Koloidi: modelski sistemi za atomsko in statistično fiziko

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Predstavil bom povzetek raziskav opravljenih v zadnjih štirih letih na Univerzi v Konstanzu ter na Univerzi v Graz-u. Področje raziskav so raztopine električno nabitih koloidnih delcev raztopljenih v monovalentnem elektrolitu, njihove ravnovesne strukture in termodinamske lastnosti. Poseben poudarek bo na prepletu eksperimenta in teorije ter na dejstvu, da so koloidne raztopine izjemno uspešni modelski sistemi. Kot primer bom obravnaval mnogodelčne interakcije med koloidi ter opazovanje nastajanja skupkov koloidov na periodičnem substratu.

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Colloids: model systems for atomic and statistical physics

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The work presented here has been done in the last four years and focused on charged stabilized colloidal suspenssions. The overlap of experimental and theoretical approach will be emphasized and the properties of colloidal suspensions which make them very promising model systems for atomic and statistical physics discussed. Specifically, many-body interactions among colloids and cluster formation of colloids on a patterned substrate will be presented.

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Resonances in Planetary Systems

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Resonances occur in any dynamical system when it has more than one degree of freedom and when it is not integrable. Such resonances may stabilize or destroy the regular motion, which depends on the initial conditions of the system. In the dynamics of planetary motions we have different types of resonances which are 1. mean motion resonances (=MMR) 2. secular resonances (=SR) and 3. spin orbit resonances. The first one occurs when the periods of two celestial bodies (it can be also a planet and an asteroid) are close to a rational number, where the ratio can be expressed with small numbers. The second one is important when we take into account that two planets perturb each other and therefore the line of the nodes (which is the line of the intersection of the two planes of motions) are slowly changing. Because also the direction of the perihelion (which is the shortest distance to the SUN) is slowly moving we have different types of the secular resonances. The third one is important when we do not ignore that the shape of a planet is not a perfect sphere. In this discussion we will concentrate on the first and second type of resonances, which play an important role not only in our own Solar system but also in extrasolar planetary systems.

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Matematično modeliranje interakcije med kalcijem, calmodulinom in miozin kinazo

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Kontrakcija gladkih mišičnih celic se prične s fosforilacijo miozina, kar sproži premik prečnih mostičkov v akto- miozinskem motorju. Fosforilacija miozina je v veliki meri odvisna od aktivnosti miozin kinaze (MLCK). Le-ta postane aktivna šele, ko je nanjo vezan kompleks kalcija s kalmodulinom (CaM). Na podlagi splošne teorije postane MLCK aktivna šele ob povišanih koncentracijah kalcija v citoplazmi, ko naj bi bila na kalmodulinu zasedena vsa štiri vezavna mesta za kalcij. Kompleks Ca_4CaM naj bi potem reagiral z MLCK in jo aktiviral, kar bi nadalje sprožilo fosforilacijo miozina, delovanje prečnih mostičkov in posledično tudi silo v mišici. Novejši eksperimenti so pokazali, da z MLCK ne reagira samo kompleks Ca_4CaM, temveč tudi kompleks Ca_2CaM in tudi prosti CaM. To nas je vzpodbudilo k izgradnji nove kinetične sheme omenjenih interakcij med kalcijem, CaM in MLCK ter matematično modeliranje in analiziranje le teh. V tem letu je bil objavljen tudi rezultat prve direktne eksperimentalne meritve aktivnosti MLCK v odvisnosti od koncentracije kalcija, s katero lahko sedaj neposredno primerjamo naše modelne rezultate. V predavanju bom na kratko predstavil omenjeni matematični model in rezultate.

Mathematical modelling of interactions between calcium, calmodulin and myosin light chain kinase

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Activation of myosin light chain kinase (MLCK) by calcium/calmodulin results in phosphorylation of regulatory light chain of myosin II (rMLC) that plays an important role in initiation of smooth muscle contraction and other cellular processes linked to secretion and contraction in smooth- and in non-muscle cells. According to popular general theory an increase in cytosolic calcium concentration, initiates calcium binding to the four binding sites of calmodulin (CaM). The Ca_4CaM complex then interacts with and activates MLCK. Then, MLCK activated phosphorylates the 20-kDa light chains of myosin II, which subsequently triggers cross-bridge cycling and the development of stress. Based on the recent experimental results it has been suggested, that not only Ca_4CaM but also $Ca^{2+} - freeCaM$ or Ca_2CaM complex can interact with MLCK. The first direct measurement of MLCK activity and the recent experiments that revealed completely novel characteristics of interactions between Ca^{2+}/CaM and MLCK stimulated us to construct a novel kinetic scheme of these interactions, to model it mathematically and to compare the model results with the most recent experimental results of MLCK activity. In my talk I will present the results of our study on that topic.

Atosekundna spektroskopija notranjih atomskih lupin

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Atomsko stanje z vrzeljo v notranji lupini razpade v času od nekaj deset atosekund do nekaj femtosekund. Nedavno je bila prvič posneta časovna slika tega razpada, četudi posredno, z modulacijo energije izletelih elektronov. V načrtovanem rentgenskem laserju na proste elektrone, ki ga bodo do leta 2012 zgradili v Hamburgu, bo atosekundna časovna ločljivost neposredno dosegljiva. Ta lastnost, skupaj z izjemno svetlostjo in koherenco novega izvira rentgenske svetlobe, pomeni novo paradigmo v atomski spektroskopiji, tako v vsebini eksperimentov kot v potrebni opremi. Med drugim lahko pričakujemo neposredno opazovanje molekularnih preureditev in študij novih agregatnih stanj snovi.

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Attosecond spectroscopy of atomic inner shells

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An atomic inner-shell vacancy state decays on the time scale from a few tens of attoseconds to a few femtoseconds. Recently, the time evolution of the decay has been recorded for the first time, albeit indirectly, with modulation of the energy of ejected electrons. In the planned free electron x-ray laser, to be built by 2012 at DESY, Hamburg, the attosecond time-resolution will be directly accessible. The resolution, together with coherence and enormous brilliance of the new x-ray source, introduces a new paradigm in atomic spectroscopy, in the experimental subject as well as in the necessary equipment. Direct observation of molecular rearrangements and study of new states of matter will be possible.

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Naboj na neidealni meji kovine in polprevodnika

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Študij lastnosti stika med kovino in polprevodnikom navadno poteka iz dveh smeri. Začetna stanja formiranja meje med kovino in polprevodnikom pri epitaksni rasti monoatomne plasti kovine na podlagi polprevodnika se raziskujejo z mikroskopskimi metodami površinske fizike (fotoelektronska spektroskopija, STM, BEEM), medtem ko se že stabilna plast kovine z debelino nekaj 100 nm raziskuje z analizo makroskopskih merjenj električnega toka skozi mejo in kapaciteto stika.

Neidealnost stikov med kovinami in polprevodniki se makroskopsko običajno izraža v odstopanju izmerjenih in pričakovanih tokovnih in kapacitivnih karakteristik. Vzrok za diskrepanco gre iskati v zapleteni elektronski strukturi neidealnega stika kjer pomembno vlogo igrajo lokalizirana elektronska stanja na meji med kovino in polprevodnikom, ki povzročajo dodatni lokalizirani naboj in vplivajo na transport naboja skozi stik.

V prispevku bom predstavil nekaj pristopov k reševanju problema povezave med mikroskopskimi lastnostmi elektronske strukture in transportom naboja, posebej se bom osredotočil na model z dvema lokaliziranima stanjima v neurejenem polprevodniku.

On charge at nonideal metal-semiconductor interface

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The physical properties of metal-semiconductor contacts are usually studied using two different approaches. The early stages of metal-semiconductor interface formation are detected with the surface physics methods (PES, STM, BEEM) while the properties of well formed interface (with a few 100 nm thick metal overlayer) are studied analyzed using macroscopically measured charge transport characteristics.

The measured charge transport characteristics (current and capacitance) of metal-semiconductor contacts do not usually follow the ideal characteristics predicted by transport theories. To resolve the discrepancy one has to consired the complex electronic structure of the nonideal metal-semiconductor contact where the crucial role is played by the localized states at the metal-semiconductor interface causing the additional localized interface charge influencing the charge transport through the contact.

In this contribution we will consider few attempts to solve the problem of the relation between the microscopic electronic structure and charge transport with special emphasis on the model with two localized states at disordered semiconductor interface.

Dosežki Laboratorija fizika kompleksnih sistemov v letu 2004

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V letu 2004 smo člani laboratorija Fizika kompleksnih sistemov teoretično preučevali (i) anihilacijo defektov [1-4], (ii) fiziko vzorcev [5] in (iii) vpliv naključnega nereda na fazno obnašanje tekoče kristalnih (TK) faz [6-10]. Slednje raziskave so močno vezane na vzporedno eksperimentalno delo [8-10], ki se izvaja na Odseku za fiziko trdne snovi na Institutu Jožef Stefan v Ljubljani. Raziskave so bile izvedene v okviru bilateralnih projektov z Rusijo, Italijo, Brazilijo, Avstrijo, Romunijo, Grčijo, Indijo in ESF mreže Cosmology in the laboratory. V nadaljevanju na kratko podajamo poglavitne rezultate našega dela.

Anihilacija defektov : Numerično smo preučevali anihilacijo nematičnih točkovnih [1,2] in smektičnih robnih [3,4] defektov v vseh režimih, s poudarkom na potrkovnem režimu. Določili smo področje, v katerem velja klasični opis defektov. Samo v slednjem režimu lahko zanemarimo notranjo strukturo defektov in jih obravnavamo kot delce, ki sodelujejo preko umeritvenih polj.

Fizika vzorcev : Razvili smo novo metodo [5], ki omogoca določitev kritičnih pogojev nastanka vzorcev in njihovo strukturo v nematični TK fazi. Metoda velja za primer zveznih strukturnih prehodov.

Vpliv nereda na fazno obnašanje : Razvili smo približno metodo [6,7], ki omogoča napoved faznega obnašanja in kvalitativnih strukturnih lastnosti TK faz v poroznih sredstvih. Pri tem smo uporabili modele, ki so bili razviti za opis nastanka domenskih struktur v zgodnjem vesolju in v magnetizmu. Metodo smo uporabili za razlago poskusov [8-10], pri katerih smo opozovali fazno obnašanje TK ograjevih v kontrolirana porozna stekla.

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Achievements of the Laboratory of complex systems in 2004

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In 2004 we have investigated (i) annihilation of defects [1-4], (ii) patterns [5] and (iii) influence of random disorder on phase behavior in liquid crystal (LC) phases [6-10]. The latter study is closely linked to parallel experimental investigations [8-10] carried out at the Jožef Stefan Institute in Ljubljana. Our research was supported by the bilateral projects with Russia, Italy, Austria, Romania, Greece, India and the ESF project Cosmology in the laboratory. In the following we briefly list our main results that were published in 2004.

Annihilation of defects : We have studied numerically annihilation of nematic point [1,2] and smectic line [3,4] LC defects in all time regimes, emphasizing the post-collision stadium. We have determined the conditions in which classical description of defects is applicable. In this regime the internal structure of defects can be ignored. Consequently defects can be treated as particles interacting via gauge fields.

Patterns : We have developed a new method [5] that enables determination of critical conditions and the structure of the pattern destabilizing an initial nematic LC structure via a continuous structural phase transition.

Disordered LC phases : We have developed an approximative method [6,7] yielding qualitative and to some extent also quantitative predictions on phase behavior of LC phases confined to random environments. Our approach is based on models that were originally developed to study domain patterns in cosmology and magnetism. We have used our method in interpreting our experimental results [8-10] where we have studied phase behavior of LC phases confined to controlled porous glasses.

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Na lovu za novimi hadronskimi stanji

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Pri eksperimentu Belle ob elektronsko-pozitronskem trkalniku KEKB iščemo med drugim tudi dokaze za eksotična hadronska stanja, takšna, ki ne ustrezajo običajnim vezanim stanjem treh kvarkov oziroma kvarka in antikvarka. Poročal bom o stanju raziskav, predvsem o lastnostih nenavadvega stanja X(3872).

Hunting for new hadronic states

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At the Belle experiment we are searching for exotic hadronic states which do not corrspond to the usual three-quark or quark-antiquark bound states. An overview of the status of research will be given, in particular of the recently discovered unusual X(3872) state.

The Astrophysical Jet Sources

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During the past 40 years, astronomers have mapped several hundreds of jet sources, of extents between $\leq 10^{15}$cm and $\geq 10^{25}$cm, whose central engines may all be fast-rotating magnets. The family of jet sources consists of four classes; (1) binary neutron stars (and BHCs), (2) binary forming white dwarfs, (3) very young stars (YSOs), and (4) the very centers of (active) galaxies (AGN). Their jets are all knotty, have opening angles $\leq 1\%$, and blow balloons (lobes, cocoons) of typical axis ratios 1:5; they are often one-sided, and occasionally expand superluminally. Their cores tend to be very luminous, broadband, and highly variable, with core/lobe power ratios of $10^{2\pm2}$, indicating jet-forming efficiencies of 1%. I shall argue that all these jet sources are powered by relativistic $e^{\pm}$ pair plasma, originating from magnetic reconnections, which performs a mono-energetic **E** x **B**-drift, of bulk Lorentz factor $\gamma = 10^{3\pm1}$, through self-rammed vacuum channels.

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Sipanje tahion-graviton v okviru teorije strun

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Predstavil bom sipanje tahion-graviton v okviru teorije strun. Izračunali smo amplitudo sipanja dveh brezmasnih zaprtih strun in dveh zaprtih strun, ki predstavljata tahion. Izračun je bil izpeljan v limiti šibkega gravitacijskega polja (1). Za graviton, ki vstopa v proces sipanja, predpostavimo, da je njegova transverzalna hitrost enaka nič in da se nahaja v prostoru Aichelburg-Sexl metričnega tenzorja (2). Obravnavali smo sipalno amplitudo štirih zaprtih strun najnižjega reda, ki izhajajo iz ploskev s pozitivnim Eulerjevim številom. Za izračun sipalne amplitude smo uporabili dva vertex operatorja za tahion in dva vertex operatorja za graviton. Vsak vertex operator zaprte strune ima svojo sklopitveno konstanto, ki je povezana z normaliziranim vertex operatorjem gravitacijske sklopitve, $K = \pi\alpha' q_c' = 2\pi q_c$. Amplitudo sipanja smo izračunali na krogli. Pri izračunu sipalne amplitude smo upoštevali ohranitev gibalne količine, mase in pogoj za fizikalna stanja $k_i e_i = 0$.

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A tachyon-graviton scattering amplitude within the framework of string theory

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The paper deals with the tachyon-graviton scattering within the framework of string theory. We calculated the scattering amplitude for two massless closed strings and two closed string tachyons. The calculation was carried out in the limit of weak gravitational field (1). The source graviton is taken to have vanishing transverse velocity and it produces the Aichelburg-Sexl metric (2). We considered the lowest order scattering amplitude of four closed strings, coming from surfaces with positive Euler number. For scattering amplitude calculation two tachyon and two graviton vertex operators were used. Each vertex operator has his closed string coupling constant which relates the normalization of the vertex operator to the gravitational coupling, $K = \pi\alpha' q_c' = 2\pi q_c$. The scattering amplitude was calculated on the sphere, using momentum conservation, mass-shell condition and physical state condition $k_i e_i = 0$.

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Pomen fleksibilnosti dinamicnih sistemov za kontrolo kaosa

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Fleksibilnost je pomembna lastnost dinamičnih sistemov. Kot matematično mero za fleksibilnost dinamicnega sistema predlagamo lokalno divergenco, pri čemer moramo dobljene rezultate primerno ovrednotiti in interpretirati v skladu s tipom dinamičnega sistema. Izkazalo se je, da fleksibilnost dinamičnih sistemov odločilno vpliva na njihove sklopitvene lastnosti, povečanje robustnosti pri dodanem šumu in razlagi konstruktivne in destruktivne vloge šuma pri stohastični resonanci [1-6]. V najnovejših raziskavah smo pokazali, da je fleksibilnost dinamicnih sistemov pomembna tudi pri kontroli kaosa [7]. Kontrola kaosa je eno pomembnejših raziskovalnih področij zadnjega desetletja [8], ki je pomembno vplivalo na številne aplikacije kaotičnih sistemov. Sprva nezaželeno kaoticno obnašanje sistemov je s kontrolo kaosa postalo sinonim za fleksibilno adaptacijo eksperimentalnih sistemov, ki jo je moč doseči s kontrolo ene izmed nestabilnih orbit in s tem zagotoviti optimalno delovanje sistema v danih okoliščinah. Šibka stran vseh dosedanjih algoritmov za kontrolo kaosa [9-11] je v tem, da se omejujejo le na nestabilne periodične orbite, ki so del kaotičnega atraktorja. Kljub dejstvu, da je kaotični atraktor sestavljen iz neskončno mnogo nestabilnih periodičnih orbit, je njihova realna eksperimentalno uporabna variabilnost velikokrat majhna. V smislu reševanja tega problema smo na podlagi predhodnih študij fleksibilnosti in robustnosti dinamičnih sistemov [1-6] razvili algoritem, ki omogoča detekcijo in kontrolo dodatnih nestabilnih periodičnih orbit, ki niso del kaotičnega atraktorja [7]. S tem smo uspeli dodatno razširiti aplikativnost algoritmov za kontrolo kaosa tudi na sisteme, ki v osnovi ne premorejo velikega števila kvalitativno različnih oscilatornih režimov.

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The role of flexibility of dynamical systems for chaos control

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Flexibility is an important property of dynamical systems. We measure the flexibility with the local divergence. The results have to be evaluated and interpreted very carefully in dependence on the type of the dynamical system. In our previous studies [1-6], we have shown that the flexibility of dynamical systems plays an important role in determining coupling properties of dynamical systems, enhancing the robustness by noise, and explaining the constructive and destructive role of noise in case of stochastic resonance. Most recently, we have shown that the flexibility of dynamical systems also plays an important role in chaos control [7]. In the last decade, chaos control theory became one of the most popular fields of research, which has contributed to numerous applications of chaotic systems [8]. The control of chaotic systems became a synonym for a flexible adaptation of experimental systems to a specific oscillatory regime, which can be obtained by controlling one of the unstable periodic orbits (UPOs) present in the chaotic attractor. A deficiency of the existing algorithms [9-11] is that the control is limited only to UPOs that are part of the chaotic attractor. Although every chaotic attractor consists of infinitely many UPOs, their diversity and, hence, their practical experimental applicability is often moderate. In order to solve these problems, we have developed a new algorithm for detecting and controlling additional UPOs that are not part of a chaotic attractor [7]. Herewith, we have enhanced the applicability of chaos control methods also to those systems that are not characterised by numerous qualitatively different oscillatory regimes.

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Nelinearna analiza časovnih vrst - izgledi v izobraževanju in raziskovanju

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Metode za nelinearno analizo časovnih vrst omogočajo določitev karakterističnih lastnosti sistema, npr. invariantnih količin kot je največji Lyapunov eksponent ali števila aktivnih prostorskih stopenj, zgolj z analizo časovnega poteka ene izmed njegovih spremenljivk. Tako so v številnih pogledih bolj primerne in nadrejene matematičnemu modeliranju. Še posebej pri poučevanju kompleksnih pojavov v nelinearnih dinamičnih sistemih, na dodiplomski kot tudi podiplomski ravni, predstavljajo metode za nelinearno analizo časovnih vrst odlično alternativo za matematično modeliranje, saj zagotavljajo direktnejšo povezavo med eksperimentom in teorijo. Tudi pri raziskovalnem delu predstavljajo te metode velikokrat prvi korak k spoznavanju in analizi obravnavanega sistema. Predvsem kompleksne večdimenzionalne sisteme je težko matematično modelirati zaradi zapletenosti procesov, ki ustvarjajo opazovano dinamiko. Tako je vpogled v lastnosti takšnega sistema brez vpletanja matematičnega modeliranja lahko ključen za uspeh raziskovalnega projekta. Glede na njihovo pomembnost in uporabnost, bom predstavil kratek pregled osnovnih metod za nelinearno analizo časovnih vrst, ki so neobhodne za uspešno in relevantno raziskovalno delo. Predstavil bom t.i. embedding teorem in izpostavil pomembnost testov za stacionarnost in determinizem opazovanega sistema. Nadalje bom predstavil tudi preprost algoritem za izračun največjega Lyapunovega eksponenta in nakazal algoritem za izračun celotnega spektra Lyapunovih eksponentov. Rezultate omenjenih metod bom prestavil sočasno za dva sistema, in sicer za paradigmatičnem Lorenzov sistem, ter za kratek elektrokardiografski zapis. Izpostavil bom tudi zanimive aspekte rezultatov, ki nudijo globlji vpogled v dinamiko človeškega srca.

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Nonlinear time series analysis - prospects in education and research

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Methods of nonlinear time series analysis enable the determination of characteristic properties of a system, e.g. invariants such as the maximal Lyapunov exponent or the number of active degrees of freedom, solely by analysing the time course of one of its variables. Therefore, there are superior to mathematical modelling, both from the educational as well as the investigative point of view. Particularly for undergraduate students, methods of nonlinear time series analysis present an excellent alternative to mathematical modelling, since they enable the introduction of basic concepts directly from the experimental data, thus guaranteeing a better link between real-life phenomena and the theory. Furthermore, in scientific research, these methods can provide insights into the dynamics of complex systems, where mathematical modelling is often extremely difficult due to the complexity of underlying processes. In view of their importance, I will present a brief survey of essential nonlinear time series analysis methods that are required for further analyses. In particular, I will present the embedding theorem, and discuss the importance of stationarity and determinism tests. Moreover, I will present a simple algorithm for calculating the maximal Lyapunov exponent, as well as outline the algorithm for calculating the whole Lyapunov exponent spectra. I will simultaneously demonstrate applications of discussed methods on the paradigmatic Lorenz system and on a short continuous electrocardiographic recording. Additionally, I will discuss interesting aspects of results that provide insights into the dynamics of the human heart.

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Ali je kaos lahko koristen v kvantni mehaniki?

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Predstavil bom nekaj osnovnih lastnosti kvantne informacije in manipuliranja z njo, ki je postalo znano kot kvantno računalništvo. Za ilustracijo bom razložil protokol kvantnega teleportiranja in pokazal, da kvantne informacije ni mogoče klonirati. Potem se bom osredotočil na problem kvantnega kaosa v časovni sliki. Pokazal bom, da kvantni kaos lahko karakteriziramo z ozirom na stabilnost časovnega razvoja glede na male variacije hamiltonke oz. Hamiltonovega operatorja. Videli bomo, da je kvantna evolucija, v nasprotju s klasično, bolj stabilna za sisteme s kaotično klasično limito kot za regularne sisteme. To spoznanje lahko uporabimo za načrtovanje učinkovitih in robustnih kvantnih algoritmov.

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When chaos is useful in quantum mechanics

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I shall review some of the basic properties of quantum information, and of manipulation with quantum information which is known as quantum computing. I will work out the so-called *quantum teleportation*, and demostrate *no-clonning* of quantum information, as two illustrative examples. Then I will focus on the quantum chaos in time domain and characterize it in terms of its stability against static perturbations of the Hamiltonian. It can be shown that, in quantum mechanics contrary to classical mechanics, systems which are chaotic in the classical limit are more roboust against external static perturbations than the regular ones. This implies a novel strategy in development of efficient and roboust quantum algorithms.

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Svetovno leto fizike 2005

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Svetovno leto fizike 2005 sovpada s praznovanjem 100-letnice Einsteinovega čudežnega leta, to je leta, v katerem je objavil tri temeljna dela: o teoriji relativnosti, o Brownovem gibanju in o fotoefektu.

V predavanju bom predstavil aktivnosti, ki se bodo odvijale v prihodnjem letu. Njihov namen je popularizirati fiziko, ki sicer med mladimi velja za razmeroma nepriljubljeno in togo vedo, kot tudi navdahniti novo generacijo znanstvenikov. Predstavil bom predvsem slovenski projekt, v okviru katerega se pripravlja verižni eksperiment.

Na koncu bom predstavil še promocijo in študij fizike v letu 2004 ter načrte za prihodnje leto.

World Year of Physics 2005

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The World Year of Physics 2005 coincides with the centennial celebration of Albert Einstein's "miraculous year", when he published the theory of relativity, explained the Brownian motion and discovered the photo effect.

In my talk I will present the activities that will take place during the following year. Their purpose is mainly to bring the excitement of physics to the public and inspire a new generation of scientists. Among the several activities I will focus on the Slovenian project of the chain experiment.

Finally I will present the popularisation of physics in 2004, our university programme of Physics and the plans for the following year.

Teorija adiabatskih invariant

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Adiabatske invariante, označene z I, so približne konstante (invariante) gibanja danega dinamičnega sistema (ki ni nujno hamiltonski), ki se približno ohranjajo pri procesu počasne spremembe sistemskih parametrov (označenih z λ), na časovni skali dolžine T, ki je po predpostavki veliko daljša kot katerikoli tipični dinamični čas, kot je denimo čas prehoda sistema, ali pa perioda najkrajše periodične orbite itd.

To je asimptotska trditev, v tem smislu, da so adiabatske invariante tem bolje ohranjene čim bolj počasen je proces, t.j. čim bolj počasi se spreminja preklopna funkcija $\lambda(t)$ na časovni skali T, in ohranitev je ekzaktna v limiti $T \to \infty$.

Pomembno je, da se ob poljubno velikem spreminjanju sistemskih parametrov $\lambda(t)$ in njegovih dinamičnih količin kot so celotna energija, vrtilna količina itd., njihova kombinacija, vsebovana v adiabatski invarianti I, ohranja z veliko stopnjo natančnosti, kar nam omogoča izračun sprememb pomembnih količin v dinamičnih sistemih. Primeri so v nebesni mehaniki, v teoriji hamiltonskih sistemov, v gibanju nabitih delcev v magnetnih in električnih poljih itd.

Podal bom pregled splošne teorije in predstavil nekaj najnovejših rezultatov o časovno odvisnem enodimenzionalnem harmonskem oscilatorju. Ta problem je v splošnem zelo težak, saj je ekvivalenten reševanju splošne enodimenzionalne stacionarne Schrödingerjeve enačbe. Začenši z ensemblom začetnih stanj z ostro določeno energijo, izračunamo analitično porazdelitev energije končnih stanj po koncu adiabatskega procesa (časovne dolžine T), in si v podrobnosti ogledamo točnost ohranitve adiabatskih invariant.

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Theory of adiabatic invariants

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Adiabatic invariants, denoted by I, are approximate constants (invariants) of motion of a given dynamical system (not necessarily Hamiltonian), which are approximately preserved (constant) during a process of very slow change of the system's parameters (denoted by λ), on a time scale T, which is supposed to be much larger than any typical dynamical time scale such as traversal time or the period of the shortest periodic orbits etc.

This is an asymptotic statement, in the sense that the adiabatic invariants are the better preserved the slower the driving of the system, that is the more slowly the switching function $\lambda = \lambda(t)$ varies on the typical evolutionary time scale T, and the preservation is perfect in the limit $T \to \infty$.

The important point is that whilst the system's parameters $\lambda(t)$ and their dynamical quantities like the total energy, angular momentum etc, can change by arbitrarily large amounts, their combination involved in the adiabatic invariant I is very well preserved to a very high degree of accuracy, and that allows us to calculate changes of important quantities in dynamical systems. Examples are in celestial mechanics, in other Hamiltonian systems, in motion of charged particles in magnetic and electric fields, etc.

I shall review the general theory and present some very recent results on the time dependent one dimensional harmonic oscillator. This is in general very difficult problem as it is equivalent to solving the one dimensional stationary Schrödinger equation. Starting with an ensemble of initial states with the sharply defined initial energy, we shall calculate analytically the distribution of the energy of final states after an adiabatic process (of time length T), and shall investigate in detail the accuracy of the preservation of the adiabatic invariant.

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WKB vrste nekaterih potencialov

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Proučujemo nekatere lasnosti WKB vrst poljubnih analitičnih potencialov in še posebej potencialov x^N (N je sodo število) ter nekaterih drugih. Izpeljemo eksplicitni funkcionalni izraz za poljubni člen WKB vrste, kjer je potrebno rešiti samo nekatere ekzaktne rekurzivne enačbe z racionalnimi koeficienti. Izpeljemo tudi ekzaktne formule za WKB člene za lastne vrednosti energije potenciala $V(x) = x^N$, kjer je N sodo število, vendar je v tem primeru vrsta le asimptotska, ne pa tudi nujno konvergentna.

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Exact WKB expansions for some potentials

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We investigate some properties of the WKB series for arbitrary analytic potentials and then specifically for potentials x^N (N even) and some others. We find the explicit functional form for the general WKB terms, where one has only to solve a general recursion relation for the rational coefficients. We derive almost explicit formulae for the WKB terms for the energy eigenvalues of the homogeneous power law potentials $V(x) = x^N$, where N is even, in which case the WKB series is asymptotic but not necessarily convergent.

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Interakcije med možgansko, srčno in dihalno aktivnostjo

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Odjemki možganskih, srčne in dihalne aktivnosti so valovi, sestavljeni iz oscilatornih komponent ob prisotnosti stohastičnih elementov. Analiza na osnovi valčne transformacije je pokazala, da se trenutne frekvence možganskih valov [1], δ (0.5–3.5 Hz), θ (3.5–7.5 Hz), α (7.5–12.5 Hz), β (12.5–25 Hz), γ_1 (25–35 Hz), γ_2 (35–50 Hz) in γ_3 (50–100 Hz), spreminjajo s časom. Tudi frekvenca srčne aktivnosti ni konstantna. Pri zdravih osebah v sproščenem stanju njena trenutna frekvenca niha okrog 1 Hz. Dihalna aktivnost je počasnejša, s spreminjajočo se trenutno frekvenco okoli 0.2 Hz. Prikazani bodo novi pristopi, ki omogočajo poglobljen vpogled v medsebojne odvisnosti aktivnosti [2,3] ter predstavljene njihove značilnosti v budnem stanju ter med anastezijo [4-6]. Predstavljen bo tudi postopek za detekcijo budnega stanja med anastezijo, ki bi lahko omogočal da bi se temu stanja med anastezijo izognili.

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Brain, cardiac and respiratory interactions

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Brain, cardiac and respiratory activities are a continuum of waves and oscillations in the presence of stochastic components. Brain waves are relatively fast. Recent analyses based on the wavelet transform have shown that the frequency content the brain waves [1], δ (0.5–3.5 Hz), θ (3.5–7.5 Hz), α (7.5–12.5 Hz), β (12.5–25 Hz), γ_1 (25–35 Hz), γ_2 (35–50 Hz) and γ_3 (50–100 Hz), varies in time. The cardiac rhythm also varies in time. In relaxed healthy humans its instantaneous frequency fluctuates around 1 Hz. Respiration is slower, and its instantaneous frequency fluctuates around 0.2 Hz. New techniques allowing fresh insight into their mutual interactions [2,3] will be described, and the characteristics of their causal relationships in the waking state and during anaesthesia [4-6] will be reported. A new approach to the detection of awareness in anaesthesia, potentially enabling its prevention, will be discussed.

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Numerično reševanje stacionarne in časovno odvisne Schrödingerjeve enačbe

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Schrödingerjevo enačbo lahko rešujemo v časovni ali energijski sliki. V prvem primeru nas tipično zanima časovni razvoj valovne funkcije ob dani začetni vrednosti, v stacionarnem primeru pa iščemo lastna stanja in lastne energije Hamiltonovega operatorja. Med obema pristopoma obstaja formalna korespondenca, v praksi pa je seveda izbira načina reševanja odvisna od narave problema, ki ga rešujemo.

V predavanju bom predstavil dva pristopa, ki smo jih uporabili za reševanje problema kvantnega Monza biljarda, v katerem v klasični sliki delci za vse čase potujejo v isti smeri vzdolž "proge". Posplošena skalirna metoda z integriranjem po robu je uporabna za reševanje stacionarnega problema in s pridom izkorišča dejstvo, da je moč rešitev znotraj biljarda zapisati z vrednostmi na robu, kjer je potrebno zadostiti ustreznim robnim pogojem. To močno zmanjša numerično zahtevnost računov ter poveča natančnost. Takšen numeričen račun razkrije nov tip spektralne statistike, ki ga pričakujemo v družini biljardov tega tipa.

Z unitarno metodo končnih elementov je mogoče spremljati časovni razvoj valovne funkcije tako znotraj biljardov poljubnih geometrij kot tudi v drugih kvantnih sistemih. V Monza biljardu metoda pokaže kvantni obrat smeri toka na dovolj dolgi časovni skali.

Numerical methods for solving the stationary and time dependent Schrödinger equation

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The Schrödinger equation can be solved in either the time or the energy representation. In the former case we are typically interested in the time evolution of a wavefunction given its initial condition, while in the latter case we are looking for eigenstates and eigenenergies of the Hamiltonian operator. Even though there exists a formal correspondence between the two approaches, in practice the method chosen depends on the nature of the problem to be solved.

In this talk I will present two approaches that we used to solve the problem of a Monza billiard, for which in the classical picture the particles maintain the direction of their traversal along the "course". The generalized boundary integral scaling method is used to solve the stationary problem and utilizes the fact that the solution within the billiard may be expressed by values at the boundary, where a certain boundary condition must be met. This reduces the numerical difficulty of the problem and increases accuracy. Such a calculation reveals a new type of spectral statistics that is expected for the family of billiards of this type.

Using the unitary finite element method we may follow the time evolution of the wavefunction for billiards of arbitrary geometries as well as other quantum systems. In the case of the Monza billiard the method reveals a quantum reversal of flow on a long enough timescale.

Kvantno adiabatsko računanje in NP-polni problemi

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Moč klasičnih računalnikov se je do sedaj povečevala eksponentno s časom. Slej ko prej bomo torej prišli do meje, ko nadaljne izboljševanje ne bo več mogoče. Naravno vprašanje je, kje je ta meja? Vsak računski stroj deluje v skladu s fizikalnimi zakoni. Ultimativna moč bo torej v principu pogojena z omejitvami, ki jih narekujejo sami fizikalni zakoni, npr. kvantna mehanika, če je za opis delovanja naprave potrebna kvantna fizika.

Posebej zanimivo vprašanje je, kakšna je algoritmična zahtevnost posameznega problema. V grobem lahko ločimo probleme na dve skupini: (i) take katerih *rešitev* zahteva število osnovnih korakov ki narašča polinomsko z velikostjo problema, ta razred na kratko označimo s P, in (ii) probleme za katere lahko v polinomskem času *preverimo* ali je dana rešitev res rešitev, take probleme označimo z NP (nedeterministični polinomski). Za ponazoritev razlike med P in NP lahko vzamemo puzle. Sestavljanje je zelo zahtevno, preveriti moramo veliko kombinacij. Na drugi strani je preverjanje ali je dana rešitev res pravilna enostavno. Za vsak košček moramo le preveriti ali se sklada z bližnjimi. Število korakov potrebnih za preverjanje rešitve bo torej sorazmerno s številom koščkov. Posebej imeniten podrazred NP problemov so NP-polni problemi (NP-C). NP-polni problemi imajo to lastnost, da lahko vsak NP problem prevedemo na NP-C v polinomskem času. To pomeni, če najdemo polinomski algoritem za NP-C problem, imamo takoj polinomski algoritem za *vse* NP probleme. Lahko rečemo, da so NP-C problemi "najtežji" izmed NP problemov, ti pa so težji od P problemov. Trenutno vsi znani algoritmi za NP-C probleme potrebujejo eksponentno mnogo korakov, ni pa znano, ali morebiti ne obstaja kak polinomski algoritem, ki pa ga še nismo odkrili. Vprašanje ali je P=NP je glavni problem teoretičnega računalništva in tudi eden izmed sedmih t.i. problemov tisočletja, ki jih je leta 2000 razpisal znameniti Clay Mathematics Institute [1]. Skoraj enotno prepričnje je, da velja P≠NP, dokaz nasprotnega bi bilo ogromno presenečenje, ki bi imelo tudi veliko praktičnih posledic.

Pred nekaj leti se je pojavil nov tip algoritmov, takih ki za svoje izvajanje potrebujejo kvantni računalnik. Veliko pozornost je kvantno računalništvo doživelo po odkritju Petra Shora [2], ki je našel *polinomski* kvantni algoritem za faktorizacijo naravnih števil. Najboljši klasični algoritem je na drugi strani počasnejši kot polinomski, a hitrejši kot eksponentni (po drugi strani pa poznamo polinomski algoritem za problem: ali je dano število praštevilo?). Izgleda torej, da so kvantni algoritmi boljši kot klasični. Zastavlja se vprašanje, koliko močnejši so? Ali omogočajo reševanje NP-C problemov v polinomskem času?

Leta 2001 je skupina iz MIT predlagala nov tip kvantnih algoritmov [3] (kvantni adiabatski algoritmi), ki temeljijo na počasni adiabatski evoluciji iz znanega začetnega stanja v končno stanje, v katerem je zakodirana rešitev našega problema. Na osnovi numeričnih simulacij pri reševanju NP-C problema so sugerirali, da je morda kvantni adiabatski algoritem boljši kot katerikoli klasični algoritem. Njihovi podatki so kazali celo, da ima kvantni algoritem le polinomsko zahtevnost, kar bi pomenilo P=NP! Splošno prepričnje je (ni pa dokazov), da tudi kvantni adiabatski algoritmi niso sposobni rešiti NP-C problemov v polinomskem času, so pa morda boljši na določenih posebnih primerih. Lepota kvantnih adiabatskih algoritmov je ta, da se vprašanje časovne zahtevnosti algoritma prevede na vprašanje skaliranja velikosti energijske reže v spektru ustreznega kvantnega sistema. Tako se zdi, da smo zapleten problem prevedli v nekoliko znosnejšo obliko.

Predstavil bom rezultate analize skaliranja energijske reže za NP-C problem imenovan 3-SAT (študiran tudi v [3]). Numerični podatki kažejo, da velikost reže *eksponentno* pojema z velikostjo problema za določen "težek" tip problemov, ki prej ni bil znan (in je torej časovna zahtevnost eksponentna).

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Quantum Adiabatic Computation and NP-Complete problems

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The power of classical computers has been growing exponentially with time. Sooner or later we will reach a point where this growth will cease. Natural question is, where is this border? Any computational machine is governed by the laws of physics. The ultimate power is therefore in principle given by these underlying laws, for instance by quantum mechanics if quantum description is necessary.

Especially interesting question is, what is algorithmic complexity of a given problem. According to the difficulty the problems can be grossly split into two groups: (i) problems for which *finding* the solution demands a number of steps that grows polynomially with the size of the problem, this group is denoted shortly by P, and (ii) problems for which *verifying* if a given solution really solves the problem needs polynomailly number of steps, this group is denoted by NP (nondeterministic polynomial). To illustrate the difference between P and NP we can consider a jigsaw puzzle. Finding a solution is very hard, we have to check many combinations. On the other hand, verifying if we have found a solution is simple. We just have to check for every piece if it fits with its neighbors. Number of steps for verification thus grows linearly with the number of pieces. Especially important class of NP problems are the co-called NP-complete problems (NP-C). They have the property that any NP problem can be translated to a NP-C problem in a polynomial time. As a consequence, if we find a polynomial algorithm for a NP-C problem, we automatically have a polynomial algorithm for *all* NP problems. Vaguely speaking, NP-C problems are the hardest problems in NP. At present, all known algorithms for NP-C require exponentially many steps, but there is no proof that none exists. Actually, the problem whether P=NP is the main problem of theoretical computer science and is also one of the seven millenium problems [1] named by the famous Clay Mathematics Institute in 2000. There is almost a unanimous opinion that P≠NP. Proof of the contrary would be a great shock and would have many practical consequences.

Few years ago a new type of algorithms apeared, that run on a quantum computer. Quantum computation has recieved great attention after Peter Shor discovered a quantum polynomial algorithm for factorization [2]. The best classical algorithms can do the job slower than polynomially but faster than exponentially (on the other hand we have a polynomial algorithm for a problem: is a given number prime?). The

quantum algorithms therefore look to be better than classical ones. The question is, how much better are they? Are they able to solve NP-C problems in polynomial time?

In 2001 a group from MIT described a new type of quantum algorithms [3] (quantum adiabatic algorithms), which are based on a slow adiabatic evolution from a known initial state to a final state that encodes the solution of our problem. Based on numerics, they suggested that quantum adiabatic algorithms might be better than classical ones for NP-C problems. Their data even showed a polynomial time dependence for an adiabatic algorithm, implying P=NP! The prevailing opinion is (but there are no proofs) that quantum adiabatic algorithms cannot solve NP-C problems in polynomial time, but they could be better than classical ones on a certain special instances. The elegance of the adiabatic computation is that the question of algorithm complexity is translated into yhe question of energy gap for a quantum system correspoding to a given problem. It therefore seems that we have translated a compicated problem into somehow more manageble form.

I will present the anaysis of scaling of the energy gap for an NP-C problem called 3-SAT (studied also in [3]). Numerical data show, that the size of the gap decays exponentially with the size of the problem for a certain type of "hard" instances not know previously. Therefore, the time dependence of the algorithm is also exponential.

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