



## BOOK OF ABSTRACTS

# 6<sup>th</sup> Workshop on Current Problems in Physics: Zielona Góra - Lviv

23 - 25 September 2013, Zielona Góra, Poland

The Workshop on Current Problems in Physics 2013 (WCPP'13) is already the sixth in a series of meetings which represent annual forum for the Polish and Ukrainian physicists community to present their latest scientific results. Usually, the meetings are attended by representatives of other countries, too. An important feature of the conference is the possibility for young scientists to present their research results and interact with the more experienced colleagues from other countries. The Workshop will be held in Zielona Góra from 23 to 25 September 2013.

The conference is organized under the auspices of His Magnificence Rector of the University of Zielona Góra, professor Tadeusz Kuczyński.

# Conference programme

<b>Monday 23.09.2013</b>	
<b>Arrival of participants</b>	
<b>Tuesday 24.09.2013</b>	
9:00-9:10	<b>Opening ceremony</b>
<b>Session I – Chairman: G. Melikidze</b> special session on integrable systems to celebrate professor Stanislaw Kasperczuk 70th birthday	
9:10-09:30	S. Kasperczuk
09:30-10:00	M. Błaszak
10:00-10:20	A. Maciejewski
10:20-10:40	M. Przybylska
10:40-10:50	<b>Coffee Break</b>
10:50-11:10	P. Rozmej
11:10-11:20	W. Szumiński
<b>Session II – Chairman: V.M. Tkachuk</b> selected aspects of classical and quantum theory	
11:20-11:40	A. Duviryak
11:40-12:00	S. Kondej
12:00-12:20	P. Jachimowicz
12:20-12:40	M. Stetsko
12:40-13:00	A. Kuzmak
12:55-14:00	<b>Lunch</b>
<b>Session III – Chairman: W. Leoński</b> quantum optics, quantum correlations, quantum information	
14:00-14:30	R. Tanaś
14:30-14:50	V. Cao Long
14:50-15:10	A. Kowalewska-Kudłaszyk
15:10-15:30	J. K. Kalaga
15:30-15:45	T. D. Nguyen
15:45-16:00	<b>Coffee Break</b>
<b>Session IV – Chairman: K. Urbanowski</b> symmetry, fundamental interactions, cosmology	
16:00-16:30	V. M. Tkachuk
16:30-16:50	Yu. Yaremko
16:50-17:20	B. Novosyadlyj
17:20-17:40	G. Melikidze
17:40-17:55	K. Raczyńska
19:00	<b>dinner under Braniborska tower observatory</b>

<b>Wednesday 25.09.2013</b>	
<b>Session I – Chairman: K.W. Wojciechowski</b> medical applications	
9:00-9:20	J. Piskorski
9:20-9:40	S. Żurek
9:40-10:10	G. Garbacz
<b>Session II – Chairman: J. Piskorski</b> nanotechnology, nanomedicine	
10:10-10:25	B. Zapotoczny
10:25-10:40	A. Timoszyk
10:40-10:55	A. Defort
10:55-11:10	J. Mleczo
11:10-11:25	<b>Coffee Break</b>
<b>Session III – Chairman: A. Drzewiński</b> metamaterials, mechanical properties	
11:25-11:55	K.W. Wojciechowski
11:55-12:15	J. Narojczyk
<b>Session IV – Chairman: I. Vakarchuk</b> spectroscopy, luminescence, materials	
12:15-12:45	N. Guskos
12:45-13:05	B.V. Padlyak
13:05-13:20	G. Panochko
13:20-14:20	<b>Lunch</b>
<b>Session IV – Chairman: B. Novosadlyj</b> statistical physics methods, models	
14:20-14:40	A. Rovenchak
14:40-14:55	M. Zubaszewska
14:55-15:10	T. Masłowski
15:10-15:30	M. Jarosik
15:30-15:45	<b>Coffee Break</b>
15:45-16:00	B. Brzostowski
16:00-16:15	A.P. Durajski
16:15-16:30	M. Wojciechowski
16:30-16:45	D. Woźniak

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## ABSTRACTS

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# Classical and quantum Stackel systems

M. Błaszak

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In the talk is presented a theory of separability for a class of Liouville integrable hamiltonian systems with all constants of motion quadratic in momenta. Then, the so called minimal quantization procedure is applied and is analyzed the problem of quantum separability of such constructed quantum systems.

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# Application of functionalized iron oxide nanoparticles to determine catecholamines

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Magnetic iron oxide nanoparticles provide attractive possibilities in biomedical application such cell labeling and separation, target drug delivery and biosensor [1,2]. These applications require magnetic nanoparticles to be well-dispersed in liquid media, chemically stable and uniform in size. Due to the magnetic dipolar attraction, unmodified magnetite nanoparticles incline to aggregate into clusters and inhibit the advantage of the specific properties by single-domain. The aggregation associated with magnetite nanoparticles can be avoided by creating an electrostatic double layer using a surfactant steric stabilizer or silica coating [3]. In this presentation magnetic nanoparticles ( $\text{Fe}_3\text{O}_4$ ) are prepared by co-precipitation method and modify by silica using Stöber process [4]. The applications of arylboronic acids as catecholamine sensors are broad, because they are small and flexible molecules. They can form fast and reversible cyclic esters with compounds containing diol moieties in aqueous media. Arylboronic acids potentially offer non-invasive continuous blood glucose monitoring, in some cases without the need for reference measurements. The information can be provided by attachment of the boronic acid moiety (for example Alizarine S) to a proper reporting unit, which undergoes a significant change in fluorescence emission [5]. This presentation will focus on the synthesis of magnetic iron oxide nanoparticles of arylboronic acids and their important properties which eventually will make them suitable as key elements in future non-invasive continuous catecholamine sensors such an epinephrine, norepinephrine or sialic acid [6].

## References

- [1] J. Chen, Y. Miao, N. He, X. Wu, S. Li, *Biotechnology Advances* **22** (2004) 505.
- [2] J. Lee, Y. Lee, J.K. Youn, *Biocatalysts. Small* **4** 143.
- [3] Z. Lu, G. Wang, J. Zhuang, W. Yang, *Colloids and Surfaces A: Physicochem. Eng. Aspects* (2006) 140.
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# The high-pressure superconductivity in hydrogen-rich compounds

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Solid molecular hydrogen and the possibility of its metallization has fascinated condensed matter researchers since the prediction of the pressure required for metallization was proposed by Wigner and Huntington in 1935 [1],[2]. The possibility of forming metallic hydrogen using hydrogenated materials was subsequently studied and discussed [3]. The recent *ab initio* calculations suggest that the superconducting state in metallic hydrogen-rich compounds under the pressure has the critical temperatures much higher than the boiling point of liquid nitrogen. For this reason, the relevant thermodynamic parameters of the superconducting state in SiH<sub>4</sub>, Si<sub>2</sub>H<sub>6</sub>, SiH<sub>4</sub>(H<sub>2</sub>)<sub>2</sub>, GeH<sub>4</sub>, GaH<sub>3</sub>(H<sub>2</sub>)<sub>2</sub> and CaH<sub>6</sub> have been determined within the framework of the Eliashberg theory. It has been shown that for a wide range of the Coulomb pseudopotential  $\mu^* \in \langle 0, 1; 0, 3 \rangle$  the values of the ratio of the energy gap to the critical temperature ( $R_\Delta \equiv 2\Delta_0 / k_B T_C$ ), the ratio of the specific heat jump to the heat in the normal state ( $R_C \equiv \Delta C(T_C) / C^N(T_C)$ ) and the ratio connected with the thermodynamic critical field ( $R_H \equiv T_C C^N(T_C) / H_C^2(0)$ ) significantly exceed the values predicted by the BCS theory [4], [5]. This fact is connected with strong coupling electron-phonon interaction and the retardation effects existing in the analyzed systems.

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- [3] N. W. Ashcroft, *Phys. Rev. Lett.* **92**, 187002 (2004).
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- [5] R. Szcześniak, A.P. Durajski, *J. Phys. Chem. Solids* **74**, 641 (2013).



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**Difficulties in prediction of the oral drug delivery  
- about differences between theory and reality  
form pharmaceutical point of view.**

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A reliable estimation of drug delivery behavior is a prerequisite for rational and efficient development of dosage forms. It is frequently believed that this challenging goal may be achieved using standard test methods as well as different mathematical models describing the drug delivery processes. Unfortunately, the clinical data often demonstrate insufficient predictive power of the available models. The main reasons thereof are the lack of the good understanding of the gastro-intestinal (GI) physiology as well as the variability on the conditions on the drug absorption site. Interestingly, both factors cannot be realistically simulated using compendial test equipment for dissolution testing. We will briefly introduce the selected aspects of the human GI physiology, evolution and goals of dissolution testing as well as the development and use of test devices that are intended to simulate the GI conditions. The data will be discussed in the light of the test results and experiences obtained with the new dissolution stress test device that simulates physic-chemical and mechanical conditions of the GI passage of dosage forms developed by our group.

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# Pairing mechanism for the high-Tc superconductivity: symmetries and thermodynamic properties

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The pairing mechanism for the high-Tc superconductors based on the electron-phonon (EPH) and electron-electron-phonon (EEPH) interactions has been presented. On the fold mean-field level, it has been proven, that the obtained s-wave model supplements the predictions based on the BCS van Hove scenario. In particular: (i) For strong EEPH coupling and  $T < T_c$  the energy gap ( $\Delta$ ) is very weak temperature dependent; up to the critical temperature  $\Delta$  extends into the anomalous normal state to the Nemst temperature. (ii) The model explains well the experimental dependence of the ratio  $R \equiv 2\Delta(0)/kT_c$  on doping for the reported superconductors in the terms of the few fundamental parameters.

In the presented paper, the properties of the d-wave superconducting state in the two-dimensional system have been also studied. The obtained results, like for s-wave, have shown the energy gap amplitude crossover from the BCS to non-BCS behaviour, as the value of the EEPH potential increases. However, for  $T > T_c$  the energy gap amplitude extends into the anomalous normal state to the pseudogap temperature. Finally, it has been presented that the anisotropic model explains the dependence of the ratio R on doping for the considered superconductors.

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# Preparation of quantum states of two spins- $\frac{1}{2}$ in the Schmidt decomposition

A. R. Kuzmak

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We consider a system of two spins and their interaction is represented by isotropic Heisenberg Hamiltonian. Our aim is to create arbitrary quantum state of two spins having started with  $|\uparrow\downarrow\rangle$  state. We can easily prepare this state because it is an eigenvector of the system of two spins which is located in the magnetic field directed along the  $z$ -axis. The method which we suggest consist of two steps. At the first step, using the evolution operator with isotropic Heisenberg Hamiltonian we obtain the state which depends on time of evolution. At the second step, the spins are driven individually by magnetic pulse fields. Finally, we obtain arbitrary state of two qubits which can be easily represented in the Schmidt decomposition. This state is defined by time of evolution and parameters which are determined strength and direction of magnetic fields.

We propose to realize this method on the physical system of atoms which have a nuclear spin  $I$  of  $1/2$  and one valence electron. Therefore, these systems can be considered as a two-qubit systems. Factorized initial state  $|\uparrow\downarrow\rangle$  can be easily prepared for these systems [1]. We consider the system of  $^{31}\text{P}$  donor in silicon because it is system with high degree of quantum coherence, and states of this system are measured with high fidelity [1].

## References

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# EIT in Lambda configuration: multilevel model and model with structured continua

V. Cao Long, W. Leoński

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We present some new results concerning so-called *electromagnetically induced transparency* (EIT) [1] in Lambda scheme. We discuss two different models. One of them involves discrete levels [2, 3], whereas the second one contains structured continua [4]. Applying multilevel model, we reconstruct multi-peak spectra registered by Warsaw Group in a sample of cold  $^{85}\text{Rb}$  atoms trapped in MOT. Moreover, we show that the nature of the spectra exhibiting several transparency windows can be explained on a basis of the second model, that with several autoionizing states, or equivalently, with Fano structured continua.

## References

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# Kerr coupler operating on Werner-like states — entanglement creation and evolution

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We consider a problem of creation of pure entangled states in two-qubit space from initial Werner or Werner-like state by Nonlinear Quantum Scissors (NQS). NQS systems are based on Kerr-like oscillators and can operate in optical domain, but there are also examples of Kerr-like Hamiltonians used in condensed matter systems. NQS are able, under some assumptions, to restrict substantially the number of states involved in the dynamics and therefore are called quantum scissors.

Such state reduction can lead to generation of maximally, or almost maximally entangled states. It was already shown that for two Kerr-like oscillators the system with various types of interactions (linear, nonlinear and parametric) behave like two-qubit, qutrit-qubit or two-qutrit system. It was also shown that we are able to generate entangled states from initial number states within Kerr-couplers.

At present we would like to show that there is also a possibility of creating pure entangled states even though the system is initially in incoherent combination of a completely mixed state and a maximally entangled pure state (Werner or Werner-like states). We consider the influence of various types of damping processes on entanglement creation. The analytical conditions for obtaining different types of entanglement decay: asymptotic or decay in finite time and its possible revival after a significantly long time period, are presented.

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# Quantum chaos of nonlinear oscillator system and Kullback - Leibler quantum divergence

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We discuss a system containing nonlinear Kerr-like oscillator, driven by a series of ultra-short external pulses. Using Kullback - Leibler quantum divergence  $K[\rho|\sigma]$  we define linear and nonlinear quantum divergences. We analyze behavior of these divergences for various values of the parameters determining character of system's dynamics and show that they can be applied as witnesses of quantum-chaotic evolution of the system. We show that the nonlinear divergence is more sensitive for the quantum-chaotic behavior than its linear counterpart.

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# Necessary conditions for integrability of algebraic Hamiltonian systems

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Necessary conditions for integrability of algebraic Hamiltonian systems Abstract: Systems with Hamiltonian functions algebraic in coordinates and momenta are considered. For such systems the right hand sides of Hamilton equations typically are not single valued. This is why the Ziglin or the Morales-Ramis theory cannot be applied directly to study their integrability. The main idea is following. One can extend the phase space of the system in such a way that the extended system is meromorphic and Hamiltonian with respect to a certain degenerated Poisson structure. Although the proposed construction is not unique it allows to obtain necessary conditions for the integrability in the framework of differential Galois theory. Applying this approach necessary conditions for integrability of algebraic homogeneous potentials of rational homogeneity degree are obtained.

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# Maximally entangled states generation in kicked Kerr-like coupler models

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We discuss a system involving Kerr-like nonlinear coupler [1] excited by a series of ultra-short external coherent pulses. We show that despite the simplicity of the model, it can behave in non-trivial way. In particular, we discuss and compare two cases of kicked nonlinear coupler's model (with and without cross-coupling), showing that the quantum evolution of the system remains closed within a two-qubit Hilbert space. Hence, the system can be treated as *non-linear quantum scissors* [2]. Moreover, maximally entangled Bell states can be generated during the system's evolution similarly as in [3]. We show that despite the presence of damping processes, some amount of entanglement can survive in the system.

## References

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# Parameters of scalar field dark energy in the light of Planck 2013 results

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The Planck 2013 results [1] together with data on baryon acoustic oscillations (BAO) [2–4] and distance moduli of SNe Ia [5,6] are used for determination of best-fit parameters and their confidential ranges for cosmological model with cold dark matter and scalar field dark energy. The scalar field  $\phi(x^i)$  defined by the canonical Lagrangian  $\mathcal{L} = \pm\phi_{;i}\phi^{;i} + U(\phi)$  and generalized linear barotropic equation of state  $p_{de} = c_a^2\rho_{de} + C = w_{de}\rho_{de}$  presents the dynamical quintessence or phantom dark energy depending on the current value of equation of state parameter  $w_{de}$  and its value in the early or future Universe. The best-fit values of scalar field dark energy parameters and their confidential ranges, obtained using Markov chain Monte Carlo method and data [1–6], give the possibility to state that the dark energy is phantom at confidential level  $> 1\sigma$ . The confidential level of existence of dark energy of any type is very high:  $> 10\sigma$ .

## References

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# The $^3\text{He}$ impurity states in $^4\text{He}$

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We consider a set of spinless Bose-particles of mass  $m$  with coordinates  $r_1, \dots, r_N$  and an impurity atom of mass  $M$  with coordinate  $r$ . For the system of “liquid helium + impurity  $^3\text{He}$ ” full- and one-particle density matrices for all temperatures by means of the method of collective variables in the approximation of pair correlations are found. The contribution to the full density matrix that takes into account the effect of impurities on the state of the system at finite temperatures is calculated. At low temperatures this contribution is considered as a correction to the ground-state energy of the system. The input data for the numerical calculations are the Fourier coefficients of the two-particle interaction potential between liquid and impurity which are written via the structure factor  $S(k)$  of liquid  $^4\text{He}$  obtained from X-rays scattering measurements. The estimation of the effective mass of the impurity is made.

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# Investigation of the local structure of boron and lithium in some borate compounds by MAS NMR spectroscopy

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The magic angle spinning nuclear magnetic resonance (MAS NMR) spectra of the <sup>11</sup>B, and <sup>7</sup>Li isotopes in a series of un-doped glassy and crystalline borate compounds with Li<sub>2</sub>B<sub>4</sub>O<sub>7</sub>, LiB<sub>3</sub>O<sub>5</sub>, LiCaBO<sub>3</sub>, LiKB<sub>4</sub>O<sub>7</sub> and SrB<sub>4</sub>O<sub>7</sub> chemical compositions were investigated and analysed. Investigated borate glasses of high optical quality and chemical purity were obtained from corresponding polycrystalline compounds using standard glass synthesis according to [1]. The borate single crystals were obtained by Czochralski method. The main structural units (BO<sub>3</sub>, BO<sub>4</sub>, and LiO<sub>4</sub> atomic groups) and their proportions in the Li<sub>2</sub>B<sub>4</sub>O<sub>7</sub>, LiB<sub>3</sub>O<sub>5</sub>, LiCaBO<sub>3</sub>, LiKB<sub>4</sub>O<sub>7</sub> and SrB<sub>4</sub>O<sub>7</sub> glasses and crystals have been established based on the comparative analysis of the <sup>11</sup>B and <sup>7</sup>Li MAS NMR experimental spectra in them. The obtained results of MAS NMR spectroscopy show good correlation with X-ray diffraction data for local structure of the cationic sites in borate glasses and crystals with same chemical compositions [1].

## References

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# Heart Rate Asymmetry - mathematical, physiological and medical aspects

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Heart rate asymmetry (HRA) is a newly discovered phenomenon by which the behavior of decelerations and accelerations of heart rate is different. The variance based HRA states that the contribution of decelerations to short-term heart rate variability is greater than that of accelerations, and that the contribution of accelerations to long-term and total variability is greater than that of decelerations. The structure based HRA states that the runs of accelerations are longer than those of decelerations. Both types are closely related and turn out to be physiologically and medically important.

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## The inhomogeneous Suslov problem

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We consider the Suslov problem of nonholonomic rigid body motion with inhomogeneous constraints. We show that if the direction along which the Suslov constraint is enforced is perpendicular to a principal axis of inertia of the body, then the reduced equations are integrable and possess an invariant measure. Interestingly, the first integral that permits integration is transcendental and the density of the invariant measure depends on the angular velocities. Moreover, in this case, using the so-called alpha-method of Painlevé one can identify when all solutions of the system are single-valued and find their explicit form.

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# Enumeration of plane partitions with a restricted number of parts

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The quantum-statistical approach is used to estimate the number of restricted plane partitions of an integer  $n$  with the number of parts not exceeding some finite  $N$ . The analogy between this number-theoretical problem and the enumeration of microstates of the ideal two-dimensional Bose-gas is used. The conjectured expression for the number of restricted plane partitions shows a good agreement between calculated and exact values for  $n = 10 \div 20$ .

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# New nonlinear equations in the shallow water wave problem

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The classical problem of irrotational long waves on the shallow water is reconsidered. The model of ideal fluid moving under the influence of gravity is used with an appropriate perturbation approach allowing consistent treatment of small parameters. Additionally to two standard parameters which control amplitude of waves and shallowness of the system, respectively, the third one, governing the amplitude of the bottom topography is introduced. Under the assumption that the bottom does not vary rapidly with the horizontal coordinates the new nonlinear equations describing shallow water waves are derived. Several different forms of equations have been obtained for different orders in three small parameters. For the flat bottom KdV equations of different orders, depending of the order of perturbation are recovered. Some particular examples of numerical solutions to those equations are presented, as well.

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# Dirac oscillator and nonrelativistic Snyder-de Sitter algebra

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Three dimensional Dirac oscillator was considered in deformed space obeyed to deformed commutation relations known as Snyder-de Sitter algebra. Snyder-de Sitter commutation relations give rise to appearance minimal uncertainty in position as well as in momentum. To derive energy spectrum and wavefunctions of the Dirac oscillator supersymmetric quantum mechanics and shape invariance technique was applied.



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# Constrained N-body problems

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We consider a problem of mass points interacting gravitationally whose motion is subjected to certain holonomic constraints. The motion of points is restricted to certain curves and surfaces or hyper-surfaces. We illustrate the complicated behaviour of trajectories of these systems using Poincaré cross sections. For some models we prove their non-integrability analysing properties of the differential Galois group of variational equations along certain particular solutions of considered systems. Also some integrable cases are identified.

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# Quantum correlations in a two-atom system

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Quantum correlations in systems composed of several subsystems are presently the subject of intensive studies because of their crucial role in quantum information processing. It is important to have reliable measures of quantum correlations to distinguish them from classical correlations. Recently, various measures of quantum correlations have been introduced and tested. Probably the most popular of them is quantum entanglement, but there are other measures, such as quantum discord, geometric quantum discord, measurement induced disturbance and others. We will shortly discuss some of them. The simplest multipartite system is a bipartite system composed of two qubits, or two two-level atoms. In case of two-level atoms interacting with the reservoir of electromagnetic field modes in the vacuum, the evolution of the system can be described by the well known Lehmborg-Agarwal master equation. The collective evolution of the two-atom system depends on two collective parameters: collective damping  $\gamma_{12}$  and dipole-dipole interaction  $V_{12}$ , which both depend on the interatomic distance. Such a system is a good testing ground for studying evolution of quantum correlations. Nice feature of the system is the fact that, if the spontaneous emission is the only relaxation process and the system is not driven, the so called X-form of the density matrix is preserved during the evolution. Examples of time evolution of various measures of quantum correlations in the two-atom system for different initial states of the system will be given to illustrate the similarities and differences between the most popular measures of quantum correlations.

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# Optical properties of gold nanoparticles

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Gold nanoparticles (GNPs) have been considered as an important area of research due to their unique properties and their biomedical science including drug delivery, photothermal therapy, chemical sensing, tissue/tumor imaging and immune-chromatographic identification of pathogens [1-3]. Due to the recent increasing green chemistry, synthesis of GNPs must be a nontoxic and environmentally friendly. Biological methods of GNPs synthesis using plant extract or microorganisms have offered a reliable eco-friendly alternative to chemical and physical methods [4]. Metal nanoparticles have unique physical and chemical properties, which are strongly affected by particle size, size distribution, shape and particle-to-particle interaction [5, 6]. When excited with an electromagnetic field, GNPs produce an intense absorption attributed to the collective oscillation of electrons on the particle surface, termed a plasmon resonance [7, 8]. The resonant frequency is high dependent on particle size, shape and environment. For instance, the sphere geometry of GNPs allows for control of optical properties in a highly predictive manner, making them a new class of materials that are capable of tailoring radiation throughout the visible and infrared wavelength regimes [9]. Because of the mentioned factors above the GNPs could be characterized by UV-visible spectroscopy, fluorescence spectroscopy, Scanning Electron Microscopy (SEM) and Different Light Scattering (DLS).

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# Effect of the generalized uncertainty principle on Galilean and Lorentz transformations

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Generalized Uncertainty Principle (GUP) was obtained in string theory and quantum gravity and suggested the existence of a fundamental minimal length which, as was established, can be obtained within the deformed Heisenberg algebra. We use the deformed commutation relations or in classical case (studied in this paper) the deformed Poisson brackets, which are invariant with respect to the translation in configurational space. We have found the transformations relating coordinates and times of moving and rest frames of reference in the space with GUP in the first order over parameter of deformation. For the non-relativistic case we find the deformed Galilean transformation which is similar to the Lorentz one written for Euclidean space with signature  $(1, 1, 1, 1)$ . The role of the speed of light here plays some velocity  $u$  related to the parameter of deformation, which as we estimate is many order of magnitude large then the speed of light  $u \simeq 1.2 \times 10^{22}c$ . The coordinates of the rest and moving frames of reference for a relativistic particle in the space with GUP satisfy the Lorentz transformation with some effective speed of light. We estimate that the relative deviation of this effective speed of light  $\tilde{c}$  from  $c$  is  $(\tilde{c} - c)/c \simeq 3.5 \times 10^{-45}$ . Finally, note that the influence of GUP on the motion of particle and the Lorentz transformation in the first order over the parameter of deformation is hidden in  $1/c^2$  relativistic effects.

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# Theoretical study of magnetic properties of compounds containing transitional metals

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Theoretical study of magnetic properties of compounds containing transitional metals Based on first principles density functional theory (DFT) calculations, we present study of magnetic compounds. These compounds are (mostly) pentamers containing such transitional metals as iron, nickel, chromium and copper. Preliminary results for  $\text{Cu}_3\text{Cr}_2$  and  $\text{Fe}_2\text{Ni}_3$  structures are presented and discussed. These include spin density maps and energy values. The 'vanishing' of magnetic moment due to charge transfer between metallic ions is observed. These results are qualitatively in agreement with empirical results. However full quantitative explanation of the process requires further study. The computational problems that arise in the research are also discussed, primarily long computational times which result from large amount of atoms comprising the structure and methods to overcome them are presented.

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## Relativistic effects in Penning trap

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We are interested in the motion of a classical charge within a processing chamber of a Penning trap. We examine the relativistic Lagrangian and Hamiltonian dynamics and show that the radial and axial motions are coupled to each other whenever the special relativity is taken into account. We demonstrate that for  $\omega_z \neq 0$  the Hamiltonian system is not integrable in the Liouville sense in the class of functions meromorphic in coordinates and momenta. The non-integrability proof is based on analysis of differential Galois group of variational equations along a certain particular solution. Also some Poincare sections illustrating dynamics for physically important values of parameters are shown. In a specific case of oscillations along the axis of symmetry of quadruple potential the equations of motion are solved. The solution is expressed in terms of Jacobi elliptic functions. The approximation of high-energy radial oscillating mode and low-energy axial oscillating mode is analyzed. The observable relativistic effects such as radiation friction and relativistic cyclotron resonance are considered.

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# Synthesis of superparamagnetic iron oxide nanoparticles (SPIONs) in mesoporous silica materials

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Mesoporous silica materials are promising for drug delivery, e.g. [1-4]. Their high surface areas, tunable pore sizes and volumes give opportunity to carry chemicals, including drugs. Moreover, high chemical and mechanical stability of silica makes this material perfect as a template for synthesis inside the pores.

The method of the synthesis of superparamagnetic iron oxide nanoparticles (SPIONs) directly inside the pores of porous silica will be presented. It is a modification of the Massart method [5]. According to the diameter of pores, different size of iron oxide nanoparticles was obtained. The synthesized material has good magnetic properties (saturation magnetizations 0,7 - 17 emu/g, where the highest saturation magnetizations for pure iron oxides exhibit magnetite and maghemite: 90–95 emu/g and 60–80 emu/g, respectively) [6]). Estimated size of gained SPIONs diameter varies from 0.5 to 6 nm. Samples exhibit superparamagnetic properties in a wide temperature range, both at room temperature and at 2K.

Porous silica with magnetic nanoparticles have also other advantages. One of them is that magnetic silica can be controlled by external magnets; another that it can generate magnetic hyperthermia. Both advantages can be used in drug delivery systems. The recent results on the use of fabricated magnetic silica as drug delivery nanocapsules will also be mentioned.

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## Critical Casimir forces along the iso-fields

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The present study are related to recent experiments showing that plasma membranes are near a critical point in the two-dimensional Ising class. Using the numerical density-matrix renormalization-group technique and the Derjaguin approximation we determine the critical Casimir force and its potential for two discs. To verify our numerical results we analytically derive the asymptotic decay law.

The most interesting result of our calculation is a significant increase in the value of the critical Casimir force along the iso-fields which lie between the bulk coexistence and and the capillary condensation line. It may have an important consequences for lipid membranes with protein inclusions, because most probably the concentration of components of the membrane is not exactly at its critical value.

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# A characteristic structures in entropy surfaces of cardiovascular time series estimated by the Norm Component Matrix Algorithm

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Sample entropy (SampEn) is a popular complexity measure in HRV analysis. SampEn is estimated by fixing the values of the embedding dimension "m" and distance threshold "r" and traditionally SampEn is calculated with m=2 and r=0.2 times the standard deviation of the series. Attempts to extend the estimates to different (m,r) pairs are hampered by the high computational burden of the traditional algorithm. However, recently an extremely fast Norm Component Matrix (NCM) algorithm was proposed for SampEn calculation [1] which allows analyzing whole ranges of (m,r) values leading to entropy surfaces. This short lecture presents the first attempts to calculate these surfaces by NCM and discusses their properties for both synthetic and physiological time series.

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