KUMQUAT

THEORETICAL PHYSICS,
QUANTUM COMPUTING
AND COMPLEX SYSTEMS
INTERNATIONAL CONFERENCE 2021

Abstract book

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Faculty of Fundamental Problems of Technology

Wrocław University of Science and Technology

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Contents

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Invited Lectures

Theoretical Physics

Non-equilibrium processes in small and heterogeneous systems

Prof Dr Ralf Metzler

University of Potsdam, Germany

Brownian motion is a ubiquitous phenomenon at the heart of non-equilibrium statistical mechanics and physical chemistry. Based on its theoretical description in terms of the diffusion equation, Smoluchowski calculated the diffusion limitation of molecular reactions in 1916. Today, by means of superresolution microscopy scientists can resolve the production and distribution of individual proteins and visualise how microbeads or fluorescently labelled molecules diffuse in a living biological cell. These experimental observations show that new theoretical models are needed to understand how transport and regulation works in systems such as live cells or their organisations in biofilms.

In my talk I will address the fact that many molecular signalling reactions running off in cells are involving minute chemical concentrations. The resulting reaction dynamics then spans several decades of reactions times, and the meaning of chemical rates needs to be re-assessed. In particular I will introduce the concepts of geometry- and reaction-control of molecular reactions.

The second, main topic is the diffusive spreading itself, of tracer particles in complex, heterogeneous environments such as biological cells. A growing body of experiments demonstrate that heterogeneity effects cause pronounced deviations from the Gaussian displacement distribution, the central law in statistical mechanics. I will highlight several experimental examples for non-Gaussian processes and present simple theoretical concepts for their description when the diffusion is ”normal” and ”anomalous”, i.e., when the mean squared displacement no longer grows linearly in time.

Invited Lectures Theoretical Physics

How to use the Green function in BLUES

Prof Joseph Indekeu
Institute for Theoretical Physics, KU Leuven, Belgium

An analytic method is proposed which uses the Green function in an alternative way for solving nonlinear differential equations approximately. The method goes beyond linear use of equation superposition and is named BLUES. The upshot is to define a related linear problem and use its Green function in a convergent iteration procedure. Illustrations will be provided as well as comparisons with other popular methods.

Invited Lectures
Theoretical Physics

From unitary dynamics to statistical mechanics in isolated quantum chaotic systems

Dr Marcos Rigol
The Pennsylvania State University, USA

Experiments with ultracold gases have made it possible to study dynamics of (nearly) isolated quantum many-body systems, which has revived theoretical interest on this topic [1]. In generic isolated systems, one expects nonequilibrium dynamics to result in thermalization: a relaxation to states where the values of macroscopic quantities are stationary, universal with respect to widely differing initial conditions, and predictable through the time-tested recipe of statistical mechanics. However, it is not obvious what feature of a many-body system makes quantum thermalization possible, in a sense analogous to that in which dynamical chaos makes classical thermalization possible. Underscoring that new rules could apply in the quantum case, experimental studies in one-dimensional systems have shown that traditional statistical mechanics can provide wrong predictions for the outcomes of relaxation dynamics [2]. We show that isolated quantum-chaotic systems do in fact relax to states in which observables are well-described by statistical mechanics [3]. Moreover, we argue that the time evolution itself plays a merely auxiliary role as thermalization happens at the level of individual eigenstates [1,3].

[1] L. D'Alessio, Y. Kafri, A. Polkovnikov, and M. Rigol. From Quantum Chaos and Eigenstate Thermalization to Statistical Mechanics and Thermodynamics. Adv. Phys. 65, 239-362 (2016).

[2] T. Kinoshita, T. Wenger, and D. S. Weiss. A quantum Newton's cradle. Nature 440, 900 (2006).

[3] M. Rigol, V. Dunjko, and M. Olshanii. Thermalization and its mechanism for generic isolated quantum systems. Nature 452, 854 (2008).

Invited Lectures
Quantum Computing

Engineering approximate counter-adiabatic protocols in complex systems

Prof Anatoli Polkovnikov
Boston University, USA

I will first discuss adiabatic transformations in classical and quantum Hamiltonian systems. They naturally lead to emergence of the adiabatic gauge potential (AGP), which is a generator of such transformations. I will briefly discuss its properties, relation to geometry, integrability, and chaos. I will show how using the AGP one can construct counter-adiabatic protocols or more generally shortcuts to adiabaticity, allowing for arbitrary fast adiabatic transformations. Finally I will discuss how one can find and engineer approximate AGP in complex chaotic systems using variational and Floquet approaches.

Invited Lectures
Quantum Computing

Machine learning of noise-resilient quantum circuits

PhD Lukasz Cincio

Los Alamos National Laboratory, USA

Noise mitigation and reduction will be crucial for obtaining useful answers from near-term quantum computers. In this work, we present a general framework based on machine learning for reducing the impact of quantum hardware noise on quantum circuits. Our method, called noise-aware circuit learning (NACL), applies to circuits designed to compute a unitary transformation, prepare a set of quantum states, or estimate an observable of a many-qubit state. Given a task and a device model that captures information about the noise and connectivity of qubits in a device, NACL outputs an optimized circuit to accomplish this task in the presence of noise. It does so by minimizing a task-specific cost function over circuit depths and circuit structures. To demonstrate NACL, we construct circuits resilient to a fine-grained noise model derived from gate set tomography on a superconducting-circuit quantum device, for applications including quantum state overlap, quantum Fourier transform, and W-state preparation.

[1] L. D'Alessio, Y. Kafri, A. Polkovnikov, and M. Rigol. From Quantum Chaos and Eigenstate Thermalization to Statistical Mechanics and Thermodynamics. Adv. Phys. 65, 239-362 (2016).

[2] T. Kinoshita, T. Wenger, and D. S. Weiss. A quantum Newton's cradle. Nature 440, 900 (2006).

[3] M. Rigol, V. Dunjko, and M. Olshanii. Thermalization and its mechanism for generic isolated quantum systems. Nature 452, 854 (2008).

Invited Lectures
Complex Systems

Sociophysics: the hidden archaic mechanisms driving opinion dynamics

Prof Serge Galam

CEVIPOF - Centre for Political Research, Sciences Po and CNRS, Paris, France

Sociophysics, a newly established field among physicists, addresses a wide range of social and political phenomena that result from human interactions, of which opinion dynamics is a major topic. Many models have been proposed to tackle the issue including the influential Sznajd model and the seminal Galam model developed over forty years, which I will review.

Two discrete choices are competing within a population of heterogeneous agents. The dynamics is monitored via repeated local updates of individual opinions in small size groups of randomly distributed agents. At each distribution of agents, local majority rules are applied within the groups. However, agents are heterogeneous in their respective compliance of the local majority. Floaters update their choices along the local majority, contrarians oppose the local majority choice and inflexibles keep on their choices. The effect of prejudices is also incorporated quite naturally.

The dynamics is found to be either a tipping point dynamics with two competing attractors or a single attractor dynamics. The phenomenon of tiny minority spreading is thus giving an operative light, which allows building winning strategies in public debates.

The paradox of these results is to show how while free opinion dynamics is perceived as the guarantee of a democratic collective choices, it appears to be more of a dictatorial machine at the service of our primary archaisms, and this without any coercion. It is enough to have people discussing. To conclude the review of the model I will mention a series of successful predictions and a failure.

Invited Lectures
Complex Systems

Unusual convergence to a Gaussian for a diffusion profile in homogenizing strongly disordered systems

Prof Dr Igor Sokolov
Humboldt University of Berlin, Germany

The experimental possibility of single particle tracking on molecular scales in complex environments including biological media and live cells has promoted a splash of interest in the precise forms of the probability density functions (PDFs) of displacements of such classical particles diffusing in inhomogeneous surroundings. Typically, at short times, these PDFs show considerable deviations from a Gaussian shape characteristic for normal diffusion, with slow convergence to a Gaussian at long times.

The usual pathway to convergence to a Gaussian in diffusion processes proceeds is via smoothening sharp features of PDFs of displacements: the PDF, presenting at short times such sharp features first gets smooth and then, slower, approaches its final Gaussian form. In different models of diffusion in strongly disordered classical systems showing homogenization at large scales, the art of this convergence is strikingly different: the distribution at longer times retains a sharp central peak, which narrows under rescaling but does not disappear. The feature is especially pronounced in the systems where the amount of trajectories that never leave a close neighborhood of their starting point decays slowly in time. The feature is absent in the mean-field models, and seems to be a true sign of disorder. Finding such behavior in a physical or biological system should usher the experimentalist to look for the source and properties of such disorder.

[1] A. Pacheco-Pozo and I.M. Sokolov, Unusual convergence to a Gaussian for a diffusion profile in homogenizing strongly disordered systems, to appear in Phys. Rev. Lett. Preprint arXiv:2108.05176

Partners Presentations

Physics-inspired methods for efficient training of neural networks

Ph.D. Mykola Maksymenko

Research and Development Director at SoftServe Inc.

During presentation you will get to know few approaches from our recent research on applying physics-inspired methods to hyperparameter optimization and Binarized Neural Networks trainings.

Hyperparameter optimization is a practical issue, and an interesting theoretical problem in training of deep architectures. Despite recent advances commonly used methods almost universally involve training multiple and decoupled copies of the model, in effect sampling the hyperparameter space. We show that at a negligible additional cost, results can be improved by sampling nonlocal paths instead of points in hyperparameter space. To this end we interpret hyperparameters as controlling the level of correlated noise in training, which can be mapped to an effective temperature. The usually independent instances of the model are coupled and allowed to exchange their hyperparameters throughout the training. Each simulation corresponds then to a unique path in the joint hyperparameter/model-parameter space. We provide empirical tests, in particular for dropout and learning rate optimization. We observed faster training and improved resistance to overfitting, and a systematic decrease in the absolute validation error, improving over benchmark results.

Participants Speakers - Theoretical Physics

Dark-matter halo shapes from fits to SPARC galaxy rotation curves

Adriana Bariego Quintana[1], *Felipe J. Llanes-Estrada* [2], *Oliver Manzanilla Carretero* [3]

[1,2,3] Department of Theoretical Physics, Faculty of Physical Sciences, Complutense University of Madrid, Spain

We fit galactic rotation curves obtained by SPARC from dark matter haloes that are not spherically symmetric, but allowed to become prolate or oblate with a higher-multipole density distribution. This is motivated by observing that the flattening of v(r)=constant is the natural Kepler law due to a filamentary rather than a spherical source, so that elongating the distribution could bring about a smaller chi squared, all other things being equal. We compare results with different dark matter profiles and extract the best fits to the ellipticity computing cosmological simulations of dark matter haloes.

[1] Llanes-Estrada, Felipe. (2020). *Flat galaxy rotation curves naturally follow from dark matter filaments.* Proceedings of the Nancy Grace Roman Space Telescope conference 10.13140/RG.2.2.35022.41289.
[2] Allgood et al (2006). *The Shape of Dark Matter Halos: Dependence on Mass, Redshift, Radius, and Formation.* Monthly Notices of the Royal Astronomical Society. 367. 1781 - 1796. 10.1111/j.1365-2966.2006.10094.x.

Participants Speakers
Theoretical Physics

Intrinsic decoherence effect on quantum correlations in Heisenberg XXZ spin model

Anas Ait Chlih[1], *Nabil Habiballah*[1,2,3], *Mostafa Nassik*[1]

[1] EPTHE, Department of Physics, Faculty of Sciences, Ibn Zohr University, Agadir, Morocco, [2] Faculty of Applied Sciences, Ibn Zohr University, Ait-Melloul, Morocco, [3] Abdus Salam International Centre for Theoretical Physics, Strada Costiera, 11, 34151 Trieste, Italy

By taking into account the effect of intrinsic decoherence and by using Milburn's dynamical master equation, we study the temporal evolution of quantum correlations in a two-qubit XXZ Heisenberg spin chain model with Dzyaloshinskii-Moriya (DM) interaction and an external nonuniform magnetic field both directed along the z-axis. We use the concurrence (C) to detect entanglement and the local quantum uncertainty (LQU) to measure discord-like correlations. We consider three cases of initial quantum states: the mixed state, the Werner state and the pure state. For the mixed initial state and the Werner initial state, our results show that the external magnetic field strongly stimulates the effect of intrinsic decoherence which can highlight the entanglement sudden death (ESD) phenomenon, while the LQU is resistant to sudden death. In addition, the DM interaction makes the effect of intrinsic decoherence more pronounced. However, a weak DM interaction can markedly improve quantum correlations and thus cause the phenomenon of entanglement sudden revival. On the other hand, and especially for the initial "uncorrelated" state (in terms of entanglement and LQU) with a zero nonuniform magnetic field and no DM interaction, it is easier to generate a strong entanglement, but it is difficult to generate LQU. Finally, we have found that when the system is initially "uncorrelated", the nonuniform magnetic field can make the system strongly correlated for very remarkable steady state values (in particular entanglement). Other results will also be discussed.

Participants Speakers
Theoretical Physics

Noncommuting integrals of motion in XXZ model

Jakub Pawłowski[1], *Marcin Mierzejewski*[1]

[1]Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

We employ a numerical procedure for systematic identification of local (LIOM) and quasilocal (QLIOM) integrals of motion in lattice systems to the case of integrable XXZ model [1]. A generalized stiffness matrix is constructed and subsequently diagonalized. From its eigenvalues, the existence of LIOMs and QLIOMs is inferred. Special focus is placed on the case of operators that do not preserve the total magnetization i.e. $\left[\hat{S}^z_{tot}, \hat{O}\right] \neq 0$, as previous studies were restricted to the $\hat{S}^z_{tot}$ preserving subspace of operators [1]. Next, we perturb the XXZ model away from integrability and investigate how it influences the stiffness of time-averaged local and quasilocal integrals of motion taken from parent integrable model [2].

[1] Mierzejewski, M., Prelovšek, P., Prosen, T. (2015). Identifying local and quasilocal conserved quantities in integrable systems. Physical Review Letters, 114(14), 1–5.
[2] Mierzejewski, M., Prosen, T., Prelovšek, P. (2015). Approximate conservation laws in perturbed integrable lattice models. Physical Review B – Condensed Matter and Materials Physics, 92(19), 1–8.

Participants Speakers
Theoretical Physics

The fluorescence: pure physics in aid to biological sciences

Jakub Jeżowski[1]

[1]Faculty of Biochemistry, Biophysics and Biotechnology, Jagiellonian University, Krakow, Poland

Fluorescence is defined as radiant loss of energy of electron-excited molecule which is incidental to the emission of a quantum of energy as a photon. Fluorescence is a widely observed phenomenon. Proteins, chosen amino acids, natural and synthetic fluorophores play an important role in the biochemical and biophysical studies of different molecules, cells, and tissues [1].

Fluorescence is a powerful tool for studying molecular interactions because its intensity and other characteristics depend on relative location, environment, and type of fluorophore. Therefore, it can be used in studying interactions between proteins and DNA [2].

[1] J. R. Lakowicz, "Principles of Fluorescence Spectroscopy," 3rd Edition, New York, Springer, 2006. doi:10.1007/978-0-387-46312-4
[2] Deshayes, S., Divita, G. „Fluorescence technologies for monitoring interactions between biological molecules in vitro. Progress in molecular biology and translational science", 2013, doi:10.1016/B978-0-12-386932-6.00004-1

Participants Speakers
Theoretical Physics

Bayesian Analysis of Cosmic Rays data for Earthquake Predictions

Bartosz Grygielski[1],

[1]Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

Bayesian inference is a method that is able to provide us with probabilities for a given hypothesis with the use of prior knowledge and reasoning. Using this approach can help find correlations between cosmic rays and earthquakes that have been conjectured by various studies. Nevertheless, the phenomenon and its explanation have to be studied more precisely and thus I would like to briefly explain the Bayesian methodology (along with other tools for finding correlations) and share the results I have gotten while working on this topic during PPSS programme from IFJ PAN institute.

[1] A.L Morozova, M.I Pudovkin, T.V Barliaeva, Variations of the cosmic ray fluxes as a possible earthquake precursor, Physics and Chemistry of the Earth, Part A: Solid Earth and Geodesy, Volume 25, Issue 3, 2000, Pages 321-324
[2] Romanova, N.V., Pilipenko, V.A. & Stepanova, M.V. On the magnetic precursor of the Chilean earthquake of February 27, 2010. Geomagn. Aeron. 55, 219–222 (2015)
[2] Linden, W., Dose, V., & Toussaint, U. (2014). Bayesian Probability Theory: Applications in the Physical Sciences. Cambridge: Cambridge University Press.

Participants Speakers
Theoretical Physics

Cosmic web in large-scale cosmology simulations

Negin Khosravaninezhad[1]

[1]Department of Physics, Sharif University of Technology, P. O. Box 11155-9161, Tehran, Iran

Galaxies are not uniformly distributed in space. They form patterns on scales much larger than individual galaxies, referred to as the Large-Scale Structure (LSS). LSS includes galaxy clusters connected by dark matter filaments, and giant voids occupy the rest of cosmic volume —that is why astronomers speak of it as a “cosmic web.” These correlated structures depend both on cosmological parameters and the formation and evolution of galaxies by gravity. The search of these dependencies can answer more general questions about the universe. Cosmologists have tried for decades to simulate how the trillions of galaxies in the observable universe arose from clouds of gas after the big bang. As a result, in the past few years, several computer simulations of the cosmic web were performed to describe its properties according to current cosmological theories. In this presentation, I will demonstrate the role of computer simulations of the cosmic web in obtaining cosmological parameters. I will also introduce our research group in which we use simulations such as Gevolution [1] to investigate the role of the parameter M_ν (cosmic neutrino mass) in the evolution of the universe.

[1] J. Adamek, Gevolution, (2015-2020), GitHub repository, https://github.com/gevolution-code

Participants Speakers
Theoretical Physics

Hawking information paradox

Fatemeh Nouri[1]

[1]Department of Physics, Sharif University of Technology, Tehran, Iran

One of the main problems of the fundamental physics is to find a theory of quantum gravity. One motivation to study such a theory is to understand the earliest moments of the universe, where we expect that quantum effects are dominant. In the search for this theory, it is better to consider simpler problems. A simpler problem involves black holes. They also contain a singularity in their interior. Studies of black holes in the '70s showed that black holes behave as thermal objects. They have a temperature that leads to Hawking radiation. They also have an entropy given by the area of the horizon. This suggested that, from the point of view of the outside, they could be viewed as an ordinary quantum system. Hawking objected to this idea through what we now know as the "Hawking information paradox." He argued that a black hole would destroy quantum information, and that the von Neumann entropy of the universe would increase by the process of black hole formation and evaporation.

Participants Speakers
Theoretical Physics

Relatively Curved Particles - From geometry to relativity!

Aaghaz Mahajan[1]

[1]Second Year Undergraduate, Department of Physics, Indian Institute of Technology, Delhi

In this talk I will introduce how the Klein and Poincare models of Non Euclidean Geometry are used in the kinematics of high speed particles. Most of the ideas are taken from an article by Vladimir Dubrovsky [1]. I will start off by using properties of a velocity space and show that it's congruent to the Klein Model. And then I'll finally explain how the formula for relativistic addition of velocities follows from the Poincare model.

[1] Quantum V3N4 - 'Common Ground'

Participants Speakers
Theoretical Physics

Studies on Electrical and Optical Properties of ZnO/TiO2 Composite

C.M. Panchasara[1], *Bhargav Rajyaguru*[1], *Himanshu Dadhich*[1], *Nisarg Raval*[1], *N.A Chondagar*[1], *P.S. Solanki*[1], *N.A. Shah*[1,a]

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In the present communication, ZnO, TiO2 and ZnO:TiO2 (1:1) composite samples were synthesized using conventional solid-state reaction (SSR) technique. Room temperature X-Ray diffraction (XRD) measurements was performed to study the different structural phases present in the sample. The measurements of XRD samples revealed hexagonal phase structure of ZnO and Anatase phase of TiO2. Also, there was no evidence of other impure phase in the structure. Rietveld refinement analysis of XRD plots were done using Fullprof software. Optical study of pure and composite samples were performed using UV-Visible (UV-Vis) absorption spectroscopic measurement. It is evident from the UV-Vis spectra that the ZnO:TiO2 (1:1) composite sample's UV absorption gets improved which can be advantageous for practical application to degrade UV light hazards. Higher bandgap value is estimated for composite material as compared to its pure materials. Dielectric permittivity at room temperature gets reduced with increase in frequency indicating disability of dipoles to follow higher electric field. It is also observed that dielectric of ZnO:TiO2 (1:1) composite material gets reduced as compared to pure ZnO and TiO2 samples.

Participants Speakers
Theoretical Physics

Transport Properties of Manganite based Heterostructure

Bhargav Rajyaguru, Himanshu Dadhich, N.A Chondagar, C.M. Panchasara, Nisarg Raval, N.A. Shah, P.S. Solanki[a]

Department of Physics, Saurashtra University, Rajkot-360 005, Gujarat, INDIA
[a] Corresponding author: piyush.physics@gmail.com

Manganites and Multiferroic thin films are widely studied due to their various properties. In this communication, we report the results of structural and transport studies performed on LaFeO3/La0.7Ca0.3MnO3/SrTiO3 (LFO/LCMO/STO) heterostructure grown using simple, low cost, vacuum free and environment friendly chemical solution deposition (CSD) method. The XRD pattern suggests the growth of both layers of the film in the (100) crystallographic orientation of the substrate. Temperature dependent resistivity behavior under different applied magnetic fields, performed for two different geometries [current in plane (CIP) and current perpendicular to plane (CPP)], suggests the modifications in metal to insulator transition temperature (Tp) and alterations in resistivity values with applied magnetic field and measurement geometry. This also implies higher resistance across the LFO/LCMO interface (CPP) as compared to the LCMO film layer (CIP). Percolation model has been used to understand the behavior of the interface and channel of the film. These changes have been discussed in detail in the context of phase separation, charge injection and depletion region modifications. LaFeO3/La0.7Ca0.3MnO3/SrTiO3 (LFO/LCMO/STO) heterostructure grown using simple, low cost, vacuum free and environment friendly chemical solution deposition (CSD) method. The XRD pattern suggests the growth of both layers of the film in the (100) crystallographic orientation of the substrate. Temperature dependent resistivity behavior under different applied magnetic fields, performed for two different geometries [current in plane (CIP) and current perpendicular to plane (CPP)], suggests the modifications in metal to insulator transition temperature (Tp) and alterations in resistivity values with applied magnetic field and measurement geometry. This also implies higher resistance across the LFO/LCMO interface (CPP) as compared to LCMO film layer (CIP). Percolation model has been used to understand the behavior of the interface and channel of the film. These changes have been discussed in detail in the context of phase separation, charge injection and depletion region modifications.

— Participants Speakers - Quantum Computing —

Semiclassical dynamics of a strongly interacting bosons: from slave bosons perspective

Aleksander Kaczmarek[1]

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Recent advances in experiments allow to simulate dynamics of strongly interacting bosons in optical lattice, while theoretical understanding of quantum dynamics of strongly interacting systems is still quite limited. This motivates the pursue of reliable and controllable numerical methods. One possible approach to analyze such systems is to utilize truncated Wigner approximation (TWA) along with spin representation i.e. SU(3) group [1]. This paper will present different approach to TWA which utilizes slave bosons representation. I present the phase space the formulation of Bose Hubbard model for strongly interacting bosons in slave bosons representation along with discussion and proposition of initial conditions. Further I provide some of the preliminary results which indicate that this method might be promising in terms of simulating low density strongly interacting bosonic systems that are a subject of experimental research.

[1] S. M. Davidson and A. Polkovnikov, "su(3) semiclassical representation of quantum dynamicsof interacting spins,"Phys. Rev. Lett., vol. 114, p. 045701, Jan 2015.
DOI :https://doi.org/10.1103/PhysRevLett.114.045701
[2] M. Greiner, O. Mandel, T. Esslinger, T. Haansch, and I. Bloch, "Quantum phase transition from a superfluidto a mott insulator in a gas of ultracold atoms,"Nature, vol. 415, pp. 39–44, 2002.

Participants Speakers
Quantum Computing

Space-Efficient Embedding of the Clique Cover Problem for Quantum Optimization

Bence Bakó[1,2], *Zoltán Zimborás*[3,4]

[1]Department of Physics of Complex Systems, Faculty of Science, Eötvös Loránd University, HU-1117 Budapest, Pázmány Péter sétány 1/A
[2] Ericsson Research, Budapest, Hungary
[3] Wigner Research Centre for Physics, H-1525, P.O.Box 49, Budapest, Hungary
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In the era of Noisy Intermediate Scale Quantum (NISQ) devices, variational quantum algorithms may offer a way of demonstrating useful quantum advantage. Different near-term device-architectures have different strengths and weaknesses: For some it is hard to execute deep circuits, for others it is complicated to scale up the number of qubits. Due to this difference in the architectures, one should consider various alternative approaches of circuit design. For example, it is important to consider both methods when the depth of the circuit is minimized and approaches when the number of qubits can be reduced. These investigations usually lead to a trade-off between depth and qubit number. Motivated by this, we introduce a space-efficient embedding of the clique cover problem that may require deeper circuits, but in return the number of qubits is exponentially reduced in the number of cliques. We compare this new embedding with the traditional one-hot encoding and present numerical simulations for variational quantum algorithms that use both methods. Furthermore, for the variational algorithm based on the space-efficient embedding, we benchmark the performance of the stochastic gradient descent technique, as well.

[1] A. Lucas, *Ising formulations of many NP problems.* Frontiers in Physics, vol. 2, p. 5, 2014.
[2] A. Glos, A. Krawiec, Z. Zimborás, *Space-efficient binary optimization for variational computing.* arXiv preprint, 2020. arXiv:2009.07309.
[3] Zs. Tabi, K. H. El-Safty, Zs. Kallus, P. Hága; T. Kozsik, A. Glos, Z. Zimborás, *Quantum Optimization for the Graph Coloring Problem with Space-Efficient Embedding.* 2020 IEEE International Conference on Quantum Computing and Engineering (QCE), Denver, CO, USA, 2020, pp. 56-62.

- Participants Speakers - Complex Systems & ML -

Participants Speakers
Machine Learning & Neural Networks

State-of-health estimation of lithium-ion battery based on the hybrid method of neural networks

Brahim Zraibi[1] ,*Mohamed Mansouri*[1]

[1]Hassan First University of Settat, National School of Applied Sciences of Berrechid, Laboratory LAMSAD, Morocco

Lithium-ion battery state-of-health (SOH) monitoring in real-time is critical for the reliable and safe functioning of battery systems because it is a key parameter for fault diagnoses and early warnings to prevent the battery's failure, as a result, the accurate forecasting of the SOH of battery is essential for preventative maintenance, thus the cost reduction. In this study, we propose the CNN-LSTM-DNN, a hybrid approach that combines Convolutional Neural Networks (CNN), Long Short Term Memory (LSTM), and Deep Neural Networks (DNN) to improve the accuracy of SOH estimate for Lithium-ion batteries. To that end, the NASA datasets of lithium-ion batteries are used for experimental validation, in addition, the MAE and RMSE are used to evaluate the performance of prediction results. The results of the verification experiments reveal that adopting this proposed method can significantly minimize prediction error and achieve high estimation accuracy of the battery's state of health compared to the other methods in the literature.

[1] D. Zhou et al., 'Research on state of health prediction model for lithium batteries based on actual diverse data', Energy, vol. 230, p. 120851, 2021, doi: 10.1016/j.energy.2021.120851.
[2] S. Son, S. Jeong, E. Kwak, J. Kim, and K.-Y. Oh, 'Integrated Framework for SOH Estimation of Lithium-ion Batteries Using Multiphysics Features', Energy, vol. 238, p. 121712, 2021, doi: 10.1016/j.energy.2021.121
[3] K. S. R. Mawonou, A. Eddahech, D. Dumur, D. Beauvois, and E. Godoy, 'State-of-health estimators coupled to a random forest approach for lithium-ion battery aging factor ranking', J. Power Sources, vol. 484, no. November 2020, p. 229154, 2021, doi: 10.1016/j.jpowsour.2020.229154.
[4] C. Chang, Q. Wang, J. Jiang, and T. Wu, 'Lithium-ion battery state of health estimation using the incremental capacity and wavelet neural networks with genetic algorithm', J. Energy Storage, vol. 38, no. September 2020, p. 102570, 2021, doi: 10.1016/j.est.2021.102570.
[5] Z. Lyu, G. Wang, and R. Gao, 'Li-ion battery prognostic and health management through an indirect hybrid model', J. Energy Storage, vol. 42, no. July, p. 102990, 2021, doi: 10.1016/j.est.2021.102990.
[6] F. Luo, H. Huang, L. Ni, and T. Li, 'Rapid prediction of the state of health of retired power batteries based on electrochemical impedance spectroscopy', J. Energy Storage, vol. 41, no. August, p. 102866, 2021, doi: 10.1016/j.est.2021.102866.

Participants Speakers
Complex Systems

Discontinuous phase transitions in the generalized q-voter model on random graphs

Angelika Abramiuk-Szurlej, ***Arkadiusz Lipiecki***, *Jakub Pawłowski*, *Katarzyna Sznajd-Weron*

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We investigate the binary q-voter model with generalized anticonformity on random Erdős–Rényi graphs. The generalization refers to the freedom of choosing the size of the influence group independently for the case of conformity q_c and anticonformity q_a. This model was studied before on the complete graph, which corresponds to the mean-field approach, and on such a graph discontinuous phase transitions were observed for $q_c > q_a + \Delta q$, where $\Delta q = 4$ for $q_a \leq 3$ and $\Delta q = 3$ for $q_a > 3$. Examining the model on random graphs allows us to answer the question whether a discontinuous phase transition can survive the shift to a network with the value of average node degree that is observed in real social systems. By approaching the model both within Monte Carlo (MC) simulations and Pair Approximation (PA), we are able to compare the results obtained within both methods and to investigate the validity of PA. We show that as long as the average node degree of a graph is relatively large, PA overlaps MC results. On the other hand, for smaller values of the average node degree, PA gives qualitatively different results than Monte Carlo simulations for some values of q_c and q_a. In such cases, the phase transition observed in the simulation is continuous on random graphs as well as on the complete graph, whereas PA indicates a discontinuous one. We determine the range of model parameters for which PA gives incorrect results and we present our attempt at validating the assumptions made within the PA method in order to understand why PA fails, even on the random graph.

Participants Speakers
Machine Learning

Applying machine learning methods in data analysis

Mikołaj Jędrzejewski[1]

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The ALICE (A Large Ion Collider Experiment) is one of the big four experiments situated on the LHC (Large Hadron Collider) accelerator at CERN. The experiment has a broad spectrum of physics from elementary collisions to heavy ion collisions at extremely high energies up to 13 TeV. One of the main topics is the study of Quark Gluon Plasma (QGP) and its influence/ modification of the production mechanism of various hadrons (probes) such as J/ψ charmonium. Studying such complex processes within the collisions of complex systems such as Lead- Lead poses a significant challenge from the side of physics, experiment and data analysis.

In my talk I will discuss applying modern techniques in data analysis based on machine learning methods and present the results of applying Boosted Decision Tree algorithm on a given data set of J/ψ measurements from ALICE detector in order to supress unwanted background events.

Participants Speakers
Complex Systems

Three-state opinion q-voter model with bounded confidence

Maciej Doniec[1]

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The aim of this work was to analyse the three-state q-voter model with bounded confidence on the complete graph. Two kinds of agents behaved either independently and conformably. The main goal was to compare the model with and without bounded confidence. The key novel result is the appearance of two phase transitions: one between order-order phases and another between order-disorder phases. The model was analysed both numerically using Monte Carlo simulations and analytically with mean-field approximation.

Participant Posters

Theoretical Physics

Far-field CP Repulsive Forces and Where to Find Them

Khatee Zathul Arifa[1], *Martial Ducloy*[2], *David Wilkowski*[1], *Lu Bing-Sui*[1]

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We consider the problem in which a two-level excited atom interacts with a Chern insulator through the resonant Casimir-Polder (CP) interaction. A Chern insulator (CI) is a two-dimensional topological insulator that breaks time reversal symmetry and exhibits quantum anomalous Hall effect, i.e., the static limit of its Hall conductance is quantised in units of e^2/h. The resonant CP forces arise from the energy shifts of the atom's excited state, and these forces oscillate between being attractive and repulsive at different separation distances. This oscillatory behaviour is most pronounced when the interaction frequency coincides with the frequency of the CI's Van Hove singularity. We also observe that for a right circularly polarised excited atom that is located in the vicinity of a CI with Chern number $C = -1$, the CP energy shift decays monotonically with distance, which implies that it is possible to generate repulsive CP forces over a long range of separation distances. On the other hand, the CP energy shift decays in an oscillatory manner in the far-field regime when an identical atom is placed in the vicinity of a $C = 1$ Chern insulator. As this phenomenon is highly sensitive to the sign of the Chern number, it provides a novel way of detecting materials with nonzero Chern numbers. Most importantly, we believe it will aid in the quest for detecting and engineering repulsive CP forces in mesoscopic systems.

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[2] B.-S. Lu, K. Z. Arifa, and X. R. Hong, "Spontaneous emission of a quantum emitter near a Chern insulator: Interplay of time-reversal symmetry breaking and Van Hove singularity." *Phys. Rev. B* **101**, 205410 (2020).

Posters
Theoretical Physics

Solutions of Schrodinger Equation with Improved Rosen Mors Potential for Some Diatomic Molecules

Mostapha.Ferdjaoui[1]

[1]Department of Physics, Faculty of Exact Science, Constantine 1 University, Algeria)
[2]

In this work, we have investigated non-relativistic problem of Schrodinger equation subject to improved Rosen Morse potential. by using factorization method, we have obtained exact energy eigenvalues equation and radial wave functions in terms of hypergeometric function. for some diatomic molecules.

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Posters
Condensed Matter Physics

Swift Heavy Ion (SHI) Induced Modifications In Transport Properties of Manganite Based Thin Film Devices

Bhargav Rajyaguru, Himanshu Dadhich, N.A Chondagar, C.M. Panchasara, Nisarg Raval, N.A. Shah, P.S. Solanki[a]

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Scientists and Researchers explain the mechanism of metal-insulator (M-I) transition observed in manganite using various fundamental physical properties. Some of them are phase coexistence, defects surface morphology and interface modifications. Swift Heavy Ion (SHI) irradiation is an interesting tool to create artificial defects and modifications in the oxide materials through which one can achieve point defects, columnar defects and film-substrate interface modifications and, eventually, receives modifications in the transport properties. Very few reports exist on the SHI irradiation induced modifications in colossal electroresistance (CER) behaviour, based on the modifications in terms of change in gross defect states and interface modifications. By following all above aspects, in this communication, temperature dependent resistivity (transport measurements) across $LaMnO_3$ (LMO)/$La_{0.7}Ca_{0.3}MnO_3$ (LCMO)/$SrTiO_3$ (STO) thin film heterostructure have been understood. Effect of 120 MeV Ag^{9+} ions irradiation in M-I transition has been discussed in detail with the support from several structural characterizations such as XRD and AFM. Change in M-I transition behaviour as a function of ion fluence has been understood in the context of lattice strain between LMO gate electrode and LCMO active channel, surface roughness and trapping-detrapping processes. Theoretical percolation model has been used to understand the phase separation introduced by SHI irradiation. Improvement in ER has been observed in these heterostructure with irradiation.

Posters
Condensed Matter Physics

Structural And Electrical Properties of Nano-Micro Composites

Bhargav Rajyaguru, Himanshu Dadhich, N.A Chondagar, C.M. Panchasara, Nisarg Raval, N.A. Shah, P.S. Solanki[a]

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In this communication, nanostructured Na-doped LaMnO3 manganite was suc- cessfully synthesized using low cost, easy, simple, environment friendly and acetate precursor-based sol-gel method. ZnO is an insulator and have wide band gap (3.4 eV). In this study, different weight ratio of La0.85Na0.15MnO3 (LNMO) and ZnO powder were employed to prepare their composites. X–ray diffraction (XRD) measurement reveals the dual phase nature of pure ZnO and pure LNMO as well as their composites. For electrical properties frequency dependent dielectric, conductivity, impedance, resistance and reactance was performed and understood in detail. To investigate the electrical nature of all studied composites, dielectric behavior has been understand using cole-cole and universal dielectric response model and ac conductivity by jonscher's power law mechanism.

Posters
Machine Learning

Distributed training of deep learning models

Salah Eddine Loukili[1], *Abdellah Ezzati*[1], *Said Ben Alla*[1]

[1]Hassan First University of Settat, Faculty of Science and Technology, Laboratory VTE, Morocco

Recently, deep learning research has demonstrated that being able to train big models improves performance substantially. In this work, we consider the problem of training a deep neural network with billions of parameters using multiple GPUs. On a single machine with a modern GPU, training a benchmark dataset of Dogs vs Cats can take up to a day; however, distributing training across numerous machines has been seen to dramatically reduce this time. The current state of the art for a modern distributed training framework is presented in this study, which covers the many methods and strategies utilized to distribute training. We concentrate on synchronous versions of distributed Stochastic Gradient Descent, different All Reduce gradient aggregation algorithms, and best practices for achieving higher throughput and reduced latency, such as gradient compression and large batch sizes. We show that using the same approaches, we can train a smaller deep network for an image classification problem in a shorter time. Although we focus on and report on the effectiveness of these approaches when used to train convolutional neural networks, the underlying methods may be used to train any gradient-based machine learning algorithm.

[1] C. Birnie, H. Jarraya, and F. Hansteen, 'An introduction to distributed training of deep neural networks for segmentation tasks with large seismic datasets', 2021.
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[5] M. Li, J. Zhou, Q. Huang, C. Ma, Z. Huang, and Q. Guo, 'TOWARDS SCALABLE DISTRIBUTED TRAINING OF DEEP LEARNING ON PUBLIC CLOUD CLUSTERS', pp. 1–7, 2019.

Posters
Aerospace Engineering

LEO Nanosatellite: Passive thermal control

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It is well known that nanosatellites have the smallest size of the envelope, low cost, with the briefest development time. In fact, it is a completely new reduced form of traditional satellites and one of the most sought-after forms. Nevertheless, they encounter different problems such as high thermal gradients or various thermal loads from solar radiation and planetary infrared emissions. The aim of this paper is to describe the different types of thermal radiation that the nanosatellite undergoes and then to accurately simulate them. The impact on the overall spacecraft becomes apparent when the spacecraft is in orbit and when parameters shift, such as emissivity and absorptivity, which refer to the optical coatings of the nanosatellite. It should be noted that for the simplicity of the approach, a simple shape of the nanosatellite was assumed. The performed approach was a first step to getting tangible results while considering a more complex and complete shape of the nanosatellite in the future.

Posters
Physical Chemistry

Synthesis and research of properties of GGG doped by ions Sm^{3+}

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Powder samples of $Gd_3Ga_5O_{12}$ garnets (GGG) were synthetized using solid state method. For synthesized GGG garnets doped with 0,05%; 0,5%; 1%; 2,5%; 5% and 10% of Sm^{3+} recorded emission spectra in 300K and decay curves. Four narrow emission lines were noticed in luminescence spectra. $^4G_{5/2}$ luminescence lifetimes were decreasing with the increase of Sm^{3+} ions. Decay curves were mostly exponential. Absorption spectra in 300K were measured for Czochralski grown single crystal GGG doped with 10% Sm^{3+}. Judd – Ofelt parameters, branching ratios β, radiative transition probabilities A_ij and $^4G_{5/2}$ luminescence lifetime were obtained. Judd-Ofelt parameters totalled $\Omega_2 = 2{,}85 \cdot 10^{-20}$, $\Omega_4 = 4{,}78 \cdot 10^{-20}$ and $\Omega_6 = 2{,}76 \cdot 10^{-20}$. Branching ratios determined transition from $^4G_{5/2}$ to $^6H_{7/2}$ and transition from $^4G_{5/2}$ to $^6H_{9/2}$ proclaim the highest probability of occurrence of laser action for given levels. The radiative lifetime amounted to 1826,16 μs and lifetime of $^4G_{5/2}$ in GGG doped with 0,5% Sm^{3+} was 1721,7 μs. Comparing the results, the optimal addition of Sm^{3+} ions for potential laser media was 0,5%.

Posters
Condensed Matter Physics

Investigations on the Structural and Electrical Properties of Oxide Nano Particle Composite

Nisarg Raval[1], *Bhargav Rajyaguru*[1], *Himanshu Dadhich*[1], *C.M. Panchasara*[1], *N.A Chondagar*[1], *P.S. Solanki*[1], *N.A. Shah*[1,a]

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Nanocomposites possess certain properties which are superior overall, compared to their pure individual constituents in terms of their practical applications. In the present study, the nanoparticles of ZnO and CuO were prepared using low-cost sol-gel technique and, also, its composite was synthesized in the weight ratio of 1:1. The structural studies using X-Ray Diffraction show single phase nature of individual constituents and reduction in lattice parameters after the formation of its composite. The investigation on dielectric response of composite suggests the enhancement as compared to ZnO nanoparticles and reduction as compared to CuO nanoparticles which have been understood on the basis of relaxation mechanism and Universal Dielectric Response (UDR) model. The overall a.c. conductivity study reports the enhancement in conduction for composite which has been, theoretically, understood on the basis of Jonscher's power law. The impedance of nanocomposite gets suppressed while comparing to its individual components which has been explained on the basis of oxygen vacancies and annealing process done during the synthesis process.

Posters
Condensed Matter Physics

Swift Heavy Ion (SHI) Induced Modifications In Transport Properties of Manganite Based Thin Film Devices

Bhargav Rajyaguru, Himanshu Dadhich, N.A Chondagar, C.M. Panchasara, Nisarg Raval, N.A. Shah, P.S. Solanki[a]

Department of Physics, Saurashtra University, Rajkot-360 005, Gujarat, INDIA
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Scientists and Researchers explain the mechanism of metal-insulator (M-I) transition observed in manganite using various fundamental physical properties. Some of them are phase coexistence, defects surface morphology and interface modifications. Swift Heavy Ion (SHI) irradiation is an interesting tool to create artificial defects and modifications in the oxide materials through which one can achieve point defects, columnar defects and film-substrate interface modifications and, eventually, receives modifications in the transport properties. Very few reports exist on the SHI irradiation induced modifications in colossal electroresistance (CER) behaviour, based on the modifications in terms of change in gross defect states and interface modifications. By following all above aspects, in this communication, temperature dependent resistivity (transport measurements) across $LaMnO_3$ (LMO)/$La_{0.7}Ca_{0.3}MnO_3$ (LCMO)/$SrTiO_3$ (STO) thin film heterostructure have been understood. Effect of 120 MeV Ag^{9+} ions irradiation in M-I transition has been discussed in detail with the support from several structural characterizations such as XRD and AFM. Change in M-I transition behaviour as a function of ion fluence has been understood in the context of lattice strain between LMO gate electrode and LCMO active channel, surface roughness and trapping-detrapping processes. Theoretical percolation model has been used to understand the phase separation introduced by SHI irradiation. Improvement in ER has been observed in these heterostructure with irradiation.

Posters
Theoretical Physics

Introduction to curved space-time and differential geometry

The poster contains a small introduction to curved space-time and differential geometry, explanation of the solution for non-rotating and zero charged black holes, and some kind of mathematical proof of the event horizon.

To keep it interesting for everyone, I would only explain the essential things. Therefore, other students can comprehend black holes in a slightly different way than we all used to do it.