

IVAN FRANKO NATIONAL UNIVERSITY OF LVIV

**WORKSHOP ON CURRENT PROBLEMS  
IN PHYSICS**

PROGRAM AND ABSTRACT

**Lviv, 10–11 July 2012**

# 10 July 2012

09:00–09:10 Opening

Chairman: **V. Tkachuk**

09:10–09:50 *B. Bandrowski, A. Karczewska, P. Rozmej*, Fractional perturbed Volterra equations of convolution type

09:50–10:30 *O. Derzhko*, Flat-band strongly correlated lattice systems

10:30–11:10 *Yu. Sitenko, N. Vlasii*, Scattering of electron by magnetic field with cylindrical symmetry: what is new and unexpected?

11:10–11:40 Coffee-break

11:40–12:20 *G. Melikidze*, Radiative processes in relativistic magnetised plasma

12:20–13:00 *B. Novosyadlyj, O. Sergijenko*, Do the observations prefer phantom dark energy?

## Lunch

Chairman: **M. R. Dudek**

14:40–15:00 *A. Kuzmak*, Quantum brachistochrone problem for two spin-1/2

15:00–15:20 *A. Karczewska, P. Rozmej, L. Rutkowski*, Surface water waves beyond KdV case

15:20–15:40 *O. Voznyak*, Quasi-exactly solvable potentials for particle with position-dependent mass

15:40–16:00 *G. Panochko*, One-particle density matrix of the Bose-system + impurity atom at finite temperatures

16:00–16:30 Coffee-break

16:30–16:50 *M. Białoskórski, M. Bobrowski, J. Dziedzic, J. Rybicki*, Combining tight-binding and molecular dynamics methods to model the behavior of metals in the plastic regime

16:50–17:10 *S. Mudry, I. Shtablavyi, Yu. Kulyk, R. Serkiz*, Structural aspects of carbon nanotubes-based composites

## Welcome party

## 11 July 2012

Chairman: **P. Rozmej**

**09:00–09:40** *M. Stetsko*, Generalized uncertainty principle with minimal length and momentum and black hole's thermodynamics

**09:40–10:20** *M. R. Dudek, W. Wolak, B. Zapotoczny*, Non-finite difference approach to nonlinear differential equations

**10:20–11:00** *B. Padlyak, W. Ryba-Romanowski, R. Lisiecki*, Optical and EPR spectroscopy of the Nd-doped borate glasses

**11:00–11:30** Coffee-break

**11:30–12:10** *V. Tkachuk*, Deformed Heisenberg algebra with minimal length and equivalence principle

**12:10–12:50** *K. Urbanowski*, On a possible emission of cosmic  $\gamma$ -rays by long living unstable particles

### Lunch

Chairman: **O. Derzhko**

**14:40–15:00** *T. Verkholyak, J. Strečka*, Exact solution for the quantum spin-1/2 two-leg ladder with the Ising interring interaction

**15:00–15:20** *B. Brzostowski, T. Ślusarski, G. Kamienniarz*, DFT study of homo- and hetero-nuclear chromium-based molecular rings

**15:20–15:40** *M. Krasnytska, B. Berche, Yu. Holovatch*, Critical behaviour of spin models on complex networks

**15:40–16:00** *A. Rovenchak*, Towards the definition of critical temperatures in the complex-valued fractional statistics

**16:00–16:30** Coffee-break

**16:30–16:50** *R. Caruana-Gauci et al.*, Recent developments on auxetic materials

**16:50–17:10** *Yu. Yaremko*, Ultrarelativistic limit of the Lorentz–Dirac equation

**17:10–17:30** *A. Dwiryak*, On the Schrödinger equation in a compactified space

**17:30–...** Closing.

## 12 July 2012

**09:00–...** Excursion.

# FRACTIONAL PERTURBED VOLTERRA EQUATIONS OF CONVOLUTION TYPE

*B. Bandrowski*<sup>1</sup>, *A. Karczewska*<sup>1</sup> and *P. Rozmej*<sup>2</sup>

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In the paper we study the following class of perturbed Volterra equations of convolution type

$$u(x, t) = u(x, 0) + \int_0^t [g_\alpha(t-s) + (g_\alpha * k)(t-s)] \Delta u(x, s) ds + \int_0^t b(t-s) u(x, s) ds, \quad (1)$$

where  $x \in \mathbb{R}^d$ ,  $t > 0$ ,  $g_\alpha(t) = t^{\alpha-1}/\Gamma(\alpha)$ ,  $\Gamma$  is the gamma function,  $\alpha \in [1, 2]$ ,  $b, k \in L^1_{loc}(\mathbb{R}_+; \mathbb{R})$  and  $\Delta$  is the Laplace operator. The function  $g_\alpha$  corresponds to the class of equations interpolating heat and wave equations. In other words, the time derivative in differential equation corresponding to Volterra equation with that kernel represents fractional derivative of  $\alpha$  order. Functions  $b, k$  introduce some additional perturbations. Problems described by the equation (1) arise in phenomena of anomalous transport, for instant in porous materials.

The paper provides approximate numerical solutions to the considered equations. The results obtained generalize our previous results [1] from 2010. The approximation consists in the application of a finite subspace of an infinite basis in time variable and discretization in space variables. This leads to a large-scale system of linear equations with non symmetric matrix that is solved with the use of the iterative GMRES method.

The presentation bases on the paper [2].

[1] B. Bandrowski, A. Karczewska, P. Rozmej, *Int. J. Appl. Math. Computer Sci.* **20** 261 (2010).

[2] B. Bandrowski, A. Karczewska, P. Rozmej, *Numerical solutions to fractional perturbed Volterra equations*, submitted.

# FLAT-BAND STRONGLY CORRELATED LATTICE SYSTEMS

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Ten years ago J. Schulenburg et. al. [J. Schulenburg, A. Honecker, J. Schnack, J. Richter, and H.-J. Schmidt, Phys. Rev. Lett. **88**, 167207 (2002)] reported interesting results concerning the ground-state magnetization curve for some quantum Heisenberg anti-ferromagnets. They found that for a wide class of highly frustrated lattices the magnetization curve at zero temperature for this spin model exhibits a jump just at the saturation field. Later on it was recognized that the examined quantum spin systems are intimately connected to another class of strongly correlated electron models, the so-called flat-band Hubbard ferromagnets, which were discussed even earlier [A. Mielke and H. Tasaki, Commun. Math. Phys. **168**, 341 (1993)]. For both spin and electron models the considered lattices support a completely dispersionless (flat) one-particle (one-magnon or one-electron) band and the states from the flat band are the lowest-energy one-particle states. This circumstance opens an interesting perspective to construct and fully characterize *many-particle ground states* of the strongly correlated lattice systems. Moreover, it provides a possibility to map these strongly correlated systems onto corresponding (highly non-trivial) *classical* systems and as a result to use completely different methods from a tool-box of classical statistical mechanics (no Green functions, no functional integrals etc.) for a discussion of quantum many-body physics.

In the present talk I intend to discuss some recent results on flat-band strongly correlated lattice systems focusing mainly on the studies performed in collaboration with J. Richter (Magdeburg), A. Honecker (Göttingen), R. Moessner (Dresden), H.-J. Schmidt (Osnabrück), J. Schulenburg (Magdeburg), T. Krokhumalskii (Lviv), and M. Maksymenko (Lviv).

# SCATTERING OF ELECTRON BY MAGNETIC FIELD WITH CYLINDRICAL SYMMETRY: WHAT IS NEW AND UNEXPECTED?

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Quantum-mechanical scattering of nonrelativistic charged particles by a magnetic vortex of nonzero transverse size is considered. A feasible experiment can be performed involving only the particles with short, as compared to the transverse size of the vortex, wavelengths. We show that the flux of the vortex serves as a gate for the strictly forward propagation of such particles; this effect is the same for various configurations of the magnetic field distributed inside the vortex. We discuss possibilities of the experimental detection of this effect.

## RADIATIVE PROCESSES IN RELATIVISTIC MAGNETISED PLASMA

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It is well known that plasma processes play a decisive role in the generation of emission from many astrophysical objects. An excellent example of a space laboratory for plasma physics is a magnetized neutron star and its environment. If the frequency of radiation is less than that of the plasma and/or cyclotron frequencies, the radiation mechanism should be coherent. Therefore, high energy (i.e. x- and  $\gamma$ -ray) emission can usually be explained by a single-particle radiation (excluding the black-body radiation from very hot spots), but the radio and optical radiation must be generated due to some plasma instabilities. We will overview of linear and nonlinear processes in such plasmas and addresses possibilities of their application for astrophysical purposes. It should be mentioned that generation of waves is a necessary but insufficient condition for radiation mechanisms. Though the plasma waves often possess the highest growth rate, they cannot escape from the plasma. Quite often it is not enough to generate turbulence in the source, but it is also necessary to find a mechanism that ensures transformation of plasma waves into waves capable of escaping from the source and reaching the observer.

# DO THE OBSERVATIONS PREFER PHANTOM DARK ENERGY?

*B. Novosyadlyj, O. Sergijenko,*

Astronomical Observatory of Ivan Franko National University of Lviv, Ukraine

We analyze the dynamics of expansion and large scale structure formation of the Universe in the models with  $\Lambda$ -phantom scalar field as dark energy, which starts from  $\Lambda$ -term mimicry at the Big Bang inflation and slowly evolves to the Big Rip singularity. Such model of dark energy is described by the three parameters - density and EoS parameter at current epoch,  $\Omega_{de}$  and  $w_0$ , and asymptotic value of EoS parameter at a-infinity,  $w_{a-i}$  ( $a$  is the scale factor in Friedmann-Robertson-Walker metric). Their best-fit values were determined jointly with other important cosmological parameters by MCMC method using available observational data on CMB anisotropy, SNe Ia luminous distances, BAO measurements etc. They are:  $\Omega_{de} = 0.72 \pm 0.04$ ,  $w_0 = -1.043_{-0.24}^{+0.043}$  and  $w_{a-i} = -1.12_{-0.50}^{+0.12}$  (denoted by  $\mathbf{p}_1$ ) for the dataset including SDSS SNe Ia distance moduli, determined by SALT2 light curve fitting method, and  $\Omega_{de} = 0.69 \pm 0.05$ ,  $w_0 = -1.002_{-0.14}^{+0.002}$  and  $w_{a-i} = -1.19_{-0.42}^{+0.19}$  (denoted by  $\mathbf{p}_2$ ) for dataset with SDSS SNe Ia distance moduli, determined by MLCS2k2 light curve fitting method. For the model with best-fit parameters  $\mathbf{p}_1$  the Big Rip singularity occurs  $\sim 170$  Gyrs after Big Bang, while in the model with  $\mathbf{p}_2$  600 Gyrs after Big Bang. The similar simulations have been run for  $\Lambda$ CDM and the quintessential scalar field model of dark energy. It was shown that the dataset with SALT2 SNe Ia distance moduli prefers phantom scalar field with parameters  $\mathbf{p}_1$  as dark energy, while dataset with MLCS2k2 SNe Ia distance moduli prefers quintessential scalar field with parameters  $\Omega_{de} = 0.70 \pm 0.05$ ,  $w_0 = -0.83_{-0.17}^{+0.22}$  and  $w_e = -0.88_{-0.12}^{+0.88}$  ( $w_e$  is EoS parameter in early epoch). But the differences of maximal likelihoods for them are statistically insignificant. Therefore, at the current level of accuracy of cosmological observational data we cannot clearly establish the type of dark energy - quintessence, phantom or  $\Lambda$ . Perhaps the new data from current and planned observational programs will give the possibility to establish the type of dark energy.

# QUANTUM BRACHISTOCHRONE PROBLEM FOR TWO SPIN-1/2

*A. R. Kuzmak*

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We study the quantum brachistochrone evolution for a system of two spin- $\frac{1}{2}$  under the specific Hamiltonian. This Hamiltonian realizes quantum evolution in two subspaces which we express as 1.  $|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$  and 2.  $|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle$ . This allows to consider our problem for each subspace separately and lead it to the quantum brachistochrone problem for a spin- $\frac{1}{2}$  in the magnetic field. Also, we obtain the time unitary operator and conditions require to generate an entangler gate and other gates. We demonstrate that this Hamiltonian allows to reach maximally entangled states such as Bell states. This results might be important in quantum computing, quantum teleportation and quantum cryptography.

## SURFACE WATER WAVES BEYOND KdV CASE

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In the paper we study propagation of surface waves on shallow water in an approximation which goes beyond that leading to the Korteweg - de Vries equation. Our aim is to solve the Euler equations for an irrotational flow of an incompressible fluid with a free surface [1]:

$$\phi_{xx} + \phi_{yy} + \phi_{zz} = 0, \quad \text{for } -h < z < \eta(x, y, t) \quad (2)$$

$$\phi_z - (\eta_x \phi_x + \eta_y \phi_y + \eta_t) = 0, \quad \text{at } z = \eta(x, y, t) \quad (3)$$

$$\phi_t + \frac{1}{2}(\phi_x^2 + \phi_y^2 + \phi_z^2) + g\eta = 0, \quad \text{at } z = \eta(x, y, t) \quad (4)$$

$$\phi_n = 0, \quad \text{at } z = -h. \quad (5)$$

Equation (1) is the Laplace equation for the velocity potential  $\phi$ , equations (2) and (3) represent so called kinematic and dynamic boundary conditions at the fluid surface and (4) gives the boundary condition at the bottom.

Derivation of the KdV equation bases on the assumptions that the bottom is flat, that is  $h = \text{const}$ , and  $z + h \ll \lambda_0$ , where  $\lambda_0$  represents a mean value of surface wave length. Then one looks for the velocity potential in the form

$$\phi = \phi_0 + (z+h)\phi_1 + (z+h)^2\phi_2 + (z+h)^3\phi_3 + (z+h)^4\phi_4 + \dots, \quad (6)$$

where functions  $\phi_k(x, t)$ ,  $k = 0, 1, 2, \dots$  do not depend on  $z$ . Further approximations consist in neglecting terms of orders  $n > 3$  in  $(z+h)^n$  in the series (6) and abandoning some other small nonlinear terms which finally lead to the KdV equation for surface waves with soliton solutions.

We consider more general case in which  $h = h(x, y)$ , i.e. the bottom is not flat. In this case there is no analytic solution and we use numerical approach. We discuss several reasonable approximations in the spirit of the KdV approach and show that we can reproduce the KdV solutions when  $h = \text{const}$ . More detailed presentation of the solutions to the above equations will be presented soon.

[1] M. Remoissenet, *Waves called solitons* (Springer, 1993).

[2] Ł. Rutkowski, A. Karczewska, P. Rozmej, in preparation.

## QUASI-EXACTLY SOLVABLE POTENTIALS FOR PARTICLE WITH POSITION-DEPENDENT MASS

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Investigations of the quantum-mechanical system with position-dependent effective mass are an important direction of the modern physics. Particularly, such problems arises in the physics of inhomogeneously doped semiconductors, semiconductor heterostructures, quantum wells, superlattices, nuclear physics, quantum liquids, metal clusters, etc. Therefore, the methods of exact solving the quantum mechanical problems with position-dependent mass were intensively investigated using different approaches.

Supersymmetric quantum mechanics provides powerful method of the exact solving of Schrödinger equation. In the paper [1] supersymmetric method was extended to the case of the position-dependent mass.

Unfortunately, there is a limited set of potential which allows exact solvability of the Schrödinger equation, therefore concept of quasi-exact solvability was introduced, where it is possible to compute certain finite number of eigenvalues and eigenfunctions exactly, even though exact expressions for the full set of eigenvalues does not exist.

In this paper we extend the supersymmetric method for generation of the quasi-exactly solvable potentials [2] to the case of position-dependent mass. This method allows us to obtain different quasi-exactly solvable potentials with two known levels and corresponding wave functions choosing different generating functions.

In frame of this method the ground state was studied. It has been shown that position dependent mass can generate bounded ground state even in the case of constant potential.

The conditions for existence of the ground and the first excited state for the different potentials and position dependent mass have been investigated.

[1] B. Bagchi, A. Banerjee, C. Quesne, V. M. Tkachuk, J. Phys. A **38**, 2929 (2005).

[2] V. M. Tkachuk, Phys. Lett. A **245**, 177 (1998).

## **ONE-PARTICLE DENSITY MATRIX OF THE BOSE-SYSTEM + IMPURITY ATOM AT FINITE TEMPERATURES**

*G. Panochko*

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In the contribution the study of the impurity states in quantum fluids based on construction of full density matrix for all temperatures is made.

The contribution taking into account the effect of impurities on the system states is singled out for the aggregate of interacting Bose-particles and impurity atoms of  $^3\text{He}$  in the approximation of pair correlations in the expression for density matrix. Averaging over the states of the Bose-liquid the one-particle density matrix of the system is found. Its Fourier-image allows to find the momentum distribution of “liquid helium + impurity”. The estimation of the effective mass of the impurity is made.

# COMBINING TIGHT-BINDING AND MOLECULAR DYNAMICS METHODS TO MODEL THE BEHAVIOR OF METALS IN THE PLASTIC REGIME

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Ultra-precision machining of metals, the breaking of nanowires under tensile stress and fracture of nanoscale materials are examples of technologically important processes which are both extremely difficult and costly to investigate experimentally. We describe a multiscale method for the simulation of such systems in which the energetically active region is modeled using a robust tight-binding scheme and the rest of the system is treated with the molecular dynamics method. We introduce a computer code implementing the method, geared towards non-equilibrium, cross-scaled tight-binding and molecular dynamics simulations. Apart from the presentation of the method and implementation, we discuss preliminary physical results obtained and discuss their validity.

## STRUCTURAL ASPECTS OF CARBON NANOTUBES-BASED COMPOSITES

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<sup>2</sup>Scientific-Technical and Educational Center of Low-Temperature Studies,  
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Nanocomposite materials with metallic matrix and carbon nanotubes as a filler attract the attention of researchers due to their promising use in various areas of application and as an inhomogeneous systems with unique physical-chemical properties which need the more detailed studies from fundamental viewpoint.

It is unclear what is interrelation between matrix and filler structure difference and properties of composite system.

It is also interesting how the boundary matrix-nanotubes can be modified in order to improve the properties of nanocomposite.

In this work we represent the results on studying of nanocomposites which consists of carbon nanotubes covered with some metals (Cu, Ni) by means of electrolytic method.

Such nanotubes were mixed with metallic melt and then solidified upon cooling. Structure changes at formation of composite have been studied by means of X-ray diffraction method.

## GENERALIZED UNCERTAINTY PRINCIPLE WITH MINIMAL LENGTH AND MOMENTUM AND BLACK HOLE'S THERMODYNAMICS

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It is well known that Heisenberg's uncertainty principle allows one to obtain thermodynamical functions such as temperature and entropy for a black hole. We apply generalized uncertainty principle with minimal length and momentum to a Schwarzschild black hole. We calculate thermodynamical functions of a Schwarzschild black hole such as temperature, entropy and heat capacity. We also investigate emission rate relation for the black hole and show that generalized uncertainty principle leads to shorter lifetime of the black hole.

## NON-FINITE DIFFERENCE APPROACH TO NONLINEAR DIFFERENTIAL EQUATIONS

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A new efficient numerical algorithm for solving the nonlinear differential equations has been discussed. It is a generalization of the non-finite difference algorithm published for ODE [1],[2] and DDE [3]. The particular examples have been discussed of  $N$ -soliton solutions of KdV equation with  $N = 1, 2$ , and 3.

- [1] M. R. Dudek, T. Nadzieja, *Int. J. Mod. Phys. C* **16**, 413 (2005).
- [2] B. Brzostowski, M. R. Dudek, B. Grabiec, T. Nadzieja, *Phys. Stat. Solidi (b)* **244**, 851 (2007).
- [3] M. R. Dudek, T. Nadzieja, in *Series on Advances in Mathematics for Applied Sciences* **79**, ed. by M. Lachowicz, J. Miekisz (World Scientific, 2009), p. 149.

# OPTICAL AND EPR SPECTROSCOPY OF THE Nd-DOPED BORATE GLASSES

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Optical absorption, luminescence (excitation and emission) spectra as well as luminescence kinetic of the Nd<sup>3+</sup> centers in glasses with Li<sub>2</sub>B<sub>4</sub>O<sub>7</sub>:Nd, LiCaBO<sub>3</sub>:Nd, and CaB<sub>4</sub>O<sub>7</sub>:Nd compositions containing 0.5 and 1.0 mol. % Nd<sub>2</sub>O<sub>3</sub> have been investigated and analyzed. By optical and electron paramagnetic resonance (EPR) spectroscopy it was shown that the Nd impurity is incorporated in the borate glass network as Nd<sup>3+</sup> ( $4f^3$ ,  $^4I_{9/2}$ ) ions. All observed transitions of the Nd<sup>3+</sup> centers in optical absorption and luminescence spectra were identified. The oscillator strengths ( $f_{\text{teor}}$ ) and phenomenological intensity parameters  $\Omega_t$  ( $t = 2, 4, 6$ ) for glasses containing 1.0 mol. % Nd<sub>2</sub>O<sub>3</sub> are calculated using standard Judd-Ofelt theory. The radiative transitions rates ( $W_r$ ), branching ratios ( $\beta$ ), and radiative lifetime ( $\tau_{\text{rad}}$ ) for Nd<sup>3+</sup> centers in the investigated glasses have been calculated and analyzed in comparison with corresponding parameters for Nd<sup>3+</sup> centers in other borate glasses with different compositions. Measured lifetimes for Nd<sup>3+</sup> centers in the  $^4F_{3/2}$  emitting level are compared with those calculated and quantum efficiencies ( $\eta$ ) of the investigated glasses are estimated. Perspectives of application of the Li<sub>2</sub>B<sub>4</sub>O<sub>7</sub>:Nd, LiCaBO<sub>3</sub>:Nd, and CaB<sub>4</sub>O<sub>7</sub>:Nd glasses for Nd<sup>3+</sup>-lasers ( $F_{3/2} \rightarrow ^4I_{11/2}$  channel), particularly for LED-pumped Nd<sup>3+</sup>-lasers, are considered. Based on the structural data for borate glasses and corresponding crystals, the peculiarities of spectroscopic properties and local structure of the Nd<sup>3+</sup> centers in Li<sub>2</sub>B<sub>4</sub>O<sub>7</sub>:Nd, LiCaBO<sub>3</sub>:Nd, and CaB<sub>4</sub>O<sub>7</sub>:Nd glasses have been discussed.

This work was supported by the Ministry of Education, Science, Youth and Sport of Ukraine (project No. 0111U001627) and the University of Zielona Góra (Poland).

# DEFORMED HEISENBERG ALGEBRA WITH MINIMAL LENGTH AND EQUIVALENCE PRINCIPLE

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The studies in string theory and quantum gravity lead to the Generalized Uncertainty Principle (GUP) and suggest the existence of fundamental minimal length which, as it was established, can be obtained in the frame of a deformed Heisenberg algebra. First look of the motion of bodies in the deformed space in uniform gravitational field can give an impression that the bodies of different mass fall in different way and that the equivalence principle is thus broken. Taking into account the result of paper [1] for the effective parameter of deformation for center of mass of a macroscopic body as a composite system we show that in fact GUP is consistent with the equivalence principle.

[1] C. Quesne, V. M. Tkachuk, Phys. Rev. A **81**, 012106 (2010).

## ON A POSSIBLE EMISSION OF COSMIC $\gamma$ -RAYS BY LONG LIVING UNSTABLE PARTICLES

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Not all mechanisms of an emission of very high energy cosmic gamma-rays are clear. We find that charged unstable particles as well as neutral unstable particles with non-zero magnetic moment which live sufficiently long may emit electromagnetic radiation. This new mechanism is connected with properties of unstable particles at the post exponential time region. Analyzing the transition time region between exponential and non-exponential form of the survival amplitude it is found that the instantaneous energy of the unstable particle can take very large values, much larger than the energy of this state for  $t$  from the exponential time region. Basing on the results obtained for a model considered, it is shown that this purely quantum mechanical effect may be responsible for causing unstable particles to emit electromagnetic, X- or  $\gamma$ -rays at some time intervals from the transition time regions.

# EXACT SOLUTION FOR THE QUANTUM SPIN-1/2 TWO-LEG LADDER WITH THE ISING INTERRUNG INTERACTION

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The quantum spin-1/2 two-leg ladder with the anisotropic  $XYZ$  Heisenberg interaction along rungs and Ising interaction between neighboring rungs is studied rigorously. Using the unitary transformation the model is reduced to the transverse Ising chain with composite spins so that the ground state of the ladder can be determined exactly. We calculate the ground state phase diagram for the cases when the interaction between the  $x$  or  $y$  spin components is dominating on the same rungs. The limit of  $X - X$  intrarung interaction corresponds to the quantum compass ladder where this interaction may destroy the  $z$ -ordering of spins along legs. We analyze how an additional diagonal Ising interaction affects the ground state of the model.

## DFT STUDY OF HOMO- AND HETERO-NUCLEAR CHROMIUM-BASED MOLECULAR RINGS

*B. Brzostowski<sup>1</sup>, T. Ślusarski<sup>2</sup> and G. Kamieniarczyk<sup>2</sup>*

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<sup>2</sup>Faculty of Physics, A. Mickiewicz University, Poznań, Poland

Based on first principles density functional theory (DFT) calculations, as implemented in the SIESTA package, we present a comprehensive study of electronic and magnetic properties of octometallic homo- and hetero-metallic chromium-based molecular rings. We widely examine the electronic and magnetic properties of  $\text{Cr}_7\text{MF}_8(\text{O}_2\text{CH})_{16}$  where  $\text{M} = \text{Cr}, \text{Cd}$  and  $\text{Ni}$ . The total, local and orbital projected density of states are presented, magnetic moments are calculated using different approaches as well as the electron density and spin density maps are discussed. Also, depending on  $\text{M}$ , the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) gaps for both spin channels are analyzed. All non-equivalent spin configurations with  $S = \pm 3/2$  are considered to extract exchange interaction parameter  $J$  from the spin model.

# CRITICAL BEHAVIOUR OF SPIN MODELS ON COMPLEX NETWORKS

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Potts and Ising models belong to the most popular spin models of statistical physics. In this report we discuss the case, when these models are considered not on the lattice sites, but on the sites of complex network-like structures with varying node degree  $k$ . Possible applications of spin models on complex networks can be found in various segments of physics, starting from problems of sociophysics to physics of nanosystems, whose structure is often much better described not with the geometry of the lattice but by a network.

First, we review peculiarities of the critical behaviour of the Ising model on a complex network. Then, we use the mean-field approach to analyze thermodynamical properties of the  $q$ -state Potts model on the uncorrelated scale-free network with the power-law decay of the node-degree distribution  $P(k) \sim k^{-\lambda}$ . We obtain thermodynamic functions and analyze the phase diagram of the model in different regions of the  $q - \lambda$  plane. Depending on particular values of  $q$  and  $\lambda$  one observes either the first-order or the second-order phase transition [1]. Analyzing the free energy for different  $q$  and  $\lambda$ , we observe, that behaviour of the thermodynamic functions in the vicinity of the critical point for  $1 \leq q \leq 2$  and certain values of  $\lambda$  is governed by a power-law singularities enhanced by the logarithmic corrections. For  $q = 2$ , the logarithmic corrections are observed at  $\lambda = 5$ , whereas for  $1 \leq q < 2$  they appear at  $\lambda = 4$ . By our data obtained for  $q = 2$  we recover familiar results for the Ising model. For  $q = 1$  (and  $1 < q < 2$ ),  $\lambda > 4$  we recover usual mean field results for the lattice percolation exponents. Furthermore, for  $3 < \lambda < 4$  our results for the leading exponents reproduce the percolation exponents on a scale-free network [2].

We show that the logarithmic corrections exponents that appear at  $\lambda = 4$  and  $q = 1$ , describe percolation on a scale-free network with the node-degree distribution exponent  $\lambda = 4$ . For the percolation problem, we also display the scaling functions for different observables in an explicit form.

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## TOWARDS THE DEFINITION OF CRITICAL TEMPERATURES IN THE COMPLEX-VALUED FRACTIONAL STATISTICS

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The possible approaches to the definition of critical temperature are analyzed for a system of  $D$ -dimensional harmonic oscillators ( $D = 1, 2$ ) obeying the Polychronakos fractional statistics with a complex-valued parameter. The occupation number in this statistics is given by

$$n_i = \frac{1}{z^{-1}e^{\varepsilon_i/T} - e^{i\pi\nu}},$$

where  $z$  is fugacity,  $T$  is temperature, and  $\varepsilon_i$  is the energy of the  $i$ th level. The statistics parameter  $\alpha = e^{i\pi\nu}$  stays on the unit circle ( $\nu = 0 \div 1$ ).

The system of oscillators is shown to have temperature points corresponding to the non-analytical behavior of thermodynamic functions. For  $\nu \neq 1$  similarity to the Bose-condensation phenomenon is observed to some extent.

# RECENT DEVELOPMENTS ON AUXETIC MATERIALS

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Typically materials which we encounter in our everyday life have a tendency to get thinner when stretched (i.e. exhibit a positive Poisson's ratio). However, not all materials behave like this and there exist some materials and structures which get fatter when stretched (i.e. exhibit a negative Poisson's ratio). Such systems are referred to as auxetic, a word which derives from the Greek word *auxetos*, which means 'to grow'.

Auxeticity, though not a common occurrence, is a highly desirable property since it imparts on the materials several enhanced properties when compared to conventional counterparts. Amongst these properties are; increased indentation resistance, the ability to adopt dome shaped surfaces and enhanced vibration absorption properties. Due to these properties, auxetic materials have a wide variety of applications.

In this paper we present some recent developments made in the subject of auxetic materials. In particular we review the various models which are currently used to explain the Poisson's ratio (both positive and negative) in materials and structures and show that new materials can be produced to exhibit this atypical property.

## ULTRARELATIVISTIC LIMIT OF THE LORENTZ-DIRAC EQUATION

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The Fradkin's projection operators are applied to the problem of motion of a light charged particle in a very strong electromagnetic field. The equation of motion is derived which takes into account the radiation reaction (self-action). The equation on eigenvalues and eigenvectors of the electromagnetic field tensor arises as the ultrarelativistic limit of the well-known Lorentz-Dirac equation. The global structure of pulsar magnetosphere is considered in context of this equation of motion.

# ON THE SCHRÖDINGER EQUATION IN A COMPACTIFIED SPACE

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A development of the modern string theory caused deep revision in the conception of physical space. At least two characteristic features of the space anticipated by the string theory are more profound than the theory itself: the existence of a fundamental length, and the multi-dimensionality. Lack of evidence of the space multi-dimensionality is conventionally explained due to compactification of extra space dimensions. A study of peculiarities of such spaces by means of mathematically simple tools, without sophisticated techniques of the string theory, is a subject of present report.

It is considered a potential of pointlike mass or charge in the multidimensional partially compactified space. A behavior of the potential is studied at a distance much longer and much shorter than a compactification radius. It is found an explicit form of the potential in the cases of 2- and 4-dimensional space with one compact dimension. It is proposed for the first example an applied physical-engineering interpretation. The second example of the potential is used in the Schrödinger equation describing a state of particle on a 3-D brane in 4-D compactified space under the gravity of point-like mass. An energy spectrum is found via various approximation methods: variational, perturbational and numerical integration. Relativistic aspect of the problem is discussed.