Commemorating the 50th Anniversary of Universidad Autónoma Metropolitana

January 28 – 31, 2025

ABSTRACT BOOKLET

Program

January	28th	29th	30th	31th
8:30 - 9:00	**Opening Ceremony**			
9:00 - 9:45	*"How to quantify information in quantum physics"* **Vlatko Vedral**	*"Information Theoretical Concepts in the study of properties of quantum systems"* **Elvira Romera**	*"Information-theoretical quantities in the thermodynamical transcription of the density functional theory"* **Agnes Nagy**	*"From Electron Density to Information Theoretical Measures to Structural Properties in Atoms and Molecules"* **K.D.Sen**
9:45 - 10:30	*"Information-theoretic approach in density functional theory and its recent applications to chemical problems"* **Shubin Liu**	*"Exact Ansatzes for Quantum Simulations of Many-body Systems"* **David Mazziotti**	*"Dynamical Paths to Densities Optimizing LMC Statistical Measures of Complexity"* **Angel Ricardo Plastino**	*"Unbounded entropy production for repulsive-to-attractive interaction quench in long-range interacting systems"* **Barnali Chakrabarti**
10:30 - 11:05	*"Quantum Information Perspective on the Ground State Problem: What is Electron Correlation?"* **Christian Schilling**	*"Usefulness of quantum entanglement for enhancing precision in frequency estimation"* **Pablo Barberis**	*"Few-electron confined quantum systems: Precise structural and quantum information theoretic measures"* **Jayanta K. Saha**	*"Information Entropy in spatially confined atoms and few-electron harmonic quantum dot within density function formalism"* **Amlan K. Roy**
11:05 - 11:25	Coffee break	Coffee break	Coffee break	Coffee break
11:25 - 12:00	*"Multifractality and chaos in light-matter systems"* **Miguel Bastarrachea**	*"An Information-theoretical Take on Electron-Nuclear Wave Packet Dynamics"* **Peter Schurger**	*"A model of energy transport in photosynthesis"* **Roberto Quezada**	*"External field modified entropic exchange: static vs time dependent fields"* **Vinod Prasad**
12:00 - 12:35	*"Hydrogen atom under spatial and magnetic confinement: Superintegrability, Information Theory, and Neural Networks"* **Adrián Escobar**	*"An Information-Theoretic approach to characterizing concurrent processes and transition regions along the IRC: A 15-year retrospective on chemical reactions"* **Moyocoyani Molina**	*"Probing Quantum-Gravity Interplay with Bose-Einstein Condensates"* **Ivette Fuentes**	*"On the numerical integration of two-particle functions for Pair Entropies of diatomic molecules"* **Manuel Solano**
12:35 - 12:55	Coffee break	Coffee break	Coffee break	Coffee break
12:55 - 13:30	*"Entropy production rate of Quantum Markov Semigroups"* **Jorge Bolaños**	*"Applications of Information Theory to Compact Objects: Configurational Entropy as a Stability Criterion"* **Charalampos Moustakidis**	*"Entanglement Dynamics in an Optomechanical Cavity with a Type-V Qutrit and Two-Mode Field"* **Shihai Dong**	*"Information entropy in confined quantum systems"* **Neetik Mukherjee**
13:30 - 14:15	*"Variational approach to time-dependent systems: Surface tension of quantum droplets"* **Rocío Jaúregui**	*"On information, entropy, and early stone tools"* **Fernando del Río**	*"The resource of Non-stabilizerness: An introduction and application to Quantum Rabi Model"* **Ernesto Benítez**	*"Title"* **Paul Ayers (to be confirmed)**
14:15 - 16:00	Lunch break	Lunch break	Lunch break	Lunch break
16:00 - 16:35	*"Propagators in Information Field Theory"* **Roberto Flores-Moreno**	*"Towards entropic uncertainty relations in non-regular Hilbert spaces"* **Angel García Chung**	*"Kullback-Leibler divergence in Machine Learning: Its relation to cross entropy and application to Boltzmann machines"* **Roberto Bernal**	*"Some generalities of the applications of information theory in chemistry"* **Nelson Flores**
16:35 - 17:10	*"Informational characterization of chemical hypergraphs"* **Humberto Laguna**	*"Information-theoretic concepts to elucidate local and non-local aspects of chemical phenomena"* **Rodolfo Esquivel**	*"Construction and analysis of information measures through Diophantine equations"* **Saúl Salazar**	*"Uncertainties and statistical correlations in quantum systems"* **Robin Sagar**
17:10 - 17:40				**Round table: Future perspectives for UAM**

Table of Contents

January 28th

Opening ceremony **8:30 - 9:00 H**

Universidad Autónoma Metropolitana

Participants:

Dr. Román Linares Romero. Director of the Division of Basic Sciences and Engineering.
Dr. Jorge Garza Olguín. Head of the Chemistry Department.
Dr. Juan Morales Corona. Head of the Physics Department.
Dr. Roberto Quezada Batalla. In representation of Dr. J. Raúl Montes de Oca, Head of the Mathematics Department.
Dr. Rodolfo Esquivel Olea. Head of the Quantum Chemistry Group.
Dr. Humberto Laguna Galindo. Chemistry Department (Moderator).

DAY 1

How to quantify information in quantum physics **9:00 - 9:45 H**

Vlatko Vedral

Oxford University

I will first talk about the general way in which information enters physics. This was historically tied with the concept of entropy and the relationship between statistical mechanics and thermodynamics. Then I will explain how quantum information differs from this originally classical concept. I will conclude by speculating how information might help us to unifying quantum physics and general relativity leading us to a new theory of physics.

Information-theoretic approach in density functional theory and its recent applications to chemical problems **9:45 - 10:30 H**

Shubin Liu

University of North Carolina at Chapel Hill

Information-theoretic approach (ITA) is the application of information theory to density functional theory (DFT) using the electron density as the probability distribution function. In this talk, we first introduce the formulation of ITA quantities including Shannon entropy, Fisher information, Ghosh–Berkowitz–Parr entropy, information gain, Onicescu information energy, etc., and then present ITA's four representations, three principles, and two identities, followed by their applications in quantifying electrophilicity, nucleophilicity, and stereoselectivity. Recent developments are outlined in topological analysis of ITA quantities, introduction of energetic information, applications to excited states and machine learning. We conclude by showcasing the big picture of our recent efforts to establish a density-based conceptual framework of chemical reactivity theory in DFT.

References:

1. Chunying Rong, Bin Wang, Dongbo Zhao, and Shubin Liu, Information-Theoretic Approach in Density Functional Theory and its Recent Applications to Chemical Problems, WIREs Comput. Mol Sci. 2020, 10(4) e1461.
2. Chunying Rong, Dongbo Zhao, Xin He, and Shubin Liu, Development and Applications of the Density-Based Theory of Chemical Reactivity, J. Phys. Chem. Lett. 2022, 13, 48, 11191–11200.
3. Xin He, Meng Li, Chunying Rong, Dongbo Zhao, Wenjian Liu, Paul W Ayers, and Shubin Liu, Some Recent Advances in Density-Based Reactivity Theory, J. Phys. Chem. A 2024, 128, 7, 1183–1196.
4. Shubin Liu (ed), Exploring Chemical Concepts Through Theory and Computation. 2024, Wiley-VCH GmbH, Weinheim, Germany.

Quantum Information Perspective on the Ground State Problem: What is Electron Correlation? **10:30 - 11:05 H**

Christian Schilling
Arnold Sommerfeld Centre for Theoretical Physics, LMU Munich

Understanding strongly interacting electrons remains a central challenge in modern quantum physics. Addressing this electron correlation problem requires harnessing both the pairwise interactions and their spatial decay. Adopting a quantum information perspective, we uncover two distinct notions of correlation and entanglement arising from the structure of realistic Hamiltonians. The first focuses on correlations between orbitals, while the second captures a more particle-centric perspective. We introduce measures to quantify these concepts and illustrate their implications for various molecular systems. Intriguingly, our findings suggest that correlations between orbitals are predominantly classical, prompting a reexamination of the role of entanglement in chemical bonding. Finally, we propose a promising connection between orbital and particle correlation, offering a potential replacement for the traditionally vague concepts of static and dynamic correlation.

Multifractality and chaos in light-matter systems **11:25 - 12:00 H**

Miguel A. Bastarrachea-Magnani
Departamento de Física, Universidad Autónoma Metropolitana, México

Multifractality is a phenomenon that emerges across a wide array of systems, from mathematical objects and biological systems [1] to the quantum world [2]. In this work, we explore multifractal behavior in the Dicke Hamiltonian [3], a paradigmatic model of quantum optics and spin-boson interaction that has become attractive in recent years for both the broad theoretical richness it apports to the study of classical and quantum equilibrium and out-of-equilibrium phenomena and its experimental applications in the context of quantum information [4]. Within the quantum-classical correspondence, quantum multifractality allows the identification of different structures in classical phase space, such as chaos [5], in an unbound Hilbert space [6].

References

[1] P. Grassberger et al., Phys. Rev. Lett. 50, 346 (1983); D. La Rocca, et al., Journal of Neuroscience Methods 309, 175 (2018).
[2] C. Monthus, J. Stat. Mech, 2016, 073301 (2016); J. Lindinger, et al., Phs. Rev. Lett. 122, 106603 (2019).
[3] R. H. Dicke, Phys. Rev. 93, 99 (1954).
[4] P. Kirton, et al., Adv. Quantum Technol. 2, 1800043 (2019).
[5] M. A. B. M. et al., Phys. Scr. 92, 054003 (2017).
[6] M. A. B. M., et al., Phys. Rev. E 109, 034202 (2024).

Hydrogen atom under spatial and magnetic confinement: Superintegrability, Information Theory, and Neural Networks **12:00 - 12:35 H**

Adrián Mauricio Escobar Granados
Departamento de Física, Universidad Autónoma Metropolitana, México

In this talk, we explore the quantum problem of a hydrogen atom confined by (I) a penetrable inverted Gaussian potential, and (II) within an impenetrable cylindrical cavity under the influence of a constant magnetic field oriented along the main cylinder's axis. Our approach combines tools from superintegrability theory, numerical techniques, and physically relevant trial functions. Additionally, we incorporate concepts from information theory to characterize quantum states and apply neural networks to optimize computational frameworks and improve predictive accuracy. The energy spectra, wavefunctions, and information-theoretic measures of the ground state are explicitly presented. We also highlight potential applications in quantum technologies and fundamental physics.

Entropy production rate of Quantum Markov Semigroups **12:55 - 13:30 H**

Jorge R. Bolaños-Servín
Departamento de Matemáticas, Universidad Autónoma Metropolitana, México

In classical Markov chains, both discrete and continuous-time, the zero entropy production rate is a key index of the reversibility of the process, it is equivalent to the well-known Kolmogorov cycle criterion and the detailed balance condition. However, when transitioning to the realm of open quantum systems, the notion of reversibility becomes more nuanced and less straightforward. In this talk, I will explore various formulations of quantum detailed balance conditions and their implications for reversibility of the evolution of open quantum systems. I will discuss how these conditions relate to the quantum entropy production rate, focusing on its characterization for GKSL generators of quantum Markov semigroups.

Variational approach to time-dependent systems: Surface tension of quantum droplets **13:30 - 14:15 H**

Rocío Jaúregui
Instituto de Física, Universidad Nacional Autónoma de México

Variational approaches are used in Physics to identify the optimal representations of a system within a given subset of functions that exhibit some of the expected properties of the system. Such an approach was used by Lord Rayleigh in 1879 to describe capillary phenomena [1]; manuscript where the concept of surface tension was also introduced. In this work, the surface tension of quantum droplets is studied and explicit expressions are found using Thouless variational approach [2]. In most circumstances, degenerate states of dilute atomic gases are realized using samples trapped by different means. However, they can also exist without a trapping potential leading to the creation of quantum droplets. Following the proposal of Petrov [3], here we consider a condensed Bose Bose mixture where the interspecies attraction becomes stronger than the geometrical average of the influtra-species repulsions. The stabilization mechanism is then provided by quantum fluctuations. Thouless variational method considers a Bogolubov scheme for the description of low energy excitations of the ground state within the random phase approximation (RPA)[4]. By the introduction of a pair variational ansatz for surface excitations of a spherical quantum droplet we obtain explicit expressions of the surface tension. One of them exhibits a dependence on the angular momentum quantum number ‘ that resembles that of Rayleigh and that of the liquid drop model of nuclei in the limit of N ! 1 nucleons. The second ansatz has an ‘-dependence similar to that predicted for atomic nuclei by Bertsch [5] and by Casas and Stringari [6] using the RPA and the density-density Green’s function formalism. The convenience of using one or the other ansatz in the description of quantum droplets that have already been generated experimentally is discussed in details, as well as, the expected consequences in binary collisions of such quantum droplets.

References

[1] Rayleigh, L.Proc. R. Soc. Lond. 29, 71 (1879).
[2] Alba-Arroyo J. E., Caballero-Benitez S. F. and Jauregui R Scientic Re- ports 12,18467 (2022)
[3] Petrov, D. S. Phys. Rev. Lett. 115, 155302 (2015)
[4] Thouless, D. J. Nuclear Phys. 22, 78 (1961).
[5] Bertsch, G. F. Phys. Rev. A 9, 819 (1974).
[6] Casas, M. and Stringari, S. J. Low Temp. Phys. 79, 135 (1990).

Propagators in Information Field Theory **16:00 - 16:35 H**

Roberto Flores Moreno
Departamento de Química, Universidad de Guadalajara

Information field theory (IFT) is a recently coined name for Bayesian field theory which emphasizes the use of field theoretical methods to access information and make decisions based on statistical inference. IFT is a statistical field theory and, therefore, is closely related to quantum field theory and the concepts of path integrals and propagators. Naturally IFT connects to information theory concepts like Shannon’s entropy and Kullback-Leibler divergence. In this talk I will share my recent experience trying to understand the role of propagators within IFT.

Informational characterization of chemical hypergraphs **16:35 - 17:10 H**

Humberto Laguna Galindo

Departamento de Química, Universidad Autónoma Metropolitana, México

A chemical hypergraph is a representation of a set of chemical reactions. Hypernodes are formed by sets of substances (which play the role of reactants or products) and hyperlinks are the chemical reactions (which connect reactants with products) and the intersections among hypernodes (chemical substances that appear in more than one reaction). In this work, a random walker in a chemical hypergraph is studied in three different regimes: equiprobable transitions between the connected hypernodes, transitions that favor the most connected nodes, and transitions that favor the smallest nodes (in chemical reactions the number of participating substances is restricted). A characterization of the random walker is carried out through network entropy, a version of Shannon entropy for networks.

January 29th

DAY 2

Information Theoretical Concepts in the study of properties of quantum systems **9:00 - 9:45 H**

Elvira Romera
Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, España

Information theoretical concepts have been proved to be an efficient tool in the study of physical systems. In particular in the study of the quantum-mechanical properties of many-particle systems. In this presentation We will describe some important applications ranging from the study of electron correlations in atomic systems to the regeneration of quantum wave packets, the study of quantum phase transitions or topological phase transitions.

Exact Ansatzes for Quantum Simulations of Many-body Systems **9:45 - 10:30 H**

David A. Mazziotti
Department of Chemistry and The James Franck Institute The University of Chicago, Chicago, IL 60601 USA

Recent advances in quantum computing have unlocked the potential for solving many-body quantum systems with verifiably exact ansatzes that scale efficiently with system size. In this lecture, I will present the development and application of exact ansatzes derived from the contracted quantum eigensolver (CQE) for treating many-fermion, many-boson, and mixed fermion-boson systems. These ansatzes solve the contracted Schrödinger equation (CSE), a reduced form of the many-body Schrödinger equation, enabling accurate simulation of ground and excited states with shallow circuits and minimal error accumulation. Applications include polaritonic chemistry, where strong light-matter coupling modifies molecular properties, and nonadiabatic dynamics at conical intersections, critical for understanding photostability in DNA base pairs. By extending the CQE to mixed systems, we address challenges in multireference and strongly correlated regimes, providing insights into chemical reactivity and energy transfer. These results demonstrate the potentially transformative impact of exact quantum algorithms on molecular and material simulations.

Usefulness of quantum entanglement for enhancing precision in frequency estimation **10:30 - 11:05 H**

Pablo Barberis

Instituto de Investigaciones en Matemáticas Aplicadas y en Sistemas, Universidad Nacional Autónoma de México

We investigate strategies for reaching the ultimate limit on the precision of frequency estimation when the number of probes used in each run of the experiment is fixed. That limit is set by the quantum Cramér-Rao bound (QCRB), which predicts that the use of maximally entangled probes enhances the estimation precision, when compared with the use of independent probes. However, the bound is only achievable if the statistical model used in the estimation remains identifiable throughout the procedure. This in turn sets different limits on the maximal sensing time used in each run of the estimation procedure, when entangled and independent probes are used. When those constraints are taken into account, one can show that, when the total number of probes and the total duration of the estimation process are counted as fixed resources, the use of entangled probes is, in fact, disadvantageous when compared with the use of independent probes. In order to counteract the limitations imposed on the sensing time by the requirement of identifiability of the statistical model, we propose a time-adaptive strategy, in which the sensing time is adequately increased at each step of the estimation process, calculate an attainable error bound for the strategy and discuss how to optimally choose its parameters in order to minimize that bound. We show that the proposed strategy leads to much better scaling of the estimation uncertainty with the total number of probes and the total sensing time than the traditional fixed-sensing-time strategy. We also show that, when the total number of probes and the total sensing time are counted as resources, independent probes and maximally entangled ones have now the same performance, in contrast to the non-adaptive strategy, where the use of independent is more advantageous than the use of maximally entangled ones.

An Information-theoretical Take on Electron-Nuclear Wave Packet Dynamics **11:25 - 12:00 H**

Peter Schürger

Institut de Chimie Physique, Université Paris-Saclay, France

Coupled electron-nuclear motion plays a crucial role in quantum chemistry, underpinning processes ranging from light-induced excitation to charge transfer and bond breaking/forming. In my talk, I present the application of information-theoretic measures to a time-dependent coupled electron–nuclear system to analyze the dynamics and correlation between both particles. For this, differential Shannon entropies are calculated that are derived from time-dependent coordinate-space and momentum-space probability densities. Two distinct scenarios are investigated: one exhibiting adiabatic Born–Oppenheimer dynamics and the other involving strong non-adiabatic transitions.. The total and single-particle entropies, as well as the mutual information are analyzed and compared to semi-analytical expressions. Our results reveal that in the adiabatic regime, correlations manifest differently in coordinate and momentum spaces, which is related to the formation of nodes. In the diabatic case, entropies can be decomposed into state-specific contributions, revealing information about the transition between adiabatic states. [Entropy. 25, 970; AIP Advances 13, 125307]

An Information-Theoretic approach to characterizing concurrent processes and transition regions along the IRC: A 15-year retrospective on chemical reactions **12:00 - 12:35 H**

Moyocoyani Molina
General Electric Aerospace

Over the past few years, our research group, led by Dr. Esquivel, has pioneered a novel approach to studying chemical reactions. By applying functional density descriptors under the framework of information theory, we were able to characterize a series of concurrent processes that occur along the intrinsic reaction coordinate (IRC). The concurrent processes can be classified as bond formation/breaking, charge transfer, and energy storage reservoirs among others. This information-theoretical approach helped us to achieve an unprecedented phenomenological description of some model reactions that goes beyond traditional thermochemical and energetic analyses, and offers a deeper understanding of chemical changes driven by the redistribution of the electron density, particularly in the vicinity of the transition state (TS). During this talk, we will not only review the groundbreaking research we have made for over 15 years in this field, but we will also share some unpublished insights from the comparative analysis of various model reactions. Our goal is not only to disseminate our findings but also to outline a roadmap for future research and inspire the next generation of chemists to build upon our foundation.

Applications of Information Theory to Compact Objects: Configurational Entropy as a Stability Criterion **12:55 - 13:30 H**

Charalampos Moustakidis
University

In a remarkable study by Gleiser and Jiang (Stability bounds on compact astrophysical objects from information-entropic measure, Phys. Rev. D 92, 044046 (2015)), the authors demonstrated that the stability regions of neutron stars, within the framework of the simple Fermi gas model, and self-gravitating configurations of complex scalar field (boson stars) with various self-couplings, obtained through traditional perturbation methods, correlate with critical points of the configurational entropy with an accuracy of a few percent. Recently (Configurational entropy as a probe of the stability condition of compact objects, Phys. Rev. D 107, 044069 (2023)) we found that, while the minimization of the configurational entropy generally anticipates qualitatively the stability point for neutron stars and quark stars, this approach lacks universal validity. In this talk, I am going to further elucidate this issue by seeking to reconcile these seemingly contradictory findings. In particular, I will present the result concerning the configurational entropy of bosonic and fermionic systems, described by interacting Fermi and boson gases, respectively, which form compact objects stabilized by gravity. I will focus mainly whether the minimization of configurational entropy coincides with the stability point of the corresponding compact objects. The results of our studies indicate a strong correlation between the stability points predicted by configurational entropy and those obtained through traditional methods, with the accuracy of this correlation showing a slight dependence on the interaction strength. Consequently, the stability of compact objects, composed of components obeying Fermi or boson statistics, can alternatively be assessed using the concept of configurational entropy.

On information, entropy, and early stone tools **13:30 - 14:15 H**

Fernando del Río Haza
Departamento de Física, Universidad Autónoma Metropolitana, México

In a recent paper [1], we quantified the information contained by Paleolithic stone tools due to their manufacturing process. The approach was based on Shannon's information theory [2] and the notion of entropy. We calculated how probable it was that such stone tools were produced by natural means, and, by implication, by our hominin ancestors. We have shown that the entropy of a stone tool can also be defined on a physical basis following Boltzmann [3, 4]. We review here the subject a point to some new developments.

References

[1] F. del Rio, R. López-Hernández and C. Chaparro Velázquez, "On information, entropy, and early stone tools", Molecular Physics, e2310644 (2024).
[2] C. E. Shannon, "The mathematical theory of communication", The Bell System Technical Journal, Vol. 27, 379–423, 623–656 (1948).
[3] L Boltzmann, "On the relationship between the second fundamental theorem of the mechanical theory of heat and probability calculations regarding the conditions for thermal equilibrium", Sitz.-Ber. K. Akad. Wiss., math.- Natur. Classe. Abt. II, LXXVI, 373-435 (1877).
[4] F del Río, "Entropy and Paleolithic stone tools", Sadi Carnot's Legacy - Celebrating 200 years of thermodynamics, École Polytechnique, Palaiseau, Paris, Sept 2024.

Towards entropic uncertainty relations in non-regular Hilbert spaces **16:00 - 16:35 H**

Ángel Alejandro Garcia Chung
Departamento de Química, Universidad Autónoma Metropolitana, México

The entropic uncertainty relations result from an intrinsic inequality between a Hilbert space and its dual. It is ubiquitous in the sense that it is not attached to any self-adjoint operator but to well-defined states in these Hilbert spaces. In this talk, I will explore whether this relation is still present in non-regular Hilbert spaces, such as those used in loop quantum cosmology.

Information-theoretic concepts to elucidate local and non-local aspects of chemical phenomena **16:35 - 17:10 H**

Rodolfo Esquivel Olea
Departamento de Química, Universidad Autónoma Metropolitana, México ; Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, Spain

Our ongoing research in various chemical domains has yielded intriguing insights into chemical phenomena through the application of both classical and quantum information theories (CIT and QIT). These insights, often beyond the reach of standard methodologies, shed light on the intricate mechanisms by which chemical (and potentially biological) phenomena occur. Notably, information-theoretic measures have proven highly effective in offering concise yet profound visual representations of systems and their processes, emphasizing key aspects such as delocalizability, order, uniformity, and complexity from CIT, as well as decoherence and non-locality from QIT. In my presentation, I will showcase examples of how the axiomatic interplay between chemical intuition and theoretical information enriches our understanding of both local and non-local chemical phenomena.

January 30th

DAY 3

Information-theoretical quantities in the thermodynamical transcription of the density functional theory **9:00 - 9:45 H**

Ágnes Nagy, professor emeritus
Department of Theoretical Physics, University of Debrecen, Hungary

Ghosh, Berkowitz and Parr [1] initiated a thermodynamical transcription of the density functional theory into a local thermodynamics and introduced a local temperature that varies from point to point. The theory, however, is not unique because the kinetic energy density is not uniquely defined. It has been shown that the phase-space Shannon information entropy takes its maximum [2] and the Fisher information attains its minimum for the case of constant temperature [3]. For Coulomb systems there is a simple relation between the total energy and phase-space Fisher information [4]. The phase-space fidelity between excited states is proportional to the position-space fidelity, with a factor of proportionality depending on the total energies. The phase-space relative entropy is equal to the position-space relative entropy plus a term depending only on the total energies. Relationship between phase-space fidelity susceptibility and Fisher information is also presented [5]. In the special case of constant inverse temperature the phase-space relative Rényi entropy is a sum of the position-space relative Rényi entropy and a term arising from the momentum space [6]. This quantity can be considered as a measure of similarity. It includes more information than the position-space measures, since it also incorporates momentum-space knowledge.

References

[1] S. K. Ghosh, M. Berkowitz and R. G. Parr, Proc. Natl. Acad. Sci. USA 81, 8028 (1984).
[2] A. Nagy, Int. J. Quantum Chem., 117, e25396(2017).
[3] A. Nagy, Chem. Phys. Lett., 695, 149 (2018).
[4] A. Nagy, J. Chem. Phys., 153, 154103 (2020).
[5] A. Nagy, Int. J. Quantum Chem., 122, e26679(2021).
[6] A. Nagy, Int. J. Quantum Chem., 124, e27226 (2023).

Dynamical Paths to Densities Optimizing LMC Statistical Measures of Complexity **9:45 - 10:30 H**

Angel Ricardo Plastino

Universidad Nacional del Noroeste de la Prov. de Buenos Aires (UNNOBA), Argentina

The celebrated LMC measure, proposed by Lopez-Ruiz, Mancini and Calbet, assigns a quantitative amount of complexity to a discrete probability distribution, or to a continuous probability density. The main idea motivating the LMC measure is the basic intuition, shared by most researchers studying complexity in natural phenomena, according to which systems exhibiting a large amount of order, or a large amount of disorder, have low or vanishing complexity. In terms of a discrete probability distribution, these situations correspond, respectively, to certainty (with one probability equal to 1, and the rest equal to 0) or to equiprobability (with all the probabilities having the same value). Consequently, the LMC measure is constructed in such a way that it vanishes in these two extreme cases, and adopts its maximum value for some intermediate regime. The denition of the LMC measure can then extended to continuous probability densities. The above mentioned "boundary" restrictions, however, are not enough to determine a unique measure of statistical complexity. In fact, researchers have introduced several statistical measures of complexity, akin to the original LMC one, dened as products of information or entropic-like quantities, that also comply with the aforementioned requirements. These measures, which we collectively refer to as "LMC-measures", have been applied by scientists to the study of diverse problems in Physics and other elds, leading to a research literature of respectable size. In spite of the intriguing results yielded by those investigations, relatively little attention has been paid to identify, and investigate, the kind of dynamical processes governing time-dependent probability densities, that evolve towards densities optimizing the LMC measures, under suitable constraints. Given the remarkable amount of phenomenological applications of the LMC measures to diverse elds, that have been developed by researchers over the years, it seems desirable to re-consider the possible dynamical origins of densities optimizing these measures. Our aim in the present contribution is to re-visit this problem, exploring the main properties of a family of evolution equations satisfying an H-like theorem based on the LMC measures. We shall present these considerations within the context of other fundamental open questions concerning the LMC measures.

Few-electron confined quantum systems: Precise structural and quantum information theoretic measures **10:30 - 11:05 H**

Jayanta Kumar Saha

Department of Physics, Aliah University, II-A/27, Action Area II, Newtown, Kolkata, West Bengal 700160, India

Few-electron confined quantum systems show several novel properties leading to significant changes in their quantum chemical behavior. A suitable model potential mimics the effect of external confinement. In this talk, I shall discuss several topics of contemporary interest in the domain of confined quantum systems e.g. large momentum oscillatory distribution for pressure-confined alkali atoms, Borromean states of three-body exotic systems, the consequence of nuclear beta decay in case of pressure-confined He atom, orbital electron trapping of the hydrogen atom using double barrier repulsive potential etc. The in-depth analysis of the methodology adopted for each case and the detailed structural and quantum information theoretic analysis will be discussed.

A model of energy transport in photosynthesis **11:25 - 12:00 H**

Roberto Quezada

Department of Mathematics, Universidad Autónoma Metropolitana, México

In the context of the theory of open quantum systems we will discuss the dynamics of quantum states in an energy transport model (photosynthesis), with a generator defined in terms of generalized discrete Fourier transform operators which induce transitions between two mutually orthogonal subspaces, similar to birth and death transitions in classical stochastic processes or creation and annihilation operators in the quantum setting. It turns out that any initial state supported on the first subspace is transported as the time increases to infinity, to a final state whose probability mass is concentrated on the second (orthogonal) subspace and there is an energy gain in the process.

Probing Quantum-Gravity Interplay with Bose-Einstein Condensates **12:00 - 12:45 H**

Ivette Fuentes
University of Southampton

The unification of quantum theory and general relativity remains one of the most profound challenges in fundamental physics. A significant obstacle is the lack of experimental data at scales where quantum and relativistic effects intersect. Developing instruments sensitive to these scales could also shed light on other pressing questions, such as the nature of dark energy and dark matter. In this talk, I will explore how Bose-Einstein condensates (BECs) can be utilized to investigate these phenomena. I will discuss the challenges in current setups to test whether gravity induces the collapse of the wavefunction. Current experimental approaches typically involve solids, such as mirrors and glass nanobeads; however, BECs, with their unbound atoms and unique quantum states, might offer distinct advantages. I will also introduce a proposal for using BECs to conduct precise tests of the two key components of the gravitational potential in Λ-gravity: the Newtonian term and the cosmological constant.

Entanglement Dynamics in an Optomechanical Cavity with a Type-V Qutrit and Two-Mode Field **12:55 - 13:30 H**

Shihai Dong
Centro de Investigación en Computación - Instituto Politécnico Nacional, México

The main objective of this work is to measure the degree of interaction of a type-V qutrit with a two-mode quantized field in an optomechanical cavity. We first deduce the Hamiltonian in the interaction picture to identify the oscillatory terms and then obtain the effective Hamiltonian analytically. By selecting initial conditions for the atom, the two-mode field, and the moving mirror, we can determine the state vector of the entire system through a first-order approximation of the effective Hamiltonian. With this information, we proceed to solve the Schrödinger equation, generating a coupled set of differential equations that is solved numerically based on the initial conditions. The atomic von Neumann entropy allows us to obtain the temporal evolution of the degree of entanglement of the qutrit in the cavity and the atomic population inversion. The results indicate that entanglement in this tripartite system, composed of the qutrit and the mirror-field subsystems, as well as the population inversion, can be manipulated by the initial state conditions of the system, the qutrit-field and mirror-field coupling coefficients, the pump field, and the dissipation rates of the two-mode field and the movable mirror, respectively.

The resource of Non-stabilizerness: An introduction and application to Quantum Rabi Model **13:30 - 14:05 H**

Ernesto Benítez Rodríguez
Departamento de Física, Universidad Autónoma Metropolitana, México

Non-stabilizerness or "magic" is a quantum resource for quantum computation, in this talk I will give you a brief introduction to the resource theory of magic, focusing on its main elements, namely, free states, free operations and resource states. Measures to quantify magic in quantum states will be reviewed, and, as final part, we will see that Quantum Rabi Model can carry magic under certain constrictions.

Kullback-Leibler divergence in Machine Learning: Its relation to cross entropy and application to Boltzmann machines **16:00 - 16:35 H**

Roberto Bernal Jaquez

Departamento de Matemáticas Aplicadas y Sistemas, Universidad Autónoma Metropolitana, México

Kullback-Leibler (KL) divergence is a fundamental measure in information theory that quantifies the difference between two probability distributions. This concept has been widely adopted in machine learning due to its central role in training probabilistic models and in optimizing targets based on comparison between distributions.

In this talk we will explore the key concepts behind KL divergence, its interpretation as a measure of discrepancy between probabilistic distributions, and its crucial role in optimizing machine learning models.

We will address its direct relationship to cross entropy, a metric frequently used in classification problems, by demonstrating how minimizing cross entropy is equivalent to minimizing KL divergence in certain contexts. To illustrate its practical application, we will delve deeper into the use of KL divergence in the context of Boltzmann machines.

Construction and analysis of information measures through Diophantine equations **16:35 - 17:10 H**

Saúl J. C. Salazar

Departamento de Química, Universidad Autónoma Metropolitana, México

The study and quantification of correlation effects are important aspects of the many-body problem. Its quantification provides a means to evaluate approximate solutions when analytical solutions are not available. In general, these effects are usually due to the interaction, or correlation, between the particles of a physical system. Previous works have studied analytical relationships of informational measures of pairs of variables such as mutual information or high orders such as total correlation and interaction information in quantum systems of harmonic oscillators. By examining the expressions of the mutual information, the total correlation, and the interaction information, it is inferred that it is possible to construct them from the definition of certain coefficients associated with linear combinations of the Shannon entropies. Therefore, in this work, we present an analysis of how to obtain these coefficients by solving Diophantine equations (equations with integer solutions). Considering the above, new correlation and higher order measures can be designed by setting some particular values of the Diophantine equations.

January 31th

DAY 4

From Electron Density to Information Theoretical Measures to Structural Properties in Atoms and Molecules **9:00 - 9:45 H**

K.D. Sen, INSA Honorary Scientist
School of Chemistry, University of Hyderabad, Hyderabad 500046, India

We present a brief review of our ongoing research interest [1-2] which originate from the application of the information theoretical measures derived tools in the area of electronic structure theory [3] .In particular, the applications relating to the (i) Slater exchange parameter (ii) mean excitation energy of atoms (iii) characteristic features of the net Shannon information entropy for confined atoms (iv) scaling properties of the information measures corresponding to a several well known quantum model potentials (v) shape complexity of H atom in external parallel electric and magnetic fields (vi) stability of H_2^+ molecule and (vii) stability of 2-electron atoms under compression will be discussed.

1. K.B.K. Raju, P.S.V. Nair and K.D. Sen, An information theoretical estimate of the exchange parameter in Xα-theory, Chem. Phys. Lett. 170, 89 (1990). First publication.
2. Koustav D. Chakladar, Santanu Mondal ,K. D. Sen and Jayanta K. Saha, Quantum-information-theoretic analysis of Zee systems under pressure confinement, Phys. Rev. A 110, 042819 (2024). Most recent publication.
3. Statistical Complexity: Applications in Electronic Structure, Ed: K.D. Sen (2011) Springer, U.K. For a collection of literature reviews up to 2010.

Unbounded entropy production for repulsive-to-attractive interaction quench in long-range interacting systems **9:45 - 10:30 H**

Barnali Chakrabarti
Department of Physics, Presidency University, 86/1 College Street, Kolkata 700073, India.

We study the non-equilibrium dynamics of a one-dimensional Bose gas with long-range interactions that decay as ($1/r\alpha$) (0.5 ¡ α ¡ 4.0). We investigate exotic dynamics of super-Tonks-Girardeau gases when the interactions are suddenly switched from strongly repulsive to strongly attractive. We find that relaxation is achieved through complex intermediate dynamics demonstrated by violent fragmentation and chaotic delocalization. We establish that the relaxed state exhibits classical gaseous characteristics and an asymptotic state associated with unbounded entropy production. The phase diagram shows an exponential boundary between the coherent quantum gas and the chaotic classical gas. We show the universality of the dynamics by also presenting analogous results for spinless fermions. Weaker quench protocols give a certain degree of control over the relaxation process. Our study showcases the complex relaxation behavior of tunable long-range interacting systems that could be engineered in state-of-the-art experiments, e.g. in trapped ions or Rydberg atoms.

Information Entropy in spatially confined atoms and few-electron harmonic quantum dot within density function formalism **10:30 - 11:05 H**

Amlan K. Roy

Department of Chemical Sciences, IISER Kolkata, Mohanpur 741246, Nadia, India

The study of confined quantum systems has been a captivating area of research since the birth of quantum mechanics. Particularly, nowadays, quantum dots (QDs) where particles are confined within nano-scale cavities, emerges as a promising area of research. QDs have garnered significant attention across diverse scientific and technological fields due to their tunable electronic properties, making them potential candidates for qubits [1]. This has spurred interest in quantum information measures quantified through some entropies, such as Shannon and Fisher entropy, for geometrically tunable few-electron systems [2-5]. Various confinement potentials, including harmonic, finite oscillator, rectangular, parabolic, and Woods-Saxon models, have been employed to trap electrons in QDs [2-5]. Among these, harmonic confinement stands out for its analytical tractability and relevance in approximating environments for few-electron systems, particularly for two-electron configurations [2-5]. Extensive studies on such systems have primarily emphasized energetic properties, while relatively fewer investigations have explored quantum information characteristics [2,5]. This gap highlights the need for systematic studies in this domain to advance the understanding of quantum confinement and its implications for quantum technologies. We incorporate the utilization of the Kohn-Sham (KS) model, which has proven to be highly effective for calculating the energy spectrum of many-electron atoms subjected to similar types of confinement [3,4,6]. Therefore, we employ the generalized pseudospectral (GPS) method [3,4] to solve the eigenvalue equations with high precision and we provide a comprehensive insight into the quantum information-theoretic aspects of confined systems by analyzing both position and momentum space information content. Results will be discussed on spatially confined atoms in impenetrable cavity as well as harmonically trapped QD.

References:

1. V. K. Dolmatov, A. S. Baltenkov, J.-P. Connerade and S. T. Manson, Rad. Phys. Chem. 70, 417 (2004).
2. S. Mondal, A. Sadhukhan, J. K. Saha and A. K. Roy, J. Phys. B 57, 175001 (2024).
3. N. Mukherjee and A. K. Roy, Int. J. Quantum Chem. 118, e25596 (2018).
4. N. Mukherjee, S. Majumdar and A. K. Roy, Chem. Phys. Lett. 691, 449 (2018).
5. S. Mondal, K. D. Sen and J. K. Saha, Phys. Rev. A 105, 032821 (2022).
6. S. Majumdar and A. K. Roy, Int. J. Quant. Chem. 121, e26616 (2021).

External field modified entropic exchange: static vs time dependent fields **11:25 - 12:00 H**

Vinod Prasad

Department of Physics, Swami Shraddhanand College, University of Delhi, India.

The comparative analysis of the uniform static and the time dependent electric fields on the quantum-information measures of the atoms under spatial confinements is discussed in detail. Also, the results of previous works where, external magnetic fields on the entropic properties of similar systems will be presented for the sake of comparison. The interaction of confined hydrogenic atoms with external electric fields unveils significant changes in their quantum mechanical properties, which includes the changes in the energies and the wave functions. This talk delves into the comparative analysis of static and time-dependent fields on the Shannon entropy of these systems, with a particular emphasis on the role of dynamic, laser-fields. We present a comprehensive study of the entropic characteristics of a dressed atom, where the atom interacts with a monochromatic laser beam. By employing a robust, non-perturbative quasi-energy formalism, we compute the dressed wave functions and quasi-energies of the laser-dressed atom, forming the basis for evaluating key entropic measures. Our findings highlight the interplay between Shannon entropy and other entropic metrics as functions of laser parameters such as frequency and intensity. We observe that transitions governed by selection rules significantly influence the levels participating in the laser–atom interaction, leading to distinct entropic signatures. Main focus is on the entropic measures in the vicinity of avoided crossings, a hallmark of the laser-driven dynamics. Furthermore, the emergence of the AC Stark effect at higher laser intensities induces the complex interplay between field strength and quantum entropy. This investigation not only provides deeper insights into the field-induced modifications in quantum systems but also establishes a framework to distinguish between the impacts of static and time dependent fields. Also, the comparisons are made among different quantum systems such as particle in a box, which is a limiting case of atom under tight confinement to the atom under soft confinements.

On the numerical integration of two-particle functions for Pair Entropies of diatomic molecules **12:00 - 12:35 H**

Juan Manuel Solano-Altamirano

Facultad de Ciencias Químicas, Benemérita Universidad Autónoma de Puebla, Puebla, Pue., México.

In order to compute informational entropies of two-particle quantities, highly-accurate numerical integration methods are needed. In this talk, we describe the details of a numerical algorithm specific for diatomic molecules, originally designed to numerically integrate 3D functions, which is adapted to integrate functions of two particles, i.e., to integrate functions in domains of the form $\Omega \times \Omega$, where $\Omega \in R^3$. The diatomic integration scheme is a cubature rule that combines Gauss-Legendre quadratures for the radial and angular parts, and the domain Ω is split into two semi-spheres, each with its own local center of coordinates. In addition, we compare the performance of the diatomic integration scheme vs. a 6D Monte Carlo integrator.

Information entropy in confined quantum systems **12:55 - 13:30 H**

Neetik Mukherjee
Department of Chemistry, Medi-Caps University, Indore, India

In recent years, information-theoretic measures such as Fisher information, Shannon entropy, and Onicescu energy have emerged as vital tools in understanding quantum systems. Among these, Shannon entropy provides a more robust bound compared to traditional uncertainty relations, highlighting its significance in quantum mechanics. This study examines the pivotal role of Shannon entropy in elucidating various phenomena, including confinement effects in double-well potentials, modifications in excited quantum states due to spatial constraints, and Compton profiles in hydrogen-like systems. Additionally, the entropy-based analysis extends to phase transitions in plasma systems, offering a unique perspective on critical phenomena. A relationship between mean excitation energy and Shannon entropy is also invoked to facilitate the derivation of a novel connection between Shannon entropy and dipole oscillator strength. These insights underscore the versatility of Shannon entropy in bridging information theory and quantum mechanics, providing a deeper understanding of quantum systems under diverse physical conditions.
References:

1. Neetik Mukherjee, Arunesh Roy and Amlan K. Roy, Ann. Phys. (Berlin) 527, 825-845, (2015).
2. Neetik Mukherjee and Amlan K. Roy, Ann. Phys. (Berlin) 528, 412-433, (2016).
3. Neetik Mukherjee, Amlan K. Roy, J Phys. B 53, 253002, (2020).
4. Neetik Mukherjee, Chandra N. Patra and Amlan K. Roy, Phys. Rev. A 104, 012803, (2021).
5. Neetik Mukherjee, Sudipta Chakraborty and Amlan K Roy, J. Phys. B 55, 145001, (2022).

Title **13:30 - 14:15 H**

Paul Ayers
Department of Chemistry and Chemical Biology, McMaster University, Canada

Abstract

Some generalities of the applications of information theory in chemistry **16:00 - 16:35 H**

Nelson Flores-Gallegos
Departamento de Ciencias Naturales y Exactas, Universidad de Guadalajara, México

In this talk, I will discuss some general aspects of informational entropies when they are applied to the study of atoms, molecules, and some simple chemical reactions. We will focus on discussing some of the informational entropies and their possible relationship among some chemistry concepts such as hardness, chemical potential, among others, which are some of the main ingredients of the chemical reactivity theory. In this regard, we also discuss the use of informational entropies to describe some simple chemical reactions, and how this concept may be linked to important chemical changes, such as the process of bond-breaking and bond-forming.

Uncertainties and statistical correlations in quantum systems **16:35 - 17:10 H**

Robin Sagar
Departamento de Química, Universidad Autónoma Metropolitana, México

A survey of recent ideas and goals behind the quantification of uncertainties and statistical correlation in quantum systems will be presented. The focus will be on ideas and connections taken from information theory.

Round table: Future perspectives for UAM **17:10 - 17:40 H**

Universidad Autónoma Metropolitana
Participants:

Dr. Miguel A. Bastarrachea-Magnani. Physics Department.
Dr. Roberto Quezada Batalla. Mathematics Department.
Dr. Rodolfo Esquivel Olea. Chemistry Department.
Dr. Robin Sagar. Chemistry Department (Moderator).