medcelično komuniciranje [2]. Ekstrahirane vzorce medcelične povezanosti analiziramo z uveljavljenimi orodji s področja teorije kompleksnih mrež. Z izračunom različnih mrežnih mer si ne pridobimo le informacij o naravi funkcionalnih medceličnih povezav, temveč lahko tudi sledimo časovnemu razvoju strukture mreže [3]. Za pridobitev še bolj poglobljenega vpogleda v delovanje Langerhansovih otočkov se poslužimo tudi matematičnega modeliranja. Izdelali smo podroben večelični matematični model sincicija celic beta, kjer posamezne celice predstavljajo vozle, povezave pa ponazarjajo medcelično komunikacijo. V model smo vključili tudi dodatne eksperimentalno ugotovljene fiziološke detajle. Naši rezultati pokažejo, da je kombinacija naprednih mikroskopskih tehnik, sodobnih analitičnih orodji in matematičnega modeliranja zelo udarno orodje, s katerim si lahko pridobimo poglobljen vpogled v delovanje Langerhansovih otočkov. Prav tako nam tovrstna metodologija nudi dobro izhodišče za preučevanje modifikacij povezanih s patofiziolokimi stanji, kot je na primer sladkorna bolezen.

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Application of complex systems approaches for studying the functional and structural organization of the pancreatic beta cell syncytium

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Methodology developed in the field of complex systems science is nowadays frequently used for the analysis of the structure and function of biological systems at different scales [1]. In our study we focus on the collective pancreatic beta cell activity in the islets of Langerhans, which triggers and regulates insulin secretion. For the characterization of the intercellular communication we build up functional networks on the basis of correlations between calcium dynamics of individual cells, which were recorded by means of confocal laser-scanning microscopy [2]. The extracted pattern of pairwise interactions between network cells, i.e. functional connections, is then scrutinized with conventional tools for network analysis. By calculating the network metrics of interest, we can not only characterize the nature of functional connectivity patterns, but can also track and analyze the temporal evolution of tissue networks [3]. In order to complement our understanding of the mechanisms that govern the functioning of islets, we make use of mathematical modelling approaches. We propose a detailed multicellular model of interconnected beta cells, which upgrades the existing modeling endeavors by incorporating additional physiological specifics. Our results demonstrate that a combination of advanced high spatial and temporal resolution confocal imaging, novel analytical tools and computational modeling is a powerful tool that enables not only a comprehensive understanding of functional mechanisms and organization of islets of Langerhans but also provides a firm framework for the examination of modifications associated with pathophysiological conditions, such as diabetes mellitus.

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Second-order hydrodynamics and universality from the gauge/string duality

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The gauge/string duality has provided us with a tool for analysing certain classes of strongly coupled field theories. In its simplest limit of a large number of colours and a large 't Hooft coupling, it enables us to compute field theory correlation functions at all energy scales, directly from classical gravity. In the hydrodynamical limit, the duality gives us both the structure of the hydrodynamical gradient expansion at all orders as well the transport coefficients of the fluid. We can therefore use it to study higher-order corrections to the one-derivative Navier-Stokes equations. After presenting the gauge/string duality, I will discuss second-order hydrodynamics and a universal result relating three of its transport coefficients at strong coupling. I will focus on higher-derivative gravity corrections to the universal relation, particularly in a non-perturbative limit in which viscosity vanishes and second-order hydrodynamics becomes dominant. Finally, the phenomenology of nearly dissipationless fluids will be discussed, using the holographic Gauss-Bonnet fluid as an example.

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Jata galaksij "Bullet" in ekstremni objekti v Hubblovem volumnu

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Velike jate in nadjate galaksij so največji gravitacijsko vezani objekti v našem vesolju. Pričakujemo, da se zaradi širjenja vesolja premikajo stran drug od drugega. V zadnjih časih so bile odkrite številne jate, ki so v procesu trčenja - nasprotno od naivnega pričakovanja. Med njimi je najbolj raziskovana in slavna "Bullet" jata galaksij. Torej, preveriti moramo ali je naš ΛCDM model vesolja zmožen generirati trke velikih jat galaksij. Ker so trki nelinearni, se predikcije ΛCDM modela testirajo v kontekstu kozmoloških simulacij N-teles. V preteklosti se je pojavil konsenz, da so trki kot je "Bullet" jata malo verjetni in jih ne pričakujemo v našem vesolju. Opis in preučevanje ekstremnih dogodkov v repih distribucij zahteva nestandardna statistična orodja (npr. Statistika ekstremnih vrednosti) in precizno poznavanje numeričnih metod v simulacijah. Nove metode, skupaj z eno od največjih kozmoloških simulacij N-teles, nas pripeljejo do sklepa, da so trki jat galaksij bolj pogosti, kot smo pričakovali v preteklosti.

The Bullet cluster and extreme objects in the Hubble volume

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Large galaxy clusters are the biggest gravitationally bound objects in our universe. They are expected to follow the Hubble flow - move away from each other due to the expansion of the universe. However, a significant number of colliding clusters has been found, with the Bullet cluster being the best studied and most famous. Therefore, our naive expectation and the concordance ΛCDM model have to be reconciled with the observation. Because of their highly non-linear nature, cluster collisions have been studied in the context of cosmological N-Body simulations and were found to be highly unlikely. Studying the extreme events in the tails of distributions requires non-standard statistical tools (e.g. Extreme Value Statistics) as well as a precise understanding of the numerical methods used in the simulations. Using improved methodology and one of the largest simulations of our universe we show that the collisions of large clusters do occur and are not as rare as previously thought.

Lattice hadron scattering: An introduction

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Recent years have seen considerable progress in ab initio QCD calculations of hadron scattering threshold parameters and scattering phase shifts in the (elastic) resonance region. The lattice approach is becoming powerful enough to even predict states in the heavy quark sector. I will discuss the methods and limitations in an introductory way, In a subsequent talk Sasa Prelovsek will present more details and recent results.

Statistical physics of isotropic-genesis nematic elastomers

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I will present an overview of nematic elastomers, which are nematic polymers that have been randomly, permanently cross-linked to form an equilibrium random solid network. I explain how such systems involve both annealed (thermal) as well as quenched (architectural) disorder. The distribution of thermal configurations of nematic polymers can be "memorized" by the elastomer at the instant of cross-linking, and I will show how a replica field theory formalism (inspired by Deam and Edwards) manages to capture this piece of physics. The random solid network restricts the motion of nematic polymer segments, and we address how this restriction modifies the liquid crystalline structure of nematic elastomers at high temperatures. In particular, we show that short-ranged oscillatory spatial correlations in the nematic alignment can emerge for a class of nematic elastomers at a sufficiently high density of cross-links.

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Wave dynamics in nonhermitian Photonics

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One of the frontiers of modern photonics is the engineering of the complex refractive index to create new composite systems with novel functionalities. In most systems optical loss has been always considered an obstacle. However, based on the recently introduced concept of parity-time (PT)-symmetry in the context of optical physics, such synthetic structures can utilize loss as an advantage and have been proven to be important for various nanophotonics applications. In this framework of open photonic systems, we also present a larger class of nonhermitian materials that are on average, lossy. These geometries exhibit transient power growth, the magnitude of which is related to the singular values of the non-normal propagator. The nontrivial wave dynamics in such nonhermitian optical structures can be understood in terms of the pseudospectra of the underlying non-normal operator. Active photonic systems that are on average lossy, are of current interest in nano-plasmonics.

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Entropija in termoelektrični pojav v rutenatih

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V snoveh temperaturni gradienti povzročijo električno polje. Ta termoelektrični pojav nastane zaradi zlomitve simetrije delec-vrzel in je uporaben v hlajenju in za koristno uporabo odvečne toplote, npr. iz avtomobilskih izpuhov. Po drugi strani meritev razmerja med električnim poljem in termalnim gradientom (Seebeckov koeficient) vsebuje pomembno informacijo o snovi in je zanimiva v bazičnih raziskavah trdne snovi. V predavanju bom obravnaval zvezo med Seebeckovim koeficientom in entropijo. Kot primer bom uporabil snov z močnimi elektronskimi korelacijami Sr_2RuO_4, ki jo bom opisal v teoriji dinamičnega povprečnega polja. Pokazal bom, da Seebeckov koeficient v ravnini ab tesno sledi rezultatu, ki sledi iz entropijskega razmisleka, Seebeckov koeficient v pravokotni ravnin c pa ne. To obnašanje razkriva poseben mehanizem, ki filtrira vrzeli in nastane kot posledica telesno centrirane rešetke.

Revealing active degrees of freedom, beating the entropy by hole filtering: lessons from thermopower in Sr2RuO4

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In materials, thermal gradients are accompanied by electrical fields. This 'thermoelectric effect' that comes from the particle-hole asymmetry can be used for solid-state refrigiration and waste heat recovery. On the fundamental side, the measurement of the ratio between the electric field and the thermal gradient (which is called Seebeck coefficient or thermopower) can be a revealing probe of the state of material. In this seminar, I will discuss the relation of thermopower to entropy. As an example, I will consider Sr2RuO4, a compound with intermediate strength of electronic correlations, which I will describe within the dynamical mean-field theory. I will argue that the in-plane thermopower reveals the active degrees of freedom which demonstrates potential of entropic interpretations of thermoelectric effect. On the other hand, the predicted c-axis thermopower is much higher and inconsistent with entropic consideration, a behavior that points to a peculiar hole-filtering mechanism.

Povezane strategije v evolucijskih igrah

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Kooperacija v človeških družbah je zelo pogosta in razširjena, in to nas pomembno ločuje od ostalih živalskih vrst. Začetki človeške kooperacije naj bi bili povezani s težavnostjo vzreje mladičev v zgodnji fazi razvoja naše vrste. Toda to že dolgo ni več problem. Vprašanje je, zakaj še vedno sodelujemo? Recipročnost je ena izmed ključnih predpostavk. Če je nekdo do nas prijazen, potem smo prijazni nazaj. Podobno, če smo izpostavljeni nepravičnosti in izkoriščevanju se maščujemo. Sodeč po teoriji močne recipročnosti naj bi bili tovrstna pozitivna in negativna recipročnost povezani. Toda je to res? Nedavni ekonomski eksperimenti zavračajo teorijo močne recipročnosti, in tudi vsakodnevne izkušnje govorijo, da ljudje bodisi primarno nagrajujemo lepo obnašanje ali pa kaznujemo grdo obnašanje, redko pa delamo z enako vnemo oboje. Pokazali bomo, kako lahko metode statistične fizike doprinesejo k razrešitvi nesoglasij med teorijo in prakso [1].

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Correlated strategies in evolutionary games

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Widespread cooperation among unrelated individuals distinguishes humans markedly from other species. The origins of our remarkable other-regarding abilities have been associated with rearing offspring that survived, which was a pressing challenge during the Paleolithic age that could not be met by individual efforts alone. But in the absence of such a challenge, what keeps us cooperating? Reciprocity is long considered an important piece of the puzzle. If someone is kind to us, we are kind in return. Similarly, if someone is unfair or exploitative, we tend to retaliate. And according to the strong reciprocity hypothesis, this positive and negative reciprocity are correlated to give us optimal evolutionary predispositions for the successful evolution of cooperation. But is this really true? Recent economic experiments reject the hypothesis, and everyday experiences leave us with the impression that people either tend to reward success or punish wrongdoing, but seldom will they do both. We show how methods of statistical physics contribute to resolving the disagreement between theory and observations [1].

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50 years of quarks

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Fifty years ago, in 1964, the notion of quarks was introduced [1]. Their interaction was formulated more than 40 years ago [2]. Still, the corresponding theory, quantum chromodynamics, cannot yet be solved comprehensively. Rather one has to resort to approximations, simulations, or models.

We discuss the development and present performance of the constituent-quark model for low-energy quantum chromodynamics [3,4], which gets by with a finite number of degrees of freedom contrary to the full quantum field theory. In particular, we address the spectroscopy of all known baryons, the structure of the nucleons exhibited under all (electromagnetic, weak, and gravitational) interactions, the electroweak structures of the other baryons with flavors up, down, and strange, as well as strong resonance decays. It turns out that by the improvements achieved over recent years a wide range of baryon properties and reactions can now be described by the relativistic constituent-quark model in rather good agreement with phenomenology and, where experimental data are missing, in reasonable congruence with results available from lattice quantum chromodynamics. The most important ingredients are relativistic invariance and a quark dynamics following from the spontaneous breaking of chiral symmetry in low-energy quantum chromodynamics. Challenging problems still exist with a proper description of resonance states and their couplings to decay channels.

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Nered in antifragilnost v coulombskih tekočinah

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Kaj se zgodi z elektrostatskimi interakcijami , ?e je gostota naboja na makromolekularnih površinah podana z netermalizirano razurejeno porazdelitvijo? Predstavil bom formalni okvir [1], ki nam omogoča, da teoretično opišemo interakcije dolgega dosega v kontekstu omejenih coulombskih tekočin z razurejenimi izvori na robovih. Monopolaren in dipolaren nered vodita v tem kontekstu do bistveno modificiranih sil med mejnimi površinami [2], ki postanejo anomalno dolgega dosega tako v normalni kot tudi v lateralni smeri. Poleg tega se pojavijo tudi anomalni navori kot posledica razurejen porazdelitve nabojev. Posledice nereda ostajajo, tudi če so mejne površine v celoti vzeto elektronevtralne in lahko kot takšni razložijo celo vrsto parazitskih efektov, ki se jih da opaziti pri meritvah Casimirjeve sile. V primeru močno sklopljenih coulombskih tekočin z netermaliziranim neredom, razurejeni izvori lahko pripeljejo celo do pojava antifragilnosti v sistemu, ko več nereda na površinah vodi k zmanjšanju termičnega nereda.

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Disorder and antifragility in Coulomb fluids

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What happens to electrostatic interactions when charge density on macromolecular surfaces is charac- terized by quenched disorder distribution? Formal framework will be presented [1] that allows for the- oretical description of long-range electrostatic interactions in the presence of quenched disordered source fields on the boundaries. Monopolar and/or dipolar surface charge disorder, in the context of confined Coulomb fluids, gives rise to fundamentally modified interactions between planar bounding surfaces [2], characterized by anomalously long-ranged normal and lateral forces as well as torques. Disorder effects persist even in the case of overall charge-neutral surfaces and can help elucidate various parasitic effects known to exist in e.g. the Casimir interaction. In the case of strongly coupled Coulomb fluids with quenched disordered source fields a peculiar type of antifragility emerges where more imposed external source disorder actually diminishes the thermal disorder in the system, allowing the system to benefit from disorder.

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Močni razpadi mezonov $D^*_{s0}(2317)$ in $D_{sJ}(2460)$

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Leta 2003 je več kolaboracij opazilo ozki rezonanci $D^*_{s0}(2317)$ in $D_{sJ}(2460)$. Pridobljeni podatki nakazujejo, da gre za mezone pozitivne parnosti in $\bar{c}s$ strukture. Zaradi prenizke mase, omenjena stanja ne morejo razpasti v nižje ležeči D mezon z emitiranjem kaona, ampak se lahko emitirjo le pioni in fotoni. Ker pioni ne vsebujejo c ali s kvarka, močni razpadi so možni le preko kiralnih zank ali efektov izospinke kršitve, kot je naprimer mešanje $\eta - \pi_0$. Eksmerimentalno so opazili tri takšne razpade: $D^{*+}_{s0}(2317) \to D^+_s\pi_0$, $D_{sJ}(2460) \to D^{*+}_s\pi_0$ in $D_{sJ}(2460) \to D_s\pi^+\pi^-$. Govorila bom o vplivu kiralnih zank na zgoraj naštete razpade z uporabo formalizma kiralne simetrije in limite težkih mezonov.

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Strong decay modes of $D^*_{s0}(2317)$ and $D_{sJ}(2460)$ mesons

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In 2003 several collaborations reported an observation of two narrow states: $D^*_{s0}(2317)$ and $D_{sJ}(2460)$. The data indicates that these are positive parity meson states with $\bar{c}s$ structure. Because of their low mass, $D^*_{s0}(2317)$ and $D_{sJ}(2460)$ can not decay into other D- meson states by emitting a kaon. Only emitting pions or photons is possible. As pions do not include strange quarks in their structure, the strong decay modes can only occur trough chiral loops or isospin violating effects like $\eta-\pi$ mixing. Three such strong decay channels of $D^*_{s0}(2317)$ and $D_{sJ}(2460)$ where observed by experiment: $D^{*+}_{s0}(2317) \to D^+_s\pi_0$, $D_{sJ}(2460) \to D^{*+}_s\pi_0$ and $D_{sJ}(2460) \to D_s\pi^+\pi^-$. Here I will talk about the effects of chiral loops in these decay modes using the formalism of heavy meson chiral Lagrangians.

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Običajni in eksotični hadroni

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Kromodinamika na mreži predstavlja ne-perturbativni pristop za študj hadronskih lastnosti ab-initio. Predstavila bom dve mezonski stanji, ki se nahajata malce pod pragom in pri katerih simulacije prvič upoštevajo vpliv praga: gre za zanimivo stanje $X(3872)$ [1], ki je morda mezonska molekula $D^0\bar{D}^{0*}$, ter za skalarni mezon $D^*_{s0}(2317)$ [2,3]. Obravnavala bom tudi čudne [4] in čarobne [5] hadronske resonance, pri katerih smo poleg mase prvič določili tudi razpadno širino. Opisala bom zahtevno iskanje eksotičnih stanj s kvarkovsko strukturo $\bar{c}c\bar{d}u$ [6], ki so bila nedavo odkrita v eksperimentu.

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Conventional and exotic hadrons

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QuantumChromoDynamics on the lattice presents a non-perturbative method to study the hadronic properties ab-initio. I will present the simulations of the mesonic states that lie slightly below thresholds, where the threshold effects are accounted for the first time. I will consider interesting state $X(3872)$ [1], which may be $D^0\bar{D}^{0*}$ molecule, and the scalar meson $D^*_{s0}(2317)$ [2,3]. The strange [4] and charmed [5] resonances will be considered, where the decay width is calculated for the first time. I will describe the challenging search for the exotic states with the quark content $\bar{c}c\bar{d}u$ [6], which have been recently discovered by several experiments.

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Točne rešitve kvantnih transportnih problemov daleč od ravnovesja in novi ohranitveni zakoni

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Anizotropna Heisenbergova veriga spinov 1/2 je osnovna paradigma sistema močno koreliranih elektronov v eni dimenziji (glej npr. [1]). Čeprav ravnovesne lastnosti modela dobro razumemo, so bile do nedavna odprta še zelo osnovna vprašanja v zvezi z neravnovesnimi, transportnimi lastnostmi, kot je npr. vprašanje [1,2], ali model dovoljuje balistični spinski transport pri končni temperaturi ali ne?

V predavanju bom na kratko orisal bistveni napredek na tem področju, ki ga je sprožilo odkritje točne rešitve kvantne master-enačbe za robno gnano Heisenbergovo verigo [3,4]. Stacionarna rešitev neravnovesne master enačbe namreč vodi do povsem novih kvazi-lokalnih ohranitvenih zakonov [3,7,10], ki posledično omogočajo strogo oceno balističnih transportnih koeficientov [6]. Takšen pristop 'neravnovesne integrabilnosti' deluje tudi za nekatere druge kvantne verige z močno interakcijo, kot je npr. Hubbardov model [8], ali Lai-Sutherlandov model verige spinov 1 [9].

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Exact solutions of quantum transport problems far from equilibrium and new conservation laws

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Anisotropic Heisenberg chain of spins 1/2 is the key paradigm of strongly correlated electrons in one dimension (see e.g. [1]). While equilibrium properties of the model are relatively well understood, even very basic questions about its non equilibrium properties were still open until very recently. A prominent example is the question [1,2] whether the model exhibits ballistic spin transport at finite temperatures or not?

In my talk I will outline the progress on this topic which has been triggered by the discovery of exact solution of quantum master equation of the boundary driven Heisenberg chain [3,4]. The steady-state solution of non-equilibrium master equation leads to novel quasi-local conservation laws [3,7,10], which in turn lead to a derivation of rigorous strict lower bounds on ballistic transport coefficients [6]. Such an approach of 'non-equilbrium integrability' works also for some other strongly interacting quantum chains, for instance, for the Hubbard model [8] or Lai-Sutherland model of spins 1 [9].

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Kvantni kaos v sistemih mešanega tipa

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Najprej bom predstavil uvod v glavne pojme kvantnega kaosa, ali bolj splošno - valovnega kaosa, nato obravnaval sisteme mešanega tipa, to so generični Hamiltonovi sistemi, ki imajo klasično regularno dinamiko za določene začetne pogoje ter kaotično dinamiko za komplementarne začetne pogoje. Tipična struktura faznega prostora je kaotično morje, ki vsebuje otoke regularnosti in stabilnosti. Nato bom predstavil nekaj najnovejših izsledkov o kvantni lokalizaciji kaotičnih stanj.

Kvantna lokalizacija klasično kaotičnih lastnih stanj je eden najpomemnejših pojavov v kvantnem kaosu, poleg značilnega vedenja statističnih lastnosti energijskih spektrov. Kvantna lokalizacija nastopi, če je t.i. Heisenbergov čas t_H danega sistema krajši od vseh klasičnih transportnih časov v danem klasičnem sistemu, se pravi, kadar je klasični transport počasnejši od kvantne časovne resolucije evolucijskega operatorja. Heisenbergov čas t_H, kot pomembna karakteristika vsakega kvantnega sistema, je namreč enak razmerju Planckove konstante $2\pi\hbar$ ter srednjega razmika med energijskimi nivoji ΔE, $t_H = 2\pi\hbar/\Delta E$.

Pokazali bomo funkcionalno povezavo med stopnjo lokalizacije ter spektralno statistiko v avtonomnih (časovno neodvisnih) sistemih, v analogiji z brcanim rotorjem, ki pa je paradigma časovno periodičnih (Floquetovih) sistemov [7], ter pristop in metodo ilustrirali v primeru družine biljardov [8,9] v dinamičnem režimu med integrabilnostjo (krog) in polnem kaosom (kardioda), kjer bomo ekstrahirali kaotična stanja. Stopnjo lokalizacije določimo z dvema lokalizacijskima merama, z uporabo t.i. Poincaré-Husimijevih funkcij (ki so Gaussovo glajene Wignerjeve funkcije v Poincaré-Birkhoffovem faznem prostoru), ki so pozitivno definitne in jih lahko obravnavamo kot kvazi-verjetnostne gostote. Prva mera A je definirana s pomočjo informacijske entropije, druga (C), pa s pomočjo korelacij v faznem prostoru Poincaré-Husimijevih funkcij lastnih stanj. Presenetljivo in zelo zadovoljivo se izkaže, da sta obe meri linearno povezani in zato ekvivalentni.

Ena od glavnih manifestacij kaosa v kaotičnih stanjih v odsotnosti kvantne lokalizacije

je porazdelitev $P(S)$ razmikov S med sosednjimi energijskimi nivoji, ki se vede pri majhnih S kot linearna funkcija $P(S) \propto S$, in govorimo o linearnem odbijanju med sosednjimi nivoji, medtem ko imamo v integrabilnih sistemih Poissonovo statistiko (eksponentno funkcijo $P(S) = \exp(-S)$), kjer odbijanja med sosednjimi nivoji ni ($P(0) = 1 \neq 0$). V povsem kaotičnem režimu s kvantno lokalizacijo pa opazimo, da je $P(S)$ pri majhnih S potenčna funkcija $P(S) \propto S^{\beta}$, z $0 < \beta < 1$. Pokazali bomo, da obstaja funkcionalna odvisnost med mero lokalizacije A in eksponentom β, namreč da je β monotona funkcija A: pri močni lokalizaciji sta A in β majhna, pri šibki lokalizaciji (skoraj povsem razširjena kaotična stanja) pa sta A in β blizu 1.

Pristop ilustriramo v primeru kaotičnih stanj za zgoraj omenjene družine biljardov, kjer lahko ločimo regularna in kaotična stanja. Ta predstavitev sloni na naših najnovejših člankih [1,4,5,7].

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Quantum chaos in the mixed-type systems

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First I shall present an introduction to the main concepts of quantum chaos, or more generally - wave chaos, and then deal with the mixed-type systems, that are the generic Hamilton systems which have classical regular dynamics for some initial conditions and chaotic dynamics for the complementary initial conditions. The typical structure of the phase space is a chaotic sea containing islands of regularity and stability of motion. Then I will present some most recent results on quantum localization of chaotic eigenstates.

Quantum localization of classical chaotic eigenstatets is one of the most important phenomena in quantum chaos, along with the characteristic behaviour of statistical properties of the energy spectra. Quantum localization sets in, if the Heisenberg time t_H of the given system is shorter than the classical transport times of the underlying classical system, i.e. when the classical transport is slower than the quantum time resolution of the evolution operator. The Heisenberg time t_H, as an important characterization of every quantum system, is namely equal to the ratio of the Planck constant $2\pi\hbar$ and the mean spacing between two nearest energy levels ΔE, $t_H = 2\pi\hbar/\Delta E$.

We shall show the functional dependence between the degree of localization and the spectral statistics in autonomous (time independent) systems, in analogy with the kicked rotator, which is the paradigm of the time periodic (Floquet) systems [7], and shall demonstrate the approach and the method in the case of a billiard family [8,9] in the dynamical regime between the integrability (circle) and full chaos (cardioid), where we shall extract the chaotic eigenstates. The degree of localization is determined by two localization measures, using the Poincaré Husimi functions (which are the Gaussian smoothed Wigner functions in the Poincaré Birkhoff phase space), which are positive definite and can be treated as quasi-probability densities. The first measure A is defined by means of the information entropy, whilst the second one, C, in terms of the correlations in the phase space of the Poincaré Husimi functions of the eigenstates. Surprisingly, and very satisfactory, the two measueres

are linearly related and thus equivalent.

One of the main manifestations of chaos in chaotic eigenstates in absence of the quantum localization is the energy level spacing distribution $P(S)$ (of nearest neighbours), which at small S is linear $P(S) \propto S$, and we speak of the linear level repulsion, while in the integrable systems we have the Poisson statistics (exponential function $P(S) = \exp(-S)$), where there is no level repulsion ($P(0) = 1 \neq 0$). In fully chaotic regime with quantum localization we observe that $P(S)$ at small S is a power law $P(S) \propto S^{\beta}$, with $0 < \beta < 1$. We shall show that there is a functional dependence between the localization measure A and the exponent β, namely that β is a monotonic function of A: in the case of the strong localization are A and β small, while in the case of weak localization (almost extended chaotic states) A and β are close to 1.

We shall illustrate the approach in the model example of the above mentioned billiard family, where we can separate the regular and chaotic states. This presentation is based on our very recent papers [1,4,5,7].

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Integrabilnost nekaterih sistemov NDE

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Obravnavamo problem iskanja sistemov z enim ali nekaj neodvisnimi prvimi integrali znotraj družin avtonomnih sistemov navadnih diferencialnih enačb odvisnih od parametrov. Metode konstruiranja prvih integralov ali dokazovanje njihovega obstoja v takšnih sistemih so prediskutirane. Med njimi je največ pozornosti usmerjene na Poincaré-Dulacovo metodo normalnih form, Darbouxjevo metodo in povezavo med integrabilnostjo in časovno reverzibilnostjo. Učinkovit računski pristop k problemu iskanja prvih integralov je predlagan. Nekateri primeri uporabe teorije in računskega pristopa so predstavljeni.

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Integrability of some systems of ODEs

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The problem of finding systems with one or few independent first integrals inside families of autonomous systems of ODEs depending on parameters is discussed. Methods to construct first integrals or prove their existence in such systems are reviewed. Among them the main attention is paid to the Poincaré-Dulac normal form method, the Darboux method and the interconnection of integrability and time-reversibility. An efficient computational technique to the problem of finding first integrals is proposed. Some examples of application of the theory and the computational approach are presented.

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Stability and periodic oscillations in the Moon-Rand System

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The Moon-Rand system is a family of ordinary differential equations in three-dimensional Euclidean space developed to model control of flexible structures. Members of the family possess an equilibrium at the origin at which the linear part has one negative and two purely imaginary eigenvalues for all values of the parameters. We describe a complete stability analysis of the origin and provide a sharp upper bound on the number of isolated periodic orbits that can be made to bifurcate from the origin when the flow restricted to any so-called local "center manifold" is a focus. (Joint work with A. Mahdi and V. G. Romanovski.)

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Stohastična simulacija prostorsko-časovne cirkadiane aktivnosti v suprakiazmatičnem jedru

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Pri sesalcih dnevni ritem uravnava cirkadiani spodbujevalnik v suprakiazmatičnem jedru v hipotalamusu, ki organizem sinhronizira s periodičnimi okoljskimi pogoji, kot je dnevno-nočni svetlobni cikel. Najpomembnejša faktorja, ki zagotavljata 24-urni cirkadiani ritem, sta sklopitev nevronske aktivnosti z okoljem in medcelična komunikacija med nevroni [1]. Natančnost na časovni skali je dosežena kljub znatni ravni fluktuacij zaradi izredno majhnih koncentracij regulacijskih molekul. Da bi preverili vpliva molekularnega šuma in medcelične povezanosti na sinhronizacijo nevronske mreže, smo izdelali večcelični stohastič-ni model suprakiazmatičnega jedra. Za opis medcelične komunikacije preko nevrotransmiterjev smo uporabili relativno realno sklopitveno shemo, ki temelji na eksperimentalnih ugotovitvah in izkazuje lastnosti mreže malega sveta [2,3]. Naši rezultati kažejo, da so nevronske mreže robustne na znotrajcelične fluktuacije in da jih lahko učinkovito vzbujamo s svetlobnimi cikli, kljub znatni meri stohastičnosti, pri čemer je koherenca oscilacij odvisna od narave medcelične komunikacije. Poleg tega smo pokazali, da vzorci nevronske aktivnosti oblikujejo lokalne sinhronizirane gruče, ki so bolj izrazite pri časovno kratkih fotoperiodah (zima) kot pri dolgih dnevih (poletje). S tem smo pokazali, da sezonske adaptacije cirkadianih ritmov ne vključujejo le reorganizacijo nevronske aktivnosti na časovni skali [3,4], temveč tudi na prostorski.

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Stohastic simulation of the spatio-temporal circadian activity in the suprachiasmatic nucleus

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In mammals, daily rhythms are driven by the circadian pacemaker in the suprachiasmatic nucleus (SCN) of the hypothalamus, which synchronizes an organism to periodically recurring environmental conditions, such as the solar day-night cycle. The coupling of the SCN neuronal activity with the environment and the intercellular communication between SCN neurons are the most important factors that ensure the precise 24h timing of the circadian rhythmicity, despite significant fluctuations in chemical activities due to very small numbers of regulatory molecules in individual cells [1]. We have developed a biochemically detailed stochastic multicellular model of the SCN in order to investigate the impact of molecular noise and intercellular connectivity on the circadian network synchronization. We have proposed a small-world coupling scheme for the intercellular communication via neurotransmitters [2,3]. Our findings reveal that the SCN network operates firmly despite significant levels of molecular noise, whereby the coherence of circadian dynamics relies significantly on the cell-to-cell interactions. We additionally show that the SCN neuronal activity patterns form localized clusters of synchronous behavior. This effect of spatial clustering is more pronounced in short days than in long photoperiods, thereby indicating that seasonal adaptation encompasses not only redistributions of the neuronal activity on the temporal level [3,4], but also on the spatial scale.

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Tridimenzionalne faze tekočih kristalov iz paličastih molekul

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Tekočekristalna faza je značilna za snovi, ki jih tvorijo močno anizotropne molekule. Največkrat je urejenost molekul v tekočekristalnih fazah eno ali dvodimenzionalna. Kljub izraziti anizotropni obliki molekul pa pogosto opazimo tekočekristalne faze s tridimenzionalno (3D) kubično ali tetragonalno strukturo [1]. 3D tekočekristalne faze pogosto sestojijo iz zlomljenih smektičnih plasti ali stolpcev molekul. Tvorba in vrsta 3D faz je močno odvisna od molekularnih parametrov, saj že npr. majhne spremembe v dolžini ogljikovodikovih repov lahko ključno vplivajo na fazno obnašanje sistema. Zelo pomemben vpliv imata tudi kiralnost in optična čistost.

Simetrijo kubične ali tetragonalne faze brez težav določimo z rentgenskim (rtg) sipanjem. Določitev notranje strukture kristalografske osnovne celice pa je veliko zahtevnejši problem. Z inverzno Fourierovo transformacijo rtg spektra lahko rekonstruiramo elektronsko gostoto v osnovni celici. Toda pri rtg sipanju dobimo le amplitudo strukturnega faktorja (kot koren iz intenzitete), izgubimo pa informacijo o fazi strukturnega faktorja. Problem lahko odpravimo tako, da skonstruiramo 3D model elektronske gostote in izračunamo Fourierovo transformacijo. Ustrezen model bo dal razmerja amplitud med vrhovi, ki so primerljiva z izmerjenimi, hkrati pa dobimo še faze vrhov. Elektronsko gostoto nato rekonstruiramo z uporabo eksperimentalno izmerjenih amplitud vrhov in teoretično dobljenih faz. Običajno je dovolj, če uporabimo le nekaj (dva do štiri) najvišjih vrhov, saj ostali ne vplivajo bistveno na elektronsko gostoto.

Predstavili bomo sistematično raziskavo vpliva kiralnosti, optične čistosti, doline oglikovodikovih repov in njihove razvejanosti na 3D faze, ki jih tvorijo tekoči kristali iz paličastih molekul [2]. Poudarek bo na predstavitvi teoretičnih modelov in njihovi uporabi za identifikacijo struktur v kubičnih in tetragonalnih fazah.

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Three-dimensional phases of liquid crystals formed of rod-like molecules

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Thermotropic liquid crystalline cubic and tetragonal phases are three-dimensionally (3D) ordered, highly symmetric structures, which can be formed also by strongly anisotropic mesogenic molecules. They are relatively common among the rod-like, polycatenar, polyhydroxy and dendritic molecules [1]. The 3D density modulated phases are usually made from strongly distorted smectic layers or columns, depending on the type of constituent molecules. Formation of the 3D phases is very sensitive to molecular factors, e.g. even small changes in the length of terminal chains might have a crucial effect on the behavior of the system. Chirality and optical purity play an important role, as well.

Identification of the symmetry of cubic or tetragonal phases is usually straightforward from the X-ray diffraction pattern. On the other hand, revealing the internal structure of crystallographic unit cell is an intriguing task. It could be done by the reconstruction of the electron density map through the reverse Fourier transform of the X-ray pattern, however in a standard X-ray experiment only information related to the amplitude of structure factor (related to the square root of signal intensity) is available, while the information about the structure factor phase is lost. Moreover, for cubic phases multiplicity of signals is high and peaks belonging to the same multiplicity set might have different phases. One way to solve this problem is to construct a model of a 3D electron density distribution and calculate its Fourier transform. An appropriate model should yield the signal amplitude ratios close to the experimental ones. Finally, the electron density map is reconstructed using experimental amplitudes and theoretically obtained phases. Usually it is enough to use only few signals of the highest intensity; the other peaks do not affect the electron density significantly.

In the talk we will report on detailed X-ray diffraction studies that enabled a reconstruction of the electron density distribution in cubic as well as, for the first time, in tetragonal LC phases. Systematic studies of the effect of chirality, optical purity, length of terminal chains and their branching on the 3D packing of rod-like mesogenic molecules were conducted [2].

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