

СЕМІНАР ІЗ СУЧАСНИХ ПРОБЛЕМ ФІЗИКИ
(Львів, 25–27 жовтня 2021 року)

WORKSHOP ON CURRENT PROBLEMS IN PHYSICS
(Lviv, 25–27 October 2021)

On 25–27 October 2021, the Physics Faculty of the Ivan Franko National University of Lviv hosted the Workshop on Current Problems in Physics. Representatives from scientific institutions of Ukraine and Poland participated in the Workshop, which was the thirteenth meeting of this series. The talks covered quantum mechanics, condensed matter physics, statistical physics, astrophysics, and some other subjects. The abstracts of the presentations are given below.

OPERATOR EXPANSIONS, LAYER SUSCEPTIBILITY AND TWO-POINT FUNCTIONS

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It appears that in boundary conformal field theories in general d dimensions (BCFT $_d$), there exists a one-to-one correspondence between the boundary operator expansion of the two-point correlation function $G(x, x')$ in terms of boundary conformal blocks and a series expansion of the layer susceptibility $\chi(z, z')$ in powers of the variable $\zeta = z/z'$. This general property allows direct identification of the boundary-operator spectrum and expansion coefficients from the layer susceptibility. Moreover, it opens a new way for efficient calculations of two-point correlators in BCFTs.

As an example, an explicit expression is derived for the correlation function $G(x, x') = \langle \phi_i(x) \phi^i(x') \rangle$ of the $O(N)$ model at the extraordinary transition in $d = 4 - \varepsilon$ dimensional semi-infinite space to order $O(\varepsilon)$. Through the bootstrap equation, the bulk operator product expansion of $G(x, x')$ gives access to the spectrum of the bulk CFT. Thus, the averaged anomalous dimensions of scalar composite operators of the $O(N)$ model are obtained, to order $O(\varepsilon^2)$. They agree with the known results both in ε and large- N expansions.

SPECTRAL SINGULARITIES IN ROTATION-TIME-SYMMETRIC AND PASSIVE PARITY-TIME-SYMMETRIC SYSTEMS

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There is increasing interest in investigating non-Hermitian systems, which can display spectral singularities known as exceptional points (EP). Typically, researchers investigate quantum systems exhibiting parity-time (PT) symmetry, which have balanced loss and gain terms, to find EPs. However, incoherent gain terms are not easy to implement experimentally, and therefore, PT-symmetric systems are not perfect for finding and investigating EPs. On the other hand, the emergence of EPs is not limited to PT-symmetric systems.

In this talk, I am going to discuss how to find passive quantum systems which are described by Hamiltonians involving only loss terms. I am going to show that the frame in which the eigenstates scale with

time, which we call *Equilibrium Frame*, is very useful in this task [1]. I am also going to introduce *Rotation-Time* symmetry, which is a generalization of PT symmetry [2], to broaden the class of Hamiltonians, in which one can easily expect the emergence of EPs.

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ESTIMATION OF ENERGY LEVELS OF SPIN SYSTEMS ON IBM'S QUANTUM COMPUTER THROUGH THE STUDIES OF MEAN VALUE EVOLUTION

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The method for estimation of the energy levels of spin systems on a quantum computer based on the studies of evolution of mean value is proposed [1,2]. On the basis of the obtained result, the energy levels of spin systems (a spin in the magnetic field, a spin chain in the magnetic field, Ising model on squared lattice) have been detected on IBM's quantum computers [3]. The method opens a possibility to achieve quantum supremacy in solving the eigenvalue problem for many-spin systems with the development of multi-qubit quantum computers.

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EFFECT OF SILVER CO-DOPING ON ENHANCEMENT OF THE Pr³⁺ LUMINESCENCE IN Li₂B₄O₇ GLASS

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Spectroscopic and luminescent properties of the Pr-doped and Pr-Ag co-doped borate glasses of Li₂B₄O₇ (Li₂O–2B₂O₃) composition are studied and discussed [1] using electron paramagnetic resonance (EPR), optical absorption, luminescence (emission, excitation, decay kinetics) spectroscopy, and Judd-Ofelt analysis. Optical absorption spectra of the investigated glasses reveal several *4f–4f* absorption bands of the Pr³⁺ (*4f²*, ³H₄) ions. Silver co-doping leads to a significant increase in optical absorption in the visible and partly NIR regions due to effects of light scattering and surface plasmon resonance (SPR) absorption induced by silver nanoparticles.

The orange-red Pr³⁺ emission band with a maximum at 601 nm (¹D₂ → ³H₄ transition) and lifetime 22 μs dominates in the luminescence spectra. An increase in the intensity of the Pr³⁺ luminescence by 40 % and 3–4 times was observed in the Li₂B₄O₇:Pr,Ag glass upon excitation respectively at 445 nm (³H₄ → ³P₂ transition) and different photoexcitation in the UV region. Based on the obtained experimental results and the Judd–Ofelt theory we calculated experimental and theoretical oscillator strengths (*f_{exp}* and *f_{theor}*), phenomenological parameters (Ω_2 , Ω_4 , and Ω_6), radiative properties (*A_{rad}*, β , τ_{rad}), and quantum efficiencies (η) of the Pr³⁺ luminescence.

Presence of the isolated Ag⁺ (*4d¹⁰*, ¹S₀) ions, small non-plasmonic Ag aggregates (Ag_{*m*}^{*n*} nanoclusters), and plasmonic Ag metallic nanoparticles in the Li₂B₄O₇:Pr,Ag glass was proposed based on the detailed analysis of optical absorption, luminescence spectra and decay curves. The observed enhancement of

luminescence intensity and the increase in the stimulated emission cross-section and quantum efficiency of luminescence in the $\text{Li}_2\text{B}_4\text{O}_7:\text{Pr},\text{Ag}$ glass are explained by the energy transfer from single Ag^+ ions and Ag aggregates to the Pr^{3+} ions as well as the local-field effect induced by Ag metallic nanoparticles. Silver co-doping is a promising approach to improving luminescent properties of the Pr^{3+} ions in borate glasses.

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LASER-INDUCED SELF-ORGANIZATION IN AMORPHOUS-NANOCRYSTALLINE MATERIALS

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In condensed matter physics, an amorphous material is a solid that lacks the long-range order. Amorphous metals can be produced through extremely rapid cooling (in the order of 10^6 K/s). The rapid cooling is too fast for crystals to form, resulting in disordered atomic-scale structure. The amorphous state is metastable and the processes of self-organization of the structure occur under external influences. The metastable configuration of the atoms gives the material the possibility to choose one pathway among many to change its free energy when, by providing some energy, the system is pushed to modify the quasi-equilibrium states in one of the multiple states of higher/lower energy. The self-organization leads to a new structure of the non-crystalline materials, the so-called nanostructure. Self-organization such as nanocrystallization or, in some cases, formation of laser-induced periodic surface structures (LIPSS), takes place in nonequilibrium conditions under laser irradiation.

Our research is devoted to the impact of laser irradiation (wavelength 1060 nm) on the structure evolution of amorphous FeNbCuSiB, CoFeMnMoBSi, and AlNiSi alloys [1, 2, 3]. In irradiated zones and surroundings, different structural transformations occurred depending on the laser parameters. Structure and phase transitions have been studied using X-ray diffraction, AFM and SEM methods.

LIPSS is a phenomenon of self-organized formation by linearly polarized ultrashort laser pulses with the duration about pico- or femtoseconds. LIPSS were observed on the surfaces of numerous materials including amorphous metal alloys [4]. LIPSS have gained an increasing attention since these structures allow surface nanostructuring and functionalization of optical, mechanical, and chemical surface properties.

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PHOTOIONIZATION MODELLING OF NEBULAR OBJECTS WITH DETAILED CALCULATION OF THE DIFFUSE IONIZING RADIATION TRANSFER

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We have developed the code *DiffRay-3D* [1] for solving the radiation transfer equation in nebular plasmas along any direction during further integration over a 3D volume. In present investigations, we coupled *DiffRay 3D* with popular photoionization code *Cloudy* [2]. The approach was tested on the photoionization modeling (PhM) of “simple” planetary nebulae as well as HII regions with homogeneous density distribution and spherical-symmetry assumption. The obtained ionization structure of these objects was compared with the one calculated on the basis of the usually used Outward Only approximation [3]. The impact of the selected method for diffuse ionizing radiation treatment on the ionization structure and output emission lines spectra was investigated. Important conclusions regarding the efficiency of approximate methods for diffuse ionizing radiation (DIR) calculation in the case of homogeneous models were

done. The same analysis of the impact of the selected method of DIR calculation on photoionization modeling results was performed for the models of planetary nebulae with inhomogeneous structure [4]. Based on the results, conclusions about the necessity for a detailed approach for DIR calculation in the case of objects with inhomogeneous density distribution were made. A detailed method of calculating diffuse ionizing radiation was also used for PhM of optimal models of symbiotic novae shells. It is shown that Outward Only approximation can be used in the case of such compact objects in spite of the inhomogeneity of radial density distribution.

Also, a new approach to investigating the nebular components of dwarf galaxies with the active star formation was introduced. The approach is based on multicomponent photoionization modeling (MPhM) [5–6] using the results of chemo-dynamical simulations [7] as input parameters for the determination of electron density and temperature distributions in the superwind region as well as chemical abundance distribution. As a result of the MPhM calculation using the detailed method of DIR calculation, spatial maps of emissivities and opacities were obtained. These maps were used to obtain synthetic emission lines spectra for different aperture positions. The obtained spectra were analyzed and compared to the corresponding observation results.

The reliability of the “classic” Te-method [8–9] as well as popular calibration approaches (P, N2, O3N2, R3D, S3D, R2D, S2D) [10–17] to determine the oxygen abundance in these objects was estimated in the following way. The emission line spectra for various positions of the synthetic aperture obtained as results of both MPhM methods were used to determine the oxygen abundance by various mentioned above diagnostic methods. The obtained values were compared with those adopted during MPhM from ChDS results, averaged over volume and weighted by emissivity as well as mass. In such way we evaluated the reliability of each of the abovementioned diagnostic methods to determine the oxygen abundance in the nebular environment of the star-forming dwarf galaxies.

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DIRAC δ -FUNCTION POTENTIAL IN QUASIPOSITION REPRESENTATION OF DEFORMED SPACE WITH MINIMAL LENGTH

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We consider the Dirac δ -function potential problem in the general case of deformed Heisenberg algebra leading to the minimal length. In quasiposition representation we present an exact bound solution of the problem. We obtain the condition for the energy spectrum, which similarly to the undeformed case, consists of one energy level. We solve exactly the scattering problem for δ potential and derive expressions for the reflection and transition coefficients. We find that for some resonance energy the incident wave is completely reflected. We conclude that this effect is very sensitive to the choice of deformation function.

PREPARATION OF UNIFORM MAGNETIC NANOPARTICLE FILM USING THE SESSILE DROPLET EVAPORATION METHOD

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Processes of obtaining thin uniform films of nanoparticles are extremely important in manufacturing fields including protecting layers and functional materials. Sessile drop evaporation is one of the well-known methods of nanoparticles deposition. During the evaporation of a pinned sessile droplet, an outward capillary flow appears. This phenomenon is induced by the higher rate of evaporation near the edge of the sessile droplet and the fast loss of liquid there. Nanoparticles present in suspension are transported towards the edge of the droplet, leading to the formation of a ring-like pattern, usually called the coffee-ring effect [1, 2]. In the present research, a stable suspension of magnetic iron oxide nanoparticles was tested for pattern formation during evaporation as a sessile droplet. The impact of the electric and magnetic fields on suppressing undesired ring-like deposit at the edge of droplet was investigated.

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POTTS MODEL WITH INVISIBLE STATES ON A SCALE-FREE NETWORK

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We investigate a critical behaviour of q -state Potts model with invisible states on an annealed scale-free network (where the probability of a randomly chosen vertex having a degree k is governed by the power-law $P(k) \propto k^{-\lambda}$). This model introduces r invisible states such that if spin lies in one of them, it does not interact with the rest of the system (to describe the competition between the energy and the entropy) [1].

We confirm the previously obtained results and conclusions, namely that the number of invisible states can change the universality class of models on graphs, in particular, on a complete graph [2] or even on a scale-free network [3], when the degree distribution decay exponent plays an important role.

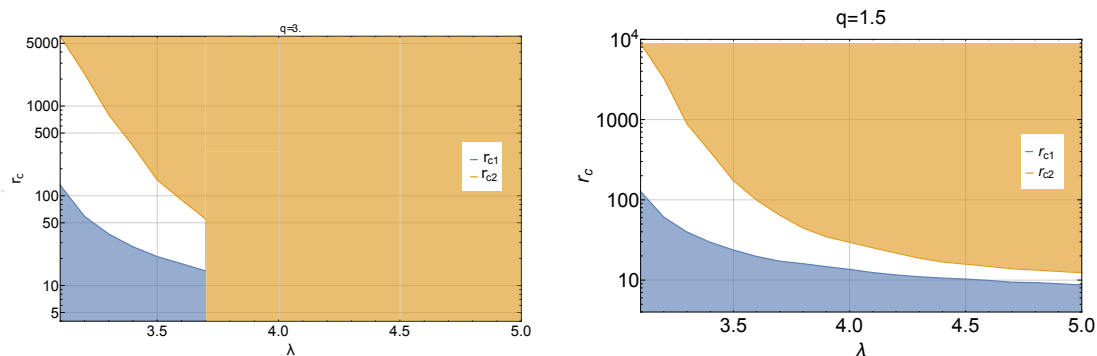


Figure. Phase diagrams for q -state Potts model in r - λ plane. In the lower (blue) region — only 2nd order phase transition (PT) occurs; in the region in-between — 1st and 2nd order PT; in the upper region (yellow) only 1st order PT [4].

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RELATION OF ENTANGLEMENT OF MULTI-QUBIT GRAPH STATES WITH A VERTEX DEGREE AND ITS DETECTION ON A QUANTUM COMPUTER

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Being an inherent feature of quantum mechanics, entanglement is widely exploited as a resource in a range of quantum information schemes. Graph states have become a focus of many recent studies due to their high degree and persistence of entanglement [1]. They find a variety of applications in quantum computing, for instance in quantum error correction, quantum cryptography and quantum machine learning.

In the present study, we consider graph states obtained as a result of the action of controlled phase shift operators on a separable multi-qubit state, in which all of the qubits are in arbitrary identical states [2]. By using the definition of the geometric measure of entanglement to quantify the entanglement of such states, we can easily evaluate this quantity on a quantum device [3], [4]. We derive an analytical expression for the geometric measure of entanglement of an arbitrary qubit l with other qubits in a graph state described by an arbitrary graph, which take the form

$$E_l = \frac{1}{2} - \frac{1}{2} \sqrt{\sin^2 \theta \left(\cos^2 \frac{\phi}{2} + \sin^2 \frac{\phi}{2} \cos^2 \theta \right)^{n_l} + \cos^2 \theta}.$$

Here n_l denotes a degree of the corresponding graph vertex, ϕ is a parameter of the phase shift operator, and θ is a parameter of the initial multi-qubit state this operator is acting on. Note, that the geometric measure of entanglement depends on the absolute values of ϕ and θ . In order to demonstrate the dependence of this quantity on the vertex degree [5], we examine graph states corresponding to graphs of different structure, namely the chain, the claw, and the complete graphs. According to the proposed quantum protocols, these states are prepared on the IBM's quantum processor *ibmq_athens* [6], and the geometric measure of entanglement of qubits corresponding to vertices of degrees 1, 2, 3, 4 with the rest of the system is detected. The results of the quantum computations are in agreement with our theoretical predictions. Deviation of experimental results from the analytical ones in the case of graph states with the structure going beyond the architecture of the quantum device is caused by the accumulation of error on an increasing number of quantum gates in the transpiled circuit.

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STUDY OF PHOTOLUMINESCENCE IN MONOCRYSTALS $\text{Gd}_{3-x}\text{Sm}_x\text{Ga}_5\text{O}_{12}$

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In recent years, oxide crystals activated by ions of three valence rare-earth ions have attracted attention as materials for the creation of LEDs with a white spectrum of radiation. Typically, the white emission color is achieved by combining in one matrix of phosphors that glow in the ultraviolet or near ultraviolet with phosphors that glow in red, green and blue. At the same time, it is problematic to search for highly efficient phosphors with emission in the red region of the spectrum, which are chemically stable and have strong absorption in the ultraviolet region. One such ion that meets these requirements is Sm^{3+} , and the matrix crystal, where the Sm^{3+} ions are placed, is an oxide crystal of the garnet-type structure, which belongs to the hexagonal class of cubic syngony with the space group $O_h^{10}\text{-Ia}3d$ containing eight $\text{A}_3\text{B}_2\text{C}_3\text{O}_{12}$ formula units per unit cell.

We have studied the photoluminescence spectra in $\text{Gd}_{3-x}\text{Sm}_x\text{Ga}_5\text{O}_{12}$ single crystals with concentrations of Sm^{3+} at 1.08×10^{21} and 2.2×10^{21} ions/cm³, which corresponded to the values of $x = 0.25$ and $x = 0.5$. Luminescence spectra were recorded in the temperature range of 5–300 K in the spectral range of 500–1100 nm. The energy structure of the Sm^{3+} Stark components in the studied spectral interval is presented. The obtained data were compared with the data from [1] for $\text{Sm}_3\text{Ga}_5\text{O}_{12}$ single crystals, and data [2] for $\text{Gd}_{3-x}\text{Sm}_x\text{Ga}_5\text{O}_{12}$ crystals with concentrations of Sm^{3+} equal to 8.6×10^{19} and 4.3×10^{20} ions/cm³, which corresponded to $x = 0.02$ and $x = 0.1$.

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RADIAL DISTRIBUTION OF CHEMICAL ELEMENTS IN THE MILKY WAY GALAXY OBTAINED USING PLANETARY NEBULAE ABUNDANCES

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We present the radial chemical abundance gradients of He/H, N/H, O/H, Ne/H, S/H, and Ar/H for the Milky Way Galaxy obtained on the basis of planetary nebulae chemical compositions (PNe). These compositions were calculated using emission line spectra of 164 galactic PNe. Emission line spectra of observed PNe envelopes were taken from Karen Kwitter [1]. Also, we used distances to them from GAIA DR2 [2]. The nebular diagnostic of these spectra was performed using PyNeb code [3]. We calculated these models along the evolutionary tracks of PNe nuclei for two types of dust grains (carbonates and silicates) as well as for various masses of progenitor stars using Gary Ferland's code Cloudy 17.01 [4]. We applied three different types of density distribution (Golovaty-Mal'kov semi-empirical law [5], hydrodynamical (private communication), and homogeneous). To take into account the unobservable ionization stages in the PNe envelopes, the ionization-correction factors were obtained using photoionization modelling of these objects. All models before usage were checked for reproduction of the observed spectra.

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DOPPLEROGRAPHY OF THE TYCHO SUPERNOVA REMNANT

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Supernovae and their remnants play an important role in modern cosmology, neutrino astrophysics and high-energy astrophysics. In the present study, the observational data of the Tycho Brahe supernova remnant (SN 1572) obtained by the Chandra Space Observatory are analyzed. Using a special software package for data analysis CIAO-4.12, images of the remnant have been produced for a number of photon energy ranges, namely, for the two brightest lines of Silicon and Sulfur. The spectra of thermal and synchrotron radiation from small regions over the whole SNR surface were extracted and analyzed. Using respective spectral models — *xsbremss* and *gauss1d* — the spectra were fitted and main characteristics of the lines were obtained. Based on the results of the research, and taking into account the Doppler effect, a 2D distribution of the velocity along the line of sight of Si (1.6–2.1 keV) and S (2.3–2.6 keV) in stellar ejecta was obtained. The constructed maps show a significant asymmetry of the supernova explosion.

PHOTOVOLTAIC EFFECT IN FERROELECTRIC $[(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.68}\text{Ti}_{0.32}]\text{O}_3$ CRYSTAL

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Nowadays photovoltaic industry, which is based on semiconductor materials, faces the fundamental limit of their efficiency. The search for a new, completely different approach to the conversion of solar energy into electricity is a task that is very important for a significant increase in the efficiency of solar cells. Under such circumstances, it is necessary to look for other pathways to perform charge separation in materials to make the next generation of photovoltaics possible. One of them is investigation of new photovoltaic materials for solar energy transformation based on the ferroelectric crystals. Existence of spontaneous polarization in the ferroelectric crystals creates an electric field in the domains which can separate photogenerated free charge carriers. Moreover, ferroelectric materials can achieve extremely high open circuit voltages in comparison to the conventional semiconductor solar cells, since the maximum voltage that can be produced by these devices is equal to the semiconductor electronic bandgap. Lead magnesium niobate lead titanate (PMN-PT) family ferroelectric crystals with the general formula $\text{Pb}[(\text{Mg}_{1/3}\text{Nb}_{2/3})_x\text{Ti}_{1-x}]\text{O}_3$ would be considered promising basic materials for the high voltage solar cells. These crystals possess large photovoltaic effect[1,2].

The studied $[(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.68}\text{Ti}_{0.32}]\text{O}_3$ ferroelectric crystal of (001) orientation was supplied by Crystal-Gmbh (Germany) in a rectangular shape with the edges along [010] and [100] directions. The silver paste electrodes were deposited in the directions parallel and perpendicular to [001]. The dielectric hysteresis loop was obtained at room temperature using an external electric field of an ultralow frequency. The samples were illuminated using a 365 nm light emission diode produced by Thorlabs Inc. The ferroelectric loops, time current, and time voltage measurements were performed using Keithley 6517A electrometer.

We observed a significant influence of the UV light on the ferroelectric properties of $[(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.68}\text{Ti}_{0.32}]\text{O}_3$ crystal, which can be explained by the dynamics of the light generated photocarriers in the internal electric field. Investigations of the ferroelectric loops under the influence of light and in darkness demonstrated widening of the FE loops for $[(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.68}\text{Ti}_{0.32}]\text{O}_3$ crystal under the UV illumination. The data obtained for parallel and perpendicular geometry of the UV light illumination allowed us to understand the origin of the photovoltaic effect in this material. The time dependence of a photovoltage reveals large photovoltaic response of the investigated sample with a jump-like increase in the signal under the UV illumination of the sample.

Acknowledgment: This work was supported by the Ministry of Education and Science of Ukraine.

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INVESTIGATION OF HEISENBERG SPIN SYSTEMS ON AN IBM'S QUANTUM COMPUTER

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The Heisenberg spin system is studied. Namely, an expression that describes the evolution of this system over time is obtained. An analytical expression was obtained for the geometric measure of the entanglement of the spin system, and the corresponding graphs of the entanglement dependence were built. A quantitative estimate for the geometric measure of entanglement is carried out by implementing a scheme of the evolution operator using quantum logic elements. The mean value of the spin is measured on a quantum computer. The results obtained for the geometric measure of the entanglement on a quantum computer are in agreement with the theoretical ones.

FILTRATION OF NANOPARTICLE AGGLOMERATES IN AQUEOUS COLLOIDAL SUSPENSIONS EXPOSED TO AN EXTERNAL RADIO-FREQUENCY MAGNETIC FIELD

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The study investigated the phenomenon of fast aggregation of single-domain magnetic iron oxide nanoparticles in stable aqueous colloidal suspensions due to the presence of a radio-frequency (RF) magnetic field. Single-domain nanoparticles have specific magnetic properties, especially the unique property of absorbing the energy of such a field and releasing it in the form of heat. The localized heating causes the colloid to become unstable, leading to faster agglomeration of nanoparticles and, consequently, to rapid sedimentation. It has been shown that the destabilization of a stable magnetic nanoparticle colloid by the RF magnetic field can be used for the controlled filtration of larger agglomerates of the colloid solution [1]. Two particular cases of stable colloidal suspensions were considered, a suspension of the bare nanoparticles in an alkaline solution and the silica-stabilized nanoparticles in a neutral solution. The obtained results are important primarily for biomedical applications and wastewater treatment.

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ON THE POSSIBILITY OF DETECTION OF MOLECULAR EMISSION FROM THE FIRST BILLION YEAR UNIVERSE

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After the cosmological recombination and before the birth of the first stars, during about a billion years, the Universe was dark and cold. Is it possible to detect some signal from there? Yes, recently EDGES has detected an absorption line in the redshifted hyperfine hydrogen 21-cm line. But, is it possible to detect molecular emission from the first billion year Universe? To answer this question, we study the creation and destruction of first molecules in the first billion year Universe life (redshift range $100 < z < 10$) and the emission of protogalaxy halos in the cosmic microwave background. We estimate the upper limits of the energy density of the first light for four models of thermal light evolution in the Cosmic Dawn using the observational constraints on the re-ionization of the intergalactic medium. We estimate its impact on the creation/destruction of first molecules as well as on the brightness temperature of protogalaxy halos in the ro-vibrational transitions (microwave range of wavelength) of the most abundant molecules H_2 , HD and HeH^+ . The results show that molecules H_2 and HD are destroyed by photodissociation processes long before the full re-ionization in the interhalo medium, in the medium of both types of halos, and for all models of the first light. Meanwhile, the number density of HeH^+ molecules illustrates an essentially more complicated dependence on the kinetic temperature of halos and the model of the first light. The time-dependence of the differential brightness temperature of protogalaxy halos mainly follows the number density of molecules and the kinetic temperature of baryonic matter. Therefore, the observations of the Dark Ages and Cosmic Dawn halos in the lines of the first molecules may be an informative probe into physical processes at the beginning of the first stars and galaxy formation in the first billion year Universe.

UNIVERSAL CAUSAL SEPARABILITY CRITERION

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The search of the most universal and physically transparent forms of separability tests for arbitrary density matrices represents one of the most fundamental challenging problems in modern quantum entanglement theory [1]. Especially, the applicability of the most famous Peres–Horodecki criterion of separability is restricted by two-qubits density matrices only [2,3], while its general physical background has not been yet clarified. However, recently a general solution of this common separability problem has been proposed by the author in Ref. 4. Here, the general physical background of the Peres–Horodecki positive partial transpose (PPT-) separability criterion has been revealed [4] for the first time. Especially,

the general physical sense of partial transpose operation was shown to be equivalent to what one could call the “*local causality reversal*” (LCR-) procedure for all separable quantum systems, or to the demonstration of a *global time arrow direction uncertainty* in all entangled cases [4]. Using these two universal causal considerations, two brand new fundamental universal probabilistic relations which encode a new heuristic causal separability criterion have been proposed for density matrices of arbitrary (even infinite) dimensionality D^N , describing arbitrary ensembles of N quantum systems of D eigenstates each [4]. Resulting general formulas have been then analyzed for the widest special type of one-parametric density matrices of arbitrary dimensionality, those modelling number N of equivalent quantum subsystems of dimensionality D in each subsystem’s Hilbert subspace, being all equally connected (EC-) with each other to an arbitrary degree by means of a single entanglement parameter p (see Ref. 4). As the result, a number of remarkable features of the entanglement thresholds $p_{\text{th}}(D, N)$ for such EC-density matrices have been described for the first time in Ref. 4. All novel results obtained for the family of arbitrary EC-density matrices are shown to be applicable to a wide range of both interacting and non-interacting (at the moment of measurement) multi-partite quantum systems, such as arrays of qubits, spin chains, ensembles of quantum oscillators, strongly correlated quantum many-body systems, etc. (see Ref. 4 for details).

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MODELING AND MEASUREMENT OF SPIN-1 ON A QUANTUM COMPUTER

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The register of quantum computers consists of a set of two-level quantum systems (qubits). To simulate one spin-1 on a quantum computer, two qubits have to be used. We propose protocols which allow one to measure the mean value of spin-1 and to measure the correlations between two certain spins. On the IBM quantum computer, we prepare the evolution of spin-1 in the magnetic field and measure its mean value. Also we prepare a system of two interaction spins and measure the correlations between them.

TWO-SPECIES REACTION-DIFFUSION SYSTEM WITH LÉVY FLIGHTS

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We analyze a two-species reaction-diffusion system with reactions $A+A \rightarrow (0, A)$ and $A+B \rightarrow A$, where both species are performing Lévy flights. The Lévy flight is a random walk in which the step-lengths obey a Lévy distribution $P(r) = r^{-d-\sigma}$ (a heavy-tailed probability distribution), with the control parameter $0 < \sigma < 2$. Previous studies of the ordinary diffusing Brownian particles have shown that for such reaction-diffusion system both the B particle density [1] and the correlation function BB [2] are characterized by nontrivial universal exponents that include an anomalous dimension for $d \leq d_c$ (fluctuation-dominated kinetics). Applying the renormalization group formalism [3], we calculate the decay exponents of the B particle decay and the correlation function BB below the critical dimension in the case of the Lévy flights. As in previous studies with the short-range diffusion hops, the two-species reaction-diffusion system with Lévy flights also exhibits an anomalous dimension in the B particle density and the BB correlation function resulting from the renormalization of the field associated with the B particles and the square of

the field, respectively. The numerical simulations of the process are performed as well, and the quantitative estimates of the decay exponents obtained are in good agreement with our analytical results [4].

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FINDING EIGENENERGIES AND EIGENFUNCTIONS OF A QUANTUM MECHANICAL SYSTEM OF BARRIERS AND WELLS IN THE QUANTUM MECHANICAL IMPEDANCE APPROACH

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It was shown how the relation between Green's function and a quantum wave impedance function can be applied for finding eigenenergies and eigenfunctions of a quantum mechanical system of barriers and wells. As the illustration, three different approaches, namely a classical approach based on a direct solving of the Schrödinger equation, a transfer matrix method, and a quantum wave impedance technique are used for the calculation of eigenenergies and eigenfunctions of a nonsymmetric single well. A comparison of these approaches gives the possibility to clarify advantages and drawbacks of each method.

OPTICAL PROPERTIES OF DOPED LiNH_4SO_4 CRYSTALS IN β -MODIFICATION

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The aim of this study was to elucidate the mechanism of the Mn ion impurity effect on the optoelectronic parameters of β -modification LiNH_4SO_4 (LAS) crystals and to establish the dependence of the temperature-spectral behavior of the refractive index and birefringence on the impurity concentration.

The impurity lithium ammonium sulfate crystals in β -modification were obtained by growth from the aqueous solution through slow evaporation of the solvent at a constant temperature of 318 K. The dispersion of refractive indices n_i was studied using the immersion and spectroscopic Obreimov methods. Temperature-spectral changes of birefringence Δn_i were studied using the spectroscopic method, which allows one to study the dispersion simultaneously in a wide spectral and temperature ranges. Studies of the refractive indices dispersion dependences of β -LAS with manganese impurity at room temperature showed that in the 300–700 nm spectral range the dispersion $n_i(\lambda)$ is normal ($dn/d\lambda < 0$) for three light polarizations $\mathbf{E} \parallel \mathbf{X}$, $\mathbf{E} \parallel \mathbf{Y}$ and $\mathbf{E} \parallel \mathbf{Z}$ and increases sharply as it approaches the absorption edge. The introduction of the impurity does not change the specifics of the spectral changes of the refractive indices for the three polarizations, but leads to an increase in their absolute values. Since the introduction of the Mn impurity increases the refractive indices in different directions unequally, it leads to an increase in the anisotropy of the optical indicatrix. This is confirmed by the increase in the A_{n-1} coefficient (to $19 \cdot 10^{-3}$), which characterizes the anisotropy of the electronic subsystem. Temperature changes of birefringence of β -LAS:Mn showed that it is quite sensitive to temperature changes in all directions

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INFLUENCE OF HYDROSTATIC PRESSURE ON STRUCTURE AND PROPERTIES OF AgAlS₂ CRYSTAL

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Within the framework of the electronic density functional theory (DFT), theoretical studies of the properties of AgAlS₂ chalcopyrite crystals were performed from the first principles. Calculations of the band-energy structure $E(k)$, total (DOS), and partial (PDOS) density of states, optical spectra, and elastic properties of AgAlS₂ crystal were performed. The effect of hydrostatic pressure on the titled compound is modelled. The influence of hydrostatic pressures in the range 0–5 GPa on the structure of electronic, optical, and elastic properties of the crystal has been studied. The analysis of anisotropy of elastic properties and its change under the action of hydrostatic pressure is carried out. An analysis of the baric change in the nature of the chemical bond was performed and discussed. The possibility of a smooth change in the chosen physical parameters using of pressure is shown.

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PHOTOIONIZATION MODELLING OF THE HII REGIONS SURROUNDING STAR-FORMING REGIONS

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We present a method of modelling HII regions around the areas of star formation. In our method, we used a “bubble” structure of HII regions, which was divided into internal and external components [1]. The internal components include the free-winding region of the superwind [2] and the superwind cavity, and the outer components include the gas layer compressed by the shock wave of the superwind and the hydrodynamically undisturbed outer part of the HII region [3]. The spectrum of the Lyman continuum, mechanical luminosity, mass loss rate, chemical abundances of the central star formation region were calculated using evolutionary-population modelling [4] and were used as input parameters for further photoionization modelling of HII regions. As a result of such modelling, the following parameters were obtained: the original Lyc spectrum, radiation fluxes at different wavelengths, the evolutionary distribution of the electron temperature, and the electron concentration of the HII region.

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QUANTUM CORRELATIONS IN \mathcal{PT} -SYMMETRIC SYSTEMS

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We consider two \mathcal{PT} -symmetric models, consisting of two or three single-mode cavities. In both models, the cavities are coupled to each other by linear interactions, forming a linear chain. Additionally, the first and last of such cavities interact with an environment [1,2].

In this communication, we focus on finding such situations for which bipartite steering can be observed for pairs of subsystems. To quantify the steering, we apply steering parameters S_{ij} defined with the use of the Cavalcanti inequality [3]

$$S_{ij} = \langle \hat{a}_i \hat{a}_j^\dagger \rangle \langle \hat{a}_i^\dagger \hat{a}_j \rangle - \langle \hat{a}_i^\dagger \hat{a}_i (\hat{a}_j^\dagger \hat{a}_j + \frac{1}{2}) \rangle,$$

where indices i and j label the subsystems, whereas \hat{a}^\dagger and \hat{a} are usual boson creation and annihilation operators, respectively. When the parameter S_{ij} is positive, the subsystem labeled by j steers that denoted by i .

In our considerations, we focus on relations between the steering generation in the models and the coupling strength, and the gain and loss of the energy. We find the values of parameters describing the system for which the steering appears.

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LOCAL STRUCTURE, SPECTROSCOPY AND PHOTOLUMINESCENCE OF THE UN-DOPED LEAD BORATE GLASSES

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The electron paramagnetic resonance (EPR), optical absorption, infrared (IR) transmission, and photoluminescence of un-doped glasses of the $\text{PbO-B}_2\text{O}_3\text{-GeO}_2\text{-La}_2\text{O}_3$ and $\text{PbO-B}_2\text{O}_3\text{-SiO}_2\text{-ZnO}$ systems were presented and analyzed according to [1]. Optical band gaps and Urbach energies for both types of glasses have been evaluated using the fundamental absorption edge analysis. The $\text{PbO-B}_2\text{O}_3\text{-GeO}_2\text{-La}_2\text{O}_3$ glass upon ultraviolet (UV) photoexcitation shows broad emission, consisting of two intense overlapping bands peaked about 465 and 610 nm. The photoexcitation spectrum of the $\text{PbO-B}_2\text{O}_3\text{-GeO}_2\text{-La}_2\text{O}_3$ glass shows an intense band peaked at 351 nm upon monitoring the emission band at 465 nm that is characterized by fast luminescence kinetics. The luminescence decay curve of the emission band at 610 nm, registered upon excitation at 357 nm, was best fitted by two-exponential approximation with lifetime values in the microsecond range. In the $\text{PbO-B}_2\text{O}_3\text{-GeO}_2\text{-La}_2\text{O}_3$ glass fast and slow recombination mechanisms were proposed for emission bands peaked about 465 and 610 nm. The $\text{PbO-B}_2\text{O}_3\text{-SiO}_2\text{-ZnO}$ glass upon excitation at 419 nm reveals only a broad emission band peaked at 593 nm that is characterised by fast luminescence kinetics. The CIE chromaticity diagram shows that the color of the observed intrinsic luminescence significantly depends on the glass composition due to the different values of the optical band gap and the location of the fundamental absorption edge in the investigated lead borate glasses. The obtained results clearly demonstrate that the studied $\text{PbO-B}_2\text{O}_3\text{-GeO}_2\text{-La}_2\text{O}_3$ and $\text{PbO-B}_2\text{O}_3\text{-SiO}_2\text{-ZnO}$ glasses belong to very perspective luminescent materials with tuneable emission in a wide visible spectral range.

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TUNNELING OF ENTANGLED PARTICLES

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We discuss the problem of tunneling of entangled particles through a potential barrier. A continuity equation for many particles is derived. As an example, two particles are considered and flow probability density is calculated. The influence of entanglement on the flow probability density is analyzed.

DETECTION OF THE PROBABILITY OF A QUANTUM STATE DETERMINATION AMONG N POSSIBLE ONES ON A QUANTUM COMPUTER

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We study the probability of determining an unknown quantum state in the case the state is one of the N eigenstates of the spin projection operator on certain N directions [1]. The probability of determining the unknown state with the smallest number of measurements is found. Also the probability of determining the unknown state for n measurements is analyzed. The results are obtained on the basis of the analytical calculations, as well as calculations on IBM's quantum computers (ibmq quito, ibmq armonk) [2].

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TRANSFER OF QUANTUM CORRELATIONS TO POPULATED QUBITS

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We discuss the process of transferring quantum correlations (entanglement) to uncorrelated qubits. Particular attention is paid to determining how the transfer process of quantum correlations depends on the initial population of the qubits. We show that depending on the initial population of the qubits, the transfer of the quantum correlations can be delayed even though the absorption of photons from the field is not sensitive to the initial population. In the absence of the initial population, the transfer of the quantum correlations begins immediately after the entangled field is turned on. In contrast, if the qubits are initially prepared in some of the excited states, the transfer is delayed by a finite time interval. A detailed discussion will be given on the dependence of the delay transfer time on the one and two photon populations, and damping rates of the qubits. The physical origin of the delayed transfer of quantum correlations is explained in terms of quantum jumps.

DISCRETE SPECTRUM IN SOFT QUANTUM WAVEGUIDES WITH AN EXPLICIT CUT-LOCUS

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We consider two-dimensional Schrödinger operators with an attractive potential in the form of an infinite channel of a fixed width and profile. The channel is built over of an unbounded curve composed of a circular arc and two straight semi-lines. Relying on a test-function argument we establish the existence of discrete eigenvalues in the system. The talk is based in the paper [S. Kondej, D. Krejcirik, J. Kriz, *Soft quantum waveguides with an explicit cut-locus*, J. Phys. A: Math. Theor. **54** (2021)].

DYNAMICS AND INTEGRABILITY ANALYSIS OF SWINGING ATWOOD'S MACHINE-LIKE SYSTEMS WITH COULOMB'S AND HOOKE'S INTERACTIONS

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Цьогоріч виповнилося 75 років професорові Національного університету “Львівська політехніка”, заслуженому діячеві науки і техніки України, докторові фізико-математичних наук Григорієві Архиповичу Ільчукові — відомому вченому в галузі проблем технологій напівпровідникових матеріалів, фізики і хімії поверхні, фізики твердого тіла.

Григорій Ільчук народився 19 листопада 1946 року в селі Кричильську Сарненського району Рівненської області. У 1964 році вступив у Львівський політехнічний інститут за спеціальністю “Напівпровідникові прилади”. По закінченні навчання 1969 року був скерований на роботу до “Спеціалізованого конструкторсько-технологічного бюро нестандартного обладнання” (місто Молодечно Мінської області) на посаду інженера. У 1970–1972 роках служив у збройних силах. Від березня 1973 року працював у Львівському політехнічному інституті на посадах інженера, старшого інженера, молодшого і старшого наукового співробітника науково-дослідної лабораторії НДЛ-10 кафедри фізики.

Григорій Ільчук навчався в аспірантурі Фізико-технічного інституту ім. А. Ф. Йоффе АН СРСР (1980–1984 рр.), де захистив дисертацію “Эпитаксиальные слои $Cd_xHg_{1-x}Te$, выращенные методом химических транспортных реакций (ХТР): получение и свойства” за спеціальністю “Фізика напівпровідників і діелектриків” і одержав науковий ступінь кандидата фізико-математичних наук.

У 1987 році він перейшов на викладацьку роботу на кафедрі фізики на посаду асистента, а 1991 року — на посаду доцента. У 2003 році вчений захистив дисертацію “Фізичні основи процесів росту з парової фази монокристалів і епітаксійних шарів A^IVB^VI та структури на їх основи” й одержав науковий ступінь доктора фізико-математичних наук за спеціальністю “Фізика приладів, елементів і систем”. Від 2003 року працює на посаді професора кафедри фізики.

Григорій Архипович Ільчук — співавтор підручників та навчальних посібників для студентів закладів вищої освіти “Фізика”, “Фізика і будівництво”, “Атомна фізика: збірник задач”, “Збірник задач з фізики” та ін., а також співавтор п’яти монографій. Професор викладає курс загальної фізики для студентів інженерно-технічних спеціальностей і курс “Вибрані розділи напівпровідникових матеріалів” для здобувачів ступеня доктора філософії спеціальності 105 “Прикладна фізика і наноматеріали”. Він розробив методiku викладання фундаментальних дисциплін, зокрема фізики, в основі якої є залучення прикладів використання законів фізики в професійній діяльності майбутніх інженерів.

Учений опублікував понад 500 наукових праць, серед яких патенти України, країн Євросоюзу, Тайваню, США, Японії. 110 наукових статей опубліковані у високореєтингових журналах, що індексуються в наукометричних базах даних Scopus та Web of Science.

Професор Григорій Ільчук є членом спеціалізованої вченої ради із захисту докторських і кандидатських дисертацій Д 35.052.13 (м. Львів). Він багаторазово опонував як кандидатські, так і докторські дисертації. Був науковим керівником успішно захищених 5 кандидатських дисертацій та є науковим консультантом захищеної 2021 року докторської дисертації.

Григорій Архипович інтенсивно займається науковими дослідженнями. Під його керівництвом успішно виконано три міжнародні наукові проекти (Тайвань), які скеровані на створення високоефективної автономної системи фотоперетворення й акумулювання сонячної енергії, складовою якої є гнучкий суперконденсатор.

У червні 2011 року відомий американський журнал “Research and Development” опублікував щорічний список переможців престижного конкурсу “Top-100 кращих досліджень і розробок світу” (The 49th Annual RandD Awards), серед яких розробка Тайванського текстильного дослідного інституту (ТТДІ) “Повністю гнучкий тканинний суперконденсатор” у номінації “Електричні прилади”. Цей суперконденсатор розробив для ТТДІ колектив учених із Національного університету “Львівська політехніка” під керівництвом Григорія Ільчука. Газета “Трибуна Чикаго” (The Chicago Tribune) називає цю премію “Оскар серед винаходів”.

Серед нагород професора Григорія Ільчука: почесне звання “Заслужений діяч науки і техніки України” (№818/2014, 21.10.2014 р.), Почесна грамота Кабінету Міністрів України (№ 18943,



27.11.2009 р.), Почесна грамота Міністерства освіти і науки України (№119139, 2007 р.), Почесна грамота Львівської обласної державної адміністрації та Львівської обласної ради (2012 р.), Почесна грамота Львівської обласної державної адміністрації (2009 р., 2012 р.), Відзнака Львівського міського голови “Почесний знак Святого Юрія” (№23, 05.05.2012 р.), Грамота Національного університету “Львівська політехніка” за значні досягнення в навчальній та науковій роботі (2004 р.), Почесна грамота Національного університету “Львівська політехніка” за визначні успіхи в педагогічній і науковій роботі та видатні заслуги перед “Львівською політехнікою” (29.11.2016 р.). Від 2019 року Григорій Льчук є керівником наукової школи “Прикладна фізика та наноматеріали”.

Редакційна колегія “Журналу фізичних досліджень”, члени наукової школи “Прикладна фізика та наноматеріали”, колеги-фізики, колектив кафедри фізики щиро вітають шановного Григорія Архиповича з ювілеєм, щиро бажають йому міцного здоров'я, щастя та натхнення, а також наснаги в здійсненні творчих задумів і плідних звершень у науковій діяльності!

Науково-дослідна група:

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