3rd Workshop on Statistical Physics

Bogotá, Colombia

August 28th – September 1st 2017

BOOK OF ABSTRACTS

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Preface

The Workshop on Statistical Physics is the third issue of a series organized by Universidad Nacional de Colombia and Universidad de los Andes. The aim of the workshop is to present to the academic community - through mini-courses - topics and research methods developed in the last 25 years that have had a strong impact in the area and that can be included in advanced graduate courses; and, to provide - through invited conferences, oral contributions and posters - a space for the local community in statistical mechanics to share their most recent research results, and give the opportunity to establish scientific exchanges and collaborations. In this way, the workshop aims to contribute to the development of Statistical Physics in Colombia.

The event is addressed to professors and researchers in the areas of statistical physics as well as graduate and undergraduate students in physics with basic knowledge in statistical mechanics.

The event combines three days of short courses (Monday to Wednesday) with two days of invited conferences and presentations of oral contributions and posters (Thursday-Friday).

Scientific Committee

José Daniel Muñoz
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Universidad de los Andes
Bogotá – Colombia

Speakers

Short Courses

Thermodynamics of Information
Juan Manuel R. Parrondo
Universidad Complutense de Madrid
Spain

Exact Analysis of the 1D KPZ Equation and Discrete Models
Tomohiro Sasamoto
Tokyo Institute of Technology
Japan

Structure, Dynamics and Emergence in Complex Networks
Jesús Gómez-Gardeñes
Universidad de Zaragoza
Spain

Invited Speakers

Carlos Alvarez (U. Rosario, Bogotá)
Alonso Botero (U. Andes, Bogotá)
Manuel Camargo (U. Antonio Nariño, Cali)
Diego Luis Gonzalez (U. Valle, Cali)
Rafael Hurtado (U. Nacional de Colombia, Bogotá)
Laura Lotero (U. Pontificia Bolivariana, Medellín)
Fernando Naranjo (U. Pedagógica y Tecnológica de Colombia, Tunja)
William Fernando Oquendo (U. Sabana, Chía)
Carlos Quimbay (U. Nacional de Colombia, Bogotá)
Luis Quiroga (U. Andes, Bogotá)
Juliana Restrepo (EIA, Medellín)
Andres Rosales (U. Nacional de Colombia, Manizales)
Gabriel Villalobos (U. Tadeo, Bogotá)
Carlos Viviescas (U. Nacional de Colombia, Bogotá)

Short Courses

Monday August 28th – Wednesday August 30th 2017

Thermodynamics of Information

R. PARRONDO, Juan Manuel [1]

[1] Universidad Complutense de Madrid

1. A bit of history: Maxwell's demon, Szilard's engine, Bennett's solution.
2. Basic concepts: Shannon information, mutual information, relative entropy.
3. Heat, work, and non-equilibrium free energy.
4. Information and the second law.
5. Fluctuation theorems for feedback systems.
6. Reversibility: optimal Maxwell demons, optimal feedback.
7. Thermodynamic cost of measurement and erasure.
8. Creating information: symmetry breaking.
9. Maxwell demons in the phase space and microcanonical Szilard engines.
10. Information flows.

References

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2. J.M.R. Parrondo, J.M. Horowitz and T. Sagawa. Thermodynamics of information. Nature Physics 11, 131-139 (2015).
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4. J.M. Horowitz and S. Vaikuntanathan. Non-equilibrium detailed fluctuation theorem for repeated discrete feedback. Physical Review E 82, 061120 (2010)
5. J.M. Horowitz and J.M.R. Parrondo. Optimizing non-ergodic feedback engines. Acta Physica Polonica B 44,803-814 (2013).
6. J.M. Horowitz, T. Sagawa and J.M.R. Parrondo. Imitating Chemical Motors with Optimal Information Motor. Physical Review Letters 111, 010602 (2013).
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8. É. Roldán, I.A. Martínez, J.M.R. Parrondo and D. Petrov. Universal features in the energetics of symmetry breaking. Nature Physics 10 457-461 (2014).

9. R. Marathe and J.M.R. Parrondo. Cooling classical particles with a microcanonical Szilard engine. Physical Review Letters 104, 245704 (2010).
10. J. M. R. Parrondo and L. Granger. Maxwell demons in phase space. European Physical Journal-Special Topics 224, 865-875 (2015).
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Exact Analysis of the 1D KPZ Equation and Discrete Models

SASAMOTO, Tomohiro [1]

[1] Tokyo Institute of Technology, Japan

The Kardar-Parisi-Zhang (KPZ) equation is a partial differential equation with noise for describing a motion of interface, and is considered to be one of the standard models in non-equilibrium statistical physics. Its fluctuations show universal scaling properties, which constitute the KPZ universality class.

Its one-dimensional version admits exact solutions. The height fluctuation scales as $t^{1/3}$ for large time t and the exponent 1/3 had been confirmed by using Bethe ansatz. In 2000 its universal distribution function was identified and turned out to be related to random matrix theory. Since then there have been vast developments on the topic.

In the lectures we explain some basics of the KPZ equation and its exact solutions. We also discuss related discrete models, and connections to random matrix theory and integrable systems.

1. Random matrix theory and TASEP

After a short introduction to the topic, we explain the basics of random matrix theory and how the totally asymmetric simple exclusion process (TASEP) is related to it.

2. Exact solutions for the KPZ equation

We explain the issue of well-posedness of the KPZ equation and the exact solution of the one-point height distribution for the narrow wedge initial condition using replica method. We also discuss some generalizations.

3. ASEP, q-TASEP and Macdonald process

Behind the solvability of the KPZ equation lies the integrability.
We introduce the Macdonald process and show how they are related to discrete models such as the asymmetric simple exclusion process (ASEP) and q-TASEP.

Structure, Dynamics and Emergence in Complex Networks

GÓMEZ-GARDEÑES, Jesús [1]

[1] Universidad de Zaragoza

In this lecture we will cover the fundamentals of complex networks. This lecture is divided in three main parts. The first part is devoted to introduce the topic of network science motivating the main questions and results about the structural characterization of real complex systems. We will also introduce models for generating synthetic complex networks. In the second part we will cover the function of complex networks, paying special attention to two key collective phenomena that appear as a product of the microscopic interactions between nodes: Epidemics and Synchronization. We will show how the complex backbone of interactions (the network) can be incorporated into well-known mean field models, such as the SIS and SIR compartmental models for epidemics and the Kuramoto model for synchronization. Finally, in the third part, we will go beyond contact networks to accommodate real data about mobility patterns. To this aim, and focusing on contagion processes, we will introduce metapopulation modeling and tackle the analysis of epidemic outbreaks in populations of commuting agents.

Outline of the lecture:

PART I :
- Introduction to network science
- Characterization of network structure- Models of networks

PART II :
- Dynamical processes on complex networks
- Spreading processes
- The heterogenenous mean field and Microscopic approaches
- Synchronization dynamics in networks- Explosive transitions in networks

PART III :
- Metapopulation models
- The Markovian formulation of metapopulation dynamics
- Multiplex complex networks
- Vector-borne diseases

Conferences Thursday Morning – August 31th 2017

Exact large deviation of a tracer position in 1D symmetric exclusion process

SASAMOTO, Tomohiro [1]

[1] Tokyo Institute of Technology, Japan

The one-dimensional symmetric simple exclusion process (SEP) is a simple and well-known stochastic interacting particle system in which many particles perform symmetric random walk with exclusion interaction.

We study the fluctuation properties of a tracer (tagged particle) in the one-dimensional SEP for a uniform density stationary initial condition. The mean position is zero and the anomalous fluctuation of order t^(1/4) has been known for a long time. We will present an exact formula for the large deviation function of its position. Our results can be generalized to the step initial condition with different densities in both direction, and can also be translated to the large deviation of the integrated current at an arbitrary position.

This is a generalization of a previous work on the current at the origin studied by Derrida and Gershenfeld, and also of another work on the single file diffusion of Brownian particles by Krapivsky, Mallick and Sadhu. Our approach uses recently developed techniques to study the one dimensional KPZ equation and asymmetric exclusion process, such as the Bethe ansatz, stochastic duality and nested contour formula for the deformed moments.

Reference:
T. Imamura, K. Mallick, T. Sasamoto, Large deviations of a tracer in the symmetric exclusion process, Phys. Rev. Lett. 118, 160601 (2017).

Critical exponents, magneto-caloric- and magneto-electrical effects, and magnetic interactions in Iron- and Cobalt-based metallic glasses

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A study of the magnetic critical behavior, and magneto-caloric and magneto-electrical effects is presented for Fe- and Co-based metallic glasses. The magnetic critical behavior and magneto-caloric effect of these systems are studied by determining the critical exponents for the zero-field magnetization (β), zero-field isothermal susceptibility (γ), critical isotherm (δ), critical temperatures T_C, and change in magnetic entropy (ΔS_M), respectively, from magnetization measurements. The magneto-electrical effects are studied by using magnetization, Hall effect, and magneto-impedance, measurements. The values obtained for the critical exponents (β, γ, δ) vary from values that correspond to universality classes of standard models with short-range interactions (i.e., Ising and Heisenberg models) to universality class of mean field model with interactions of long-range. The resulting curves for ΔS_M vs. T show a symmetric peak in the vicinity of T_C, indicating that the ferromagnetic-paramagnetic phase transition is continuous one. The magnetization, Hall effect, and magneto-impedance measurements indicate that the spin-orbit interaction plays a central role in these metallic glasses. The influence of other possible mechanisms on the values of (β, γ, δ) including exchange interaction, magnetic dipolar interaction, RKKY interaction, magneto-elastic anisotropies, and itinerancy, are also analyzed. A possible relationship, at least at the phenomenological level, between the magnetic critical behavior, magneto-caloric effect, and the spin-orbit interaction is experimentally studied.

Configurational temperature at limit states of granular materials

OQUENDO, William Fernando[1]

[1] Universidad de la Sabana

Granular media (GM) represent one paradigmatic example of complex systems where the emergent response cannot be predicted only from the (possibly) simple dynamics of the composing bodies. Furthermore, GM could behave as a gas, a liquid or a solid depending on the external conditions imposed on it. Several approaches have been attempted to understand GM, although there is still no universal model capable of explaining and predicting the response of the system under general conditions. One modern approach to GM is based on Statistical Mechanics (SM), which has been successfully applied to understand many particle systems. In spite of its huge success, the direct extension of SM to GM faces several conceptual challenges, in particular: 1) the strong dependence on initial conditions, which also increases the difficulty to define a true ensemble, and, 2) the definition and measure of the temperature, which looses is kinetic definition and becomes a quantity related with the configurations and volume, called typically the compactivity. Fortunately, for 1), there are some reference limit states in GM which are independent of the initial conditions: the state of isotropic compression and the so-called critical or steady State (CS). For instance, in the CS, the system is in a unique macroscopic state that is independent of the deformation history, but with presenting different internal states as the system evolves, thus allowing to define a statistical ensemble of internal states. Regarding 2), Aste et al have shown a convenient approach for measuring the configurational temperature from the statistics of volumes in static granular packings, generalized as the Cell theory. In this work, we present results for the measurement of the configurational temperature on a dry granular system by applying the Cell theory to both the isotropic and the critical states, under quasi-static conditions and over a broad range of microscopic sliding and rolling coefficients. The volume distribution is found to be robust over different kinds of sample preparation and external parameters, and an state equation is obtained.

EPL (Europhysics Letters) 114.1 (2016): 14004.

Statistical Mechanics in Opinion Formation Models

QUIMBAY HERRERA, Carlos José [1]

[1] Departamento de Física, Universidad Nacional de Colombia, Sede Bogotá

The study of the problem of how the opinion of an agent is formed and how this opinion can be influenced by its interactions with the other agents of a social system has been motive of great interest. This problem has been considered from different approaches in the context of the social sciences, based on microscopic or macroscopic views of the social system under consideration. From the point of view of physics, the problem of opinion formation has been studied using mainly concepts and tools of statistical mechanics. The main objective of this talk is to review the different types of opinion formation models that have been developed in the context of statistical mechanics, focusing on the possible application of these models in the description of certain social phenomena that emerge because of the opinion that agents have about something or someone in the system. We emphasize that there are few models of opinion formation based on statistical mechanics that have been applied to describe specific social phenomena.

Oral contributions Thursday Morning – August 31th 2017

Entropía y volatilidad de logretornos de volúmenes diarios de transacción de acciones como herramientas para caracterizar la dinámica de mercados bursátiles

QUIMBAY HERRERA, Carlos José [1]; GÓMEZ PINTO, Andrés Eduardo [1]

[1] Departamento de Física, Universidad Nacional de Colombia, Sede Bogotá

Como resultado del ejercicio de transacciones de compraventa diarias de acciones en los mercados bursátiles, dos de las cantidades más significativas que dan cuenta de este ejercicio son los precios de cierre y los volúmenes de transacción diarias de las acciones. Desde el punto de vista de la Econofísica, son muchas las metodologías basadas en la Mecánica Estadística que han estudiado las series de tiempo de logretornos de precios de cierre de las acciones con el fin de contribuir al entendimiento de la dinámica de los mercados bursátiles. Sin embargo, en este contexto, no se conocen trabajos realizados que hayan contribuido al entendimiento de dicha dinámica a partir del estudio de las series de tiempo de logretornos de volúmenes diarios de transacción de acciones. En este trabajo mostramos que estas últimas series de tiempo también pueden ser usadas para caracterizar la dinámica de los mercados bursátiles. Para lograr lo anterior, calculamos la entropía y la volatilidad de estas series de tiempo, usando ventanas de observación dependientes del tiempo, para diversos conjuntos de acciones pertenecientes a diferentes mercados bursátiles internacionales, encontrando que existen patrones de comportamiento en las series de tiempo de entropía y volatilidad, cuyo comportamiento es dependiente de si la acción es transada en un mercado consolidado o emergente. Con lo anterior mostramos que la entropía y la volatilidad de logretornos de volúmenes diarios de transacción de acciones son dos herramientas que pueden contribuir al entendimiento de la dinámica de los mercados bursátiles.

Leyes del capitalismo como propiedades macroscópicas en un modelo cinético de distribución de riqueza con ahorro

QUEVEDO VEGA, David Santiago [1]; QUIMBAY HERRERA, Carlos José [1]

[1] Universidad Nacional de Colombia

Partiendo de ciertas reglas de intercambio de dinero entre pares de agentes, los modelos cinéticos de distribución de dinero pueden reproducir las formas de los patrones de distribución obtenidas a partir de los datos empíricos de ingreso de la población económicamente activa de los diferentes países del mundo. En este contexto de la Econofísica, el modelo cinético de intercambio de dinero de Chakraborti y Chakrabarti ha sido motivo de crítica por parte de algunos economistas, debido a que ellos plantean que en este modelo el dinero juega el papel de la riqueza y que, a un parámetro de propensión al ahorro que es pieza fundamental del modelo, se le atribuyen equivocadamente propiedades de ahorro. En este trabajo realizamos una extensión del modelo de Chakraborti y Chakrabarti, basados en un enfoque de multiplicadores de Lagrange, que nos permite proponer un modelo de intercambio de riqueza entre pares de agentes, incluyendo al ahorro desde el punto de vista de la producción, consistentemente con su significado en la Economía. Usando las reglas de intercambio de riqueza entre pares de agentes que surgen del modelo propuesto, obtenemos que las leyes del capitalismo, formuladas por Thomas Piketty a partir del análisis estadístico de datos empíricos de riqueza y de ingreso, son obtenidas como propiedades macroscópicas estructurales, emergiendo como consecuencia de la dinámica microscópica del sistema económico considerado.

Conferences Thursday Afternoon – August 31th 2017

Stochastic Thermodynamics of Collective Cell Migration

RÄDLER, Joachim [1]

[1] LMU

Epithelial cell migration is of prominent importance in wound healing, embryonic development, and cancer progression. The dynamics in epithelial sheets were found to be highly heterogeneous, exhibiting spontaneous formation of swirls, long-range correlations, and glass-like dynamic arrest as a function of cell density. Theoretical attempts to capture the complex cellular hydrodynamics as an actively driven soft matter system are currently progressing. Here we describe experimental and theoretical approaches in order to grasp collective cell phenomena and to bridge collective dynamics to single cell dynamics. Using time-lapse microscopy we study the flow-like properties in confining geometries examining flow profiles as well as spatial and temporal correlations [1]. One of the hallmarks of active cellular matter is the spontaneous emergence of vortices. In recent experiments we examined the states of coherent angular motion of small, mesoscopic cell systems on circular micro-patterns [2]. Experiments are compared to computer simulations based on a generalized Potts model, which comprises scalar fields to account for intra-cellular cytoskeleton dynamics. The model shows that the emergence of vortex states is well reproduced and that vortex stability depends on the interplay of spatial arrangement and internal polarization of neighboring cells. It will be shown that micro-patterned surfaces in general allow for the guidance of cell behavior and hence open up novel tools to study cell dynamics [3]. Examples are cells migrating in ring-shaped micro-lanes, lanes with artificial chemical barriers and artificial dumbbells. The talk intends to provide a perspective on how artificial micro-environments can be used for high content phenotypic characterization with potential applications in cell biology and drug screening at the single cell level.

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[2] FJ Segerer, F Thüroff, AP Alberola, E Frey, and JO Rädler, Physical Review Letters 114, no. 22, 228102 (2015).

[3] C Schreiber, FJ Segerer, E Wagner, A Roidl, and JO Rädler. Scientific Reports 6, 26858 (2016).

Understanding a bleeding disorder by non-equilibrium free energy calculations

APONTE-SANTAMARÍA, Camilo [1]; LIPPOK, Svenja [2]; MITTAG, Judith [2]; OBSER, Tobias [3]; SCHNEPPENHEIM, Reinhard [3];

BALDAUF, Carsten [4]; GRÄTER, Frauke [5]; BUDDE, Ulrich [6]; RÄDLER, Joachim [2]

[1] University of Los Andes, [2] Ludwig Maximilian University, [3] University Medical Center Hamburg-Eppendorf, [4] Fritz-Haber-Institut der Max-Planck-Gesellschaft, [5] HITS gGmbh, [6] Asklepios Klinik Altona

Hemostasis is a key biological process in which platelets –flowing in our blood stream– adhere to injured blood vessels to stop bleeding. Platelets are anchored to the site of injury by the giant von Willebrand Factor (VWF) protein. Once a plug has been formed, and the injured site is closed, VWF is cleaved by the enzyme ADAMTS13, a crucial regulatory mechanism to prevent the formation of large thrombus aggregates. Several naturally occurring mutations modify this process, inducing distinct types of bleeding disorders, by unknown mechanisms. We present the first quantitative description of the dramatic destabilization of VWF caused by a one of such mutations, which strongly accelerates VWF cleavage. Molecular dynamics simulations revealed this mutation to induce structural, dynamic, and mechanical perturbations in the VWF-A2 domain. Non-equilibrium free energy calculations, performed by using the Crooks fluctuation theorem and the Bennett acceptance ratio, revealed that this mutation destabilized A2 by ~10 kJ/mol promoting its unfolding. In close agreement, fluorescence correlation spectroscopy (FCS) experiments revealed a 20-fold increase in the cleavage rate for this mutant, compared to the wild-type VWF. Cleavage was found cooperative with a cooperativity coefficient n = 2.3, suggesting that the mutant VWF gives access to multiple cleavage sites at the same time. Taken together, the enhanced cleavage activity can be readily explained by an increased availability of the cleavage site through A2-domain-fold thermodynamic destabilization. Our study therefore puts forward the combination of non-equilibrium free energy calculations and FCS, as a powerful way of examining protein stability in a clinically relevant context.

References: C Aponte-Santamaría, S Lippok, J Mittag, T Obser, R Schneppenheim, C Baldauf, F Gräter, U Buddee, and JO Rädler. Mutation G1629E increases von Willebrand factor cleavage via a cooperative destabilization mechanism. Biophys. J. 112: 57-65 (2017).

Simulation of Trypanosoma Cruzi swimming in shear flow

VILLALOBOS, Gabriel [1]; CASTILLO, Alberto [2]

[1] Universidad de Bogotá Jorge Tadeo Lozano

[2] Universidad de Bogotá Jorge Tadeo Lozano y Universidad Central

Chagas disease or American Trypanosomiasis is caused by Trypanosoma cruzi (T. cruzi), a protozoan parasite that flows within blood; while living and reproducing inside its human host for several years would cause different diseases and even death [1]. In order to fight the disease, it is crucial to understand the way the parasite moves inside the body of the host. Hereby, we present a T. cruzi bloodstream trypomastigote model aimed at studying the effect of the blood flow and Reynolds number in the parasite tropism and mechanical properties. The parasite itself is modeled using spring network models (as in [2] and [3]), and the flow by dissipative particle dynamics, DPD [4],[5]. The present work constitutes a first step towards the modeling of the interaction between the T. cruzi and the blood corpuscles.

[1] F. Villalta, J. Scharfstein, A. W. Ashton, K. M. Tyler, F. Guan, S. Mukherjee, M. F. Lima,S. Alvarez, L. M.Weiss, H. Huang, et al. Perspectives on the trypanosoma cruzi–host cell receptor interactions. Parasitology research, 104(6):1251–1260, 2009.

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[3] M. Kong, Y. Wu, G. Li, and R. G. Larson. A bead-spring model for running and tumbling of flagellatedswimmers: detailed predictions compared to experimental data for e. coli. Soft matter, 11(8):1572–1581, 2015. [4] P. Hoogerbrugge and J. Koelman. Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics. EPL (Europhysics Letters), 19(3):155, 1992.

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Poster session Thursday Afternoon – August 31th 2017

Análisis del índice de Gini y la entropía en los modelos cinéticos de distribución de ingreso con propensión al ahorro fijo.

SANTOS, Alexander [1]; QUIMBAY, Carlos Jose [2]; ALVARADO, Jose Luis [1]

[1] Universidad de los Llanos

[1] Universidad Nacional de Colombia

La implementación de simulaciones basadas en agentes ha permitido estudiar modelos cinéticos de distribución que explican la asimetría en las distribuciones de ingreso empíricas. El modelo más robusto es el propuesto por Chakraborti y Chakrabarti, en donde en cada agente intercambia dinero de forma similar al intercambio de energía en los choques elásticos de las partículas en un gas, y en el cual la cantidad intercambiada es una fracción aleatoria de dinero que no está libre de riesgo. Debido a que la forma de la distribución depende de la fracción libre de riesgo o propensión al ahorro, en este trabajo se hace un análisis de la desigualdad de las diferentes distribuciones y se relaciona con el valor de la entropía en el equilibrio. Los resultados muestran que el índice de Gini, que mide la desigualdad en las distribuciones, crece conforme al aumento del parámetro de ahorro, y que en cambio, la entropía disminuye hasta hacerse nula para la propensión máxima. Finalmente se encuentra una relación entre el índice de Gini y la entropía y se discuten sus resultados.

Modelo cinético de formación de opinión aplicado al estudio de la dinámica de variables de desarrollo organizacional definidas a partir de la percepción de los agentes del sistema

RUBIANO, Jefferson Rubiano[1]; QUIMBAY HERRERA, Carlos Jose [1]

[1] Universidad Nacional de Colombia

Desde el punto de vista de la Mecánica Estadística, diversos tipos de modelos se han desarrollado para estudiar la dinámica de la formación de opinión. Dentro de este contexto, varios tipos de metodologías de formación de opinión han sido desarrolladas basadas en modelos cinéticos donde los agentes del sistema, que intercambian opinión entre pares, juegan el papel partículas de un gas ideal que intercambian energía cinética a través de colisiones elásticas entre pares. Sin embargo, buena parte de los modelos de formación de opinión fundamentados en la Mecánica Estadística carecen de relevancia empírica al no describir fenómenos sociales reales que hayan sido originados como consecuencia de la opinión de los agentes del sistema. Teniendo en cuenta que una parte relevante del diagnóstico sobre el desarrollo organizacional proviene de la opinión de los individuos que hacen parte de la organización, en este trabajo proponemos un modelo cinético de formación de opinión que es aplicado al estudio de la dinámica de variables de desarrollo organizacional que han sido definidas a partir de la percepción que tienen los agentes que hacen parte de la organización. Por lo anterior, en este trabajo una organización es considerada como un sistema social complejo constituido por muchos agentes, en el que las variables que cuantifican un determinado tipo de desarrollo organizacional son asumidas como propiedades estructurales que emergen como consecuencia del intercambio de opinión entre pares de agentes. El modelo cinético de formación de opinión mencionado permite reproducir los valores de opinión que tienen los servidores públicos con respecto a siete variables de desarrollo organizacional de entidades colombianas del orden nacional, durante el período 2011-2016, los cuales son medidos mediante la Encuesta Sobre Ambiente y Desempeño Institucional Nacional (EDI) aplicada anualmente por el DANE.

Aging Study of Saccaromyces Cerevisiae using the Kaplan Meier Estimator

DURAN CHAPARRO, David Camilo [1]; PEDRAZA, Juan Manuel [1]

[1] Universidad de los Andes

Saccharomyces cerevisiae are model organisms for studying several phenomena in eukaryotic cells. Some examples of phenomena studied with these cells are molecular mechanisms of aging and behaviour of synthetic circuits for different purposes. Recently, different devices have been built for making such studies using microfluidic technology. We designed a novel microfluidic device and used it to study aging of Saccaromyces Cerevisiae using the Kaplan-Meier Estimator. This is a non-parametric statistic of the survival function which allows estimation of survival probability of a population during a time interval.

Analysis of brain states from fMRI data using a complex network based method approach

TAPIA HERRERA, Luis Carlos [1]; CASTELLANO, Gabriela [2]; OZELO, Helka [2]; OLIVEIRA, Marcia [2]; CORDEIRO, Monica [3]; DAMASCENO, Benito [3]; CENDES, Fernando [3]; COVOLAN, Roberto [2]; ALESSIO, Andrea [3]

[1] IFGW Unicamp

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[3] Neuroimage Laboratory, School of Medical Sciences,UNICAMP

This work presents a useful methodology to visualize and identify rain areas related with the performance of a task. For this, two different fMRI sessions were studied, one in resting state (RS) and other in a language task (LT). The BOLD time series of the two sessions were analized using a standard anatomical atlas of the brain. Two main objetives that guided this work were: 1) establish differences between the activity of the brain in resting state and the brain developing a cognitive task; 2) identify areas of the brain involved in the developing of a task, without a previous model of the task. The community structure of group connectivity matrices was explored for both conditions (RS and LT) and for different preprocessing steps. When gray matter signal regression (GSR) was performed, small changes of the community structure were observed. Approximately, the same regions were classified in the same communities before and after GSR. This means, that the community structure of the data is weakly affected by this preprocessing step. The modularity index presented significant changes between conditions (RS and LT) and between different preprocessing pipeline.

Berry Phase: a Tool to Study Quantum Phase Transitions

PADILLA-GONZÁLEZ, Daniel Camilo [1]; FRANCO, Roberto [1]; SILVA-VALENCIA, Jereson [1]

[1] Universidad Nacional de Colombia

The classical phase transitions as well as quantum phase transitions are usually classified as first and second kind transitions. This classification depends of the behavior of an *order parameter* as a function of thermodynamic or internal parameters of the system. However, this classification is not complete. In fact, there are some kind of phase transitions which cannot classify as a first or second order phase transitions as the *Kosterlitz-Thouless transition*. This new type phase transitions are characterized by some kind of *topological invariants* and the topological phases described by this invariants are robust against thermal effects or presence of impurities in the system. An example of this invariants is the Berry phase which is a non-trivial phase due to a smooth evolution of the system. In this work, we study the possibility of use the Berry phase to determine the critical points of quantum phase transition for some one dimensional systems. In particular, with aid of this topological invariant, we give a description of topological phase transitions in one dimensional models like Heisenberg model or the Su-Schrieffer-Heeger model for polyacetylene.

Biopolymer dynamics under an external shear flow studied by Brownian dynamics coarsed-grained simulations

AMAYA ESPINOSA, Helman Alirio [1]; APONTE-SANTAMARÍA, Camilo [1]

[1] Universidad de los Andes

The Von Willebrand factor (VWF) is a huge extracellular-protein biopolymer involved in hemostasis. It forms a hemostatic plug that stops bleeding by adhering platelets to sites of vascular injury. Hydrodynamic forces in the bloodstream impose a shear-stress over VWF that trigger its activation and thereby initiates the coagulation cascade.

In this work, we performed Brownian dynamics (BD) simulations at coarse-grained (CG) level resolution, to study the dynamics of VWF-like biopolymers containing specific molecular interactions under non-equilibrium conditions imposed by an external shear flow. For a randomly distributed constant density of specifically-interacting points within the polymer, the critical activation flow rate at which the biopolymer switches from a globular to a stretched conformation was established to be $5x10^{-5}$ ps^{-1}.

The obtained results will be used to complete the phase-diagram for biopolymers like VWF as a function of the strength of the molecular specific interaction, the density of interacting points within the polymer, and the flow-induced shear-rate.

Brazilian House of Representatives Analysis from Network Theory Perspective

MARENCO, Ludwing [1]; LENZ, Carlos [1]

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A new effective method for analysing a Representatives' system from the network formalism is presented. A matrix with the annual results of the roll - call vote of the Brazilian House of Representatives from 2007 to 2015 was constructed.

By measuring the correlation coefficient among the annual roll - call vote sets a Representatives' network was computed. For extracting the Minimal Spanning Tree of the Representatives' network general features of this system arises. Specifically, the concordance - opposition stance, the individual connections among Representatives, the partisan fidelity and a new way to identify the approved and disapproved draft bills, as well as, its time evolution are disclosed.

A well-defined correlation behaviour among Representatives is observed, in fact, we prove that five or six political parties are sufficient to encapsulate all political diversity in the Brazilian House of Representatives. In addition, we propose that the probability distribution of correlation values in the Brazilian House of Representatives is a combination of logistic distributions. Besides that, a new method for re-ordering correlation matrices based on the result of the Minimal Spanning Tree is enunciated.

Distribución de tamaño de islas con agregación obstaculizada

SANCHEZ MUÑOZ, Julian Andres [1]; GONZALEZ CABRERA, Diego Luis [1]; CAMARGO CHAPARRO, Manuel [2]

[1] Universidad del Valle

[2] CICBA, Universidad Antonio Nariño-Campus Farallones

Se estudia el efecto de la agregación obstaculizada en el proceso de formación de islas en un modelo unidimensional para crecimiento epitaxial con tamaño de núcleo crítico "i". En el modelo propuesto el proceso de agregación de un mónomero a una isla estable está limitado por una barrera de energía ε_a, caracterizada por una longitud característica l_a. Para l_a=0, las islas se comportan como sumideros perfectos de mónomeros y la agregación está limitada por difusión (DLA). Por otro lado, si l_a tiende a infinito, las islas se son, esencialmente, fronteras reflectivas perfectas y la agregación está limitada por reacción (ALA). A medida que se incrementa l_a, el sistema pasa suavemente de DLA a ALA. El efecto de la barrera de agregación se estudia por medio de la distribución de tamaño de islas, N_s. Esta distribución se obtiene por medio la solución de un conjunto de ecuaciones auto-consistentes basadas en una descripción aproximada de la nucleación. Los resultados obtenidos se comparan con aquellos encontrados por medio de simulaciones de Monte Carlos cinético. Se encuentra que el método auto-consistente describe apropiadamente N_s para diferentes valores de " l_a " e "i". Además la barrera ε_a tiene un efecto importante sobre N_s lo que permite, en principio, su determinación a partir de resultados experimentales.

Dyson model, exchange interaction and random graphs

ANDRAUS, Sergio [1]

[1] Chuo University

The Dyson model [1] is a multivariate stochastic process famous for its intimate relationship with the Gaussian random matrix ensembles. This model can be interpreted as a system of mutually repelling particles with a logarithmic potential, and it can be formulated as the eigenvalue process of a random matrix with Brownian motions as entries. This model can be generalized using the Dunkl differential-difference operators [2] to construct a generalized heat equation [3]. Due to the difference term in Dunkl operators, the Dunkl heat equation describes a stochastic process with particle trajectories equivalent in law to those of the Dyson model, but it includes an additional interaction term. This pair interaction exchanges the particles' positions randomly and spontaneously. Some of the properties of this interaction have been studied [4,5], but the physical meaning of the interaction remains unknown. In this presentation, we consider this interaction as a means of information transmission, and we examine its consequences. To this end, we focus on the statistical properties of information propagation in this scheme in terms of the dynamical formation of random graphs whose edges represent the exchange interactions occurred up to a given time, and we compare them with the properties of the most well-known families of random graphs.

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Effect of the lipid-protein interaction on the assembly process of the GPIb-IX complex

ORJUELA, Juan David [1]; APONTE-SANTAMARÍA, Camilo [1]

[1] Universidad de los Andes

Lipid-protein interaction are known to play key roles in living organisms. Not only protein function is altered by the surrounding lipids but conversely the proteins affect membrane behavior through its mechanical properties. Specifically, glycoprotein Ib\alpha (GPIb\alpha) forms a complex with GPIb\beta and GPIX to aid platelets' hemostasis effort, but its activity is poorly understood on a molecular level. There is evidence that suggest that lipids form a type of solvation shell which might act as a molecular glue, tethering the GPIb\alpha to the membrane under mechanical tension imposed by flows. We performed multiple microsecond coarse grained molecular dynamics simulations to observe the assembly process of the GPIX with the GPIb, identify the key residues of the interaction and test the complex's stability.

Emergence of the rho=1 Mott lobe in an anyon chain with three-body interactions

ARCILA-FORERO, Julian [1]; FRANCO, Roberto. [1]; SILVA-VALENCIA, Jereson [1]

[1] Universidad Nacional de Colombia

A quantum phase transition driven by the statistics was observed in an anyon-Hubbard model with local three-body interactions. Using a fractional Jordan-Wigner transformation, we arrived at a modified Bose-Hubbard model, which exhibits Mott insulator and superfluid phases. The absence of a Mott insulator state with one particle per site depends on the anyonic angle, and a quantum phase transition from a superfluid to a Mott insulator state is obtained for a fixed value of the hopping. The critical points were estimated with the von Neumann block entropy and increase as the hopping grows. The statistics modify the ground state, and three different superfluid regions were observed for larger values of the anyonic angle.

Entanglement in the Wigner-Weyl Representation

MURILLO MEJÍA, Miller Mateo [1]

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Despite being the first, among the fascinating set of quantum correlations that a quantum state of a composite system can display, to be identified, entanglement remains as the most intriguing one due to its central role in quantum information protocols. Even though it has being studied for the last three decades, the identification and quantification of entanglement remains an area of research. Recently, questions regarding the generation of entanglement under a classical dynamics have rise that can be better address in a phase space representation of quantum mechanics. In this work we present a review of the entanglement criteria and measures that can be formulated in the Weyl-Wigner representation, and discuss the advantages of the use of this representation for the study of entanglement in some quantum systems.

Modelamiento de fluidos inmiscibles a partir del método de Lattice Boltzmann

ACOSTA SEQUEDA, Juan Guillermo [1]; FLÓREZ JIMÉNEZ, Juan [2]; MUÑOZ CASTAÑO, Jose Daniel [3]

[1] Student

[2] Undergraduate Student

[3] Universidad Nacional de Colombia

En este trabajo se realiza un recuento del método de Lattice Boltzmann para modelar el comportamiento de dos fluidos inmiscibles en el régimen de bajos números de Reynolds y razones de densidades entre 1/10 y 10. En primer lugar, se muestra cómo se obtiene el modelo que simula el comportamiento de dos fases inmiscibles a partir del modelo que simula las ecuaciones de Navier-Stokes para una fase, y cómo se puede generalizar para n fases inmiscibles diferentes. A partir del modelo computacional se calculan variables macroscópicas, como la tensión superficial, la velocidad terminal de una burbuja al moverse dentro de un medio con presión inhomogénea, y el tiempo de decaimiento de una onda capilar. Se comparan varios de los resultados obtenidos con soluciones analíticas para estimar la precisión del modelo computacional y se plantean posibles mejoras para ser aplicadas en trabajos posteriores.

Quantum phase diagram of the AB2 fermionic chain

MURCIA CORREA, Luz Stefany [1]; Dr. FRANCO, Roberto [2]; Dr. SILVA VALENCIA, Jereson [2]

[1] Universidad Nacional de Colombia y UECCI

[2] Universidad Nacional de Colombia

In the current work we study the one-dimensional AB2 fermionic chains, where A is a lattice site with an energy level, and B is another site with a different energy level, which repeats 2-times in the unit cell. The halogen-bridged binuclear material R4[Pt2(P2O5H2)4X]•nH2O [Yam01] is described through these chains. It is important to point that these configurations can be done in the assemblage of ultracold atoms in which is possible to have a total control over the settings. We studied the AB2 chain using the density matrix renormalization group method (DMRG) for large finite system sizes L. Reconsidering the previous study performed by Torio et al. [TAJN06], in the 2006, for small lattice sizes. It was calculated the charge gap, spin gap, excitation gap, the spin and charge structure factors, ionicity, and the von Neumann entropy of the quantum theory of information, in order to characterize the fundamental ground-state of the system, in terms of the local interaction parameter (U) and the energy difference between the levels (Δ). We show that the average of the von Neumann local entropy and the block entropy, are right quantities that allows to differentiate a few stages of the model. Finally, it is concluded that the phases diagram of the AB2 fermionic chain presents two phases clearly identified. An insulating phase for small values of U, not paying attention to the value of Δ, and an insulating phase from Mott correlating for big values of U. However, it is possible to identify an intermediate phase between these two, for values of Δ and for the values less than Δ it was not possible to distinguish between the insulating region of a band and an intermediate region.

Spin-1 Bose-Hubbard model with two- and three-body local interaction

HINCAPIE, Andres [1]; Dr. SILVA-VALENCIA, Jereson [1]; Dr. FRANCO, Roberto [1]

[1] Universidad Nacional de Colombia

Using the density-matrix renormalization-group method, we studied the ground state of the one-dimensional S = 1 Bose-Hubbard model with local two- and three-body spin dependent and independent interactions. We observe a quantum phase transition from superfluid to Mott insulator state and draw the phase diagram for different parameters, recovering the asymmetry present with two-body interactions, we found that the density drives first-order (second-orded) superfluid-Mott insulator transitions for even (odd) lobes. The odd Mott insulator states were characterized with a dimerized pattern while the even ones were composed by singlets. Also, the all Mott lobes present a spin isotropy while superfluid states with even global density present a nematic order. A phase transition is reported in the superfluid phase increasing the density.

Study of Amino Acid Production Under Prebiotic Conditions Using Molecular Statistical Thermodynamics

BOURDON GARCÍA, Rubén [1]; ÁGREDA BASTIDAS, Jesús Alberto [2]

[1] Estudiante de doctorado en Ciencias - Química, Universidad Nacional de Colombia

[2] Profesor Asociado de la Universidad Nacional de Colombia

The amino acid production was a very important event for the origin of life. There are a lot of experiments, like Miller - Urey, and theoretical models to simulate the production of amino acids under early earth atmosphere conditions. In this work, we study the chemical potential of amino acid precursors and simple organic molecules which are important for the amino acid synthesis by the Strecker reaction. Chemical potentials of the species and reactions were calculated with molecular statistical thermodynamics, using independent electronic, vibrational, rotational and translational partition functions for atoms and molecules. As a test reliability of the method used for the calculations, the obtained chemical potentials of the simple an well known species contain an error less than 2% with respect to the values reported in the literature. Amino acid precursors and the Strecker reaction have an error in the chemical potential less than 40%. Which is acceptable for our purposes. With the tested tool for the thermodynamic calculations, we studied the direct and autocatalytic production of amino acids by the Strecker reaction in the standard reference conditions for gases (298.15 K and 101,325 Pa).

Conferences Friday Morning – 1st September 2017

Hunter-Gatherer Networks and Cumulative Culture

GÓMEZ-GARDEÑES, Jesús [1]

[1] Universidad de Zaragoza

Social networks in modern societies are highly structured, usually involving frequent contact with a small number of unrelated 'friends'. However, contact network structures in traditional small-scale societies, especially hunter-gatherers, are poorly characterized. We developed a portable wireless sensing technology (motes) to study within-camp proximity networks among Agta and BaYaka hunter-gatherers in fine detail. We show that hunter-gatherer social networks exhibit signs of increased efficiency for potential information exchange. Increased network efficiency is achieved through investment in a few strong links among non-kin 'friends' connecting unrelated families. We show that interactions with non-kin appear in childhood, creating opportunities for collaboration and cultural exchange beyond family at early ages. We also show that strong friendships are more important than family ties in predicting levels of shared knowledge among individuals. We hypothesize that efficient transmission of cumulative culture may have shaped human social networks and contributed to our tendency to extend networks beyond kin and form strong non-kin ties.

Human mobility at urban scale. Insights from Colombian cities.

LOTERO, Laura [1]

[1] Universidad Pontificia Bolivariana

Understanding how people move in the city is crucial for urban planning, public health and marketing, among others. One plausible way to represent this movement is by means of networks. In this presentation, I will introduce the urban mobility networks of three Colombian cities (Bogotá, Medellín and Manizales) constructed by using origin destination surveys. The networks account the trips from one zone of the city to others, including information of transportation mode, time and duration of trip and socioeconomic strata of travelers. Multimodality and social segregation were some of the patterns that emerged of the interaction of people moving though the Colombian cities under study.

Characterization of resilience in the network of Aedes-Aegypti mosquitoes in urban Zone

NARANJO, Fernando [1]

[1] Physics School UPTC

The Zika, Dengue and Chikunguña virus among others, is transmitted by the bite of the Aedes-Aegypti mosquito. The WHO warns the increase of these diseases in the coming years and since there is still no vaccine or specific treatment for these diseases, it is relevant to study the behavior of the mosquito population, versus control strategies. We present the Aedes Aegypti´s resilience study in urban areas of Colombia. We define the network based on the Skeeter-Buster model, where each node is represented by a niche of mosquitoes in the area. The state that defines the population of each node depends on the gonotrophic cycle of the species and the environmental conditions. The interactions between nodes are defined by the probability of migrating mosquitoes from one node to another and includes the mutualistic dynamics between nodes. The model also considers, the probability of creation of nodes, originated by the migrations of the vector.

We evaluate the topology of the network and calculate the measures of vitality of the complex network. We disturb the network, based on the effects about the reduction of mosquito population that generate the usual control mechanisms, like insecticides, for example. With these measures, we apply the universal resilience.

Tonal consonance and the rise of mesoscopic rules in the Marimba de Chonta music

USECHE, Jorge [1]; HURTADO, Rafael [1]; DEMMER, Federico [2]

[1] Department of Physics, Universidad Nacional de Colombia

[2] Conservatory of Music, Universidad Nacional de Colombia

Diverse macroscopic properties have been found in musical works, for example power law and exponential type distributions in complex networks of musical notes, Zipf law in musical interval frequency, and Levy distributions in correlations, among other. These properties indicate the presence of order due to rules acting at different levels; one example of these rules is the selection of the sounds for constructing a musical scale or tuning, based mainly on the consonance properties of the combination of sounds; another example is the suppression of combinations of sounds in a musical practice: the tritone was avoided or forbidden in Western sacred music from the Middle Ages to the late Renascence, due to its high dissonance level. In the traditional Marimba de Chonta music of the Pacific Coast of Colombia and Ecuador, declared intangible heritage of humanity by UNESCO, there is a set of tunings and interpretive practices that remain widely misunderstood and that are at risk of disappearing. In this talk we show how, based on the acoustic properties of a musical instrument, it is possible to understand the diversity of tunings of the Marimba de Chonta, and some interpretative practices in this music.

Controlling heat flow in nanoscale hybrid systems

RESTREPO, Juliana [1]

[1] Universidad EIA

Controlling heat flow has been a longstanding quest in solid state physics and a fundamental requisite for thermotronics. In this talk I will explore how to use nanoscale hybrid systems as possible candidates for thermal devices. In our work we consider a two level system weakly coupled to two reservoirs and investigate how their nature (normal metal, insulator and conventional superconductor) plays a role in determining the thermal characteristics of the device (JR, D. Oettinger, R. Chitra, Eur. Phys. J. B (2014) 87). We also consider the application of a Zeeman field in one of the metallic or insulating reservoirs and demonstrate how it can be used to augment rectification (M. Dominguez, JR, B. Rodriguez, R. Chitra, paper to be submitted).

Entanglement distribution in random states of identical particles

VIVIESCAS, Carlos [1]

[1] Universidad Nacional de Colombia

In contrast to the well developed and established theory of entanglement for distinguishable particles, and despite the numerous attempts and significant effort invested in it, an entanglement theory for states of indistinguishable particles still remains in a precarious condition. At this point, the main hurdles faced by the theory derive from the subtleties of the quantum correlations inherent to the statistical properties of states of indistinguishable particles.

In an attempt to illustrate basic differences between the nature of entanglement in systems of distinguishable and indistinguishable particles, we propose a measure for the entanglement of bipartite systems of indistinguishable particles which emerges as a natural extension of the G-concurrence; an existing monotone for NxN systems of distinguishable particles. As a first application of this measure we use it to characterize the entanglement distribution on particular ensembles of random states of high-dimensional bipartite systems of bosons and fermions, and compare it with known results for systems of distinguishable particles.

Time-Correlations as Probes of Quantum Order-Disorder and Topological Phase Transitions

GÓMEZ-RUIZ, F. J. [1]; MENDOZA-ARENAS, J.J. [1]; RODRÍGUEZ, F. J. [1]; TEJEDOR, C [2]; QUIROGA, Luis [1]

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[2] Departamento de Física Teórica de la Materia Condensada and IFIMAC, Universidad Autónoma de Madrid

We make use of two-time correlations (TTC) and Leggett-Garg inequalities (LGI) for probing quantum phase transitions. We focus on two different, but related, 1D systems which are candidates as quantum simulators: a chain of spins and a Kitaev model.

Starting with the thoroughly studied chain of spins we can check the capabilities of our procedure [1]. We show how purely local measurements allow to determine the quantum critical points not only of finite-order transitions but also those of infinite-order as the Kosterlitz-Thouless transition, a task not always easy with usual methods. By means of matrix product simulations of one-dimensional XXZ and XY models, we argue that finite-order quantum phase transitions can be determined by singularities at criticality of the TTC or their derivatives as well as by Leggett-Garg functions. Violation of the LGI for early times allow us to characterize an infinite-order transition of the XXZ model.

With all this baggage, we study the transitions from normal to topological phases in a Kitaev chain. Now the dichotomic magnitude to be measured is the fermion local occupation. Again, TTC show characteristic features when Kitaev chain supports Majorana zero modes. Violations of LGI are evaluated for different qubits formed by pairing local and non-local Majorana fermions in order to get insight on the physical properties of the system. We obtain analytical results which allow us to understand the fundamental aspects of TTC in topological Kitaev chains.

Finally we study the effects of coupling a cavity mode to the quantum states of the Kitaev chain.

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Conferences Friday Afternoon – September 1st 2017

Brownian Carnot Engine

R. PARRONDO, Juan Manuel [1]; MARTÍNEZ, Ignacio A. [2]; ROLDÁN, Édgar [3]; DINIS, Luis [4]; PETROV, Dmitri [5]; RICA, Raúl A. [6]

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[6] U. Granada

At the microscale, the energy transfer between a system and its surroundings becomes random and a new theoretical framework ---stochastic thermodynamics [1]--- is necessary to account for those fluctuations. In particular, stochastic thermodynamics can be used to analyze the performance of small motors, like Brownian engines or molecular machines. Here we will report on a recent experiment that reproduces the Carnot cycle with a single Brownian particle as working substance [2]. The experiment uses optical tweezers to confine the particle and a noisy electrostatic force to mimic a high temperature reservoir. To analyze this Brownian Carnot engine, we will review some basic aspects of stochastic thermodynamics and discuss fundamental differences between driven and autonomous machines that arise from their behavior under time reversal [3].

Derivative principle: a powerful tool for joint eigenvalue distributions in unitarily invariant random matrix ensembles.

BOTERO, Alonso [1]

[1] Universidad de los Andes

In unitarily invariant RMT ensembles, a surprising connection can be established between the joint distribution of the diagonal elements of the matrix and the joint eigenvalue distribution (JED). The resulting formula proves to be a powerful tool in analyzing the JED for various random matrix ensembles, particularly when the matrix elements exhibit correlations. I will show how the connection can be established using the well-known Harish-Chandra-Itzykson-Züber integral, and how for many practical applications, the computation of the JED can be reduced to the calculation of a multidimensional complex integral. Finally, I will give some illustrative applications, including the GUE and ensembles of interest in Quantum Information theory, such as the ensemble of reduced density matrices from multipartite pure states and the ensemble of the difference between two random reduced density matrices.

Island formation on one-dimensional colloidal substrates

GONZÁLEZ, Diego Luis [1]; CAMARGO, Manuel [2]

[1] Universidad del Valle

[2] CICBA, Universidad Antonio Nariño

We study the island formation in a colloidal model for epitaxial growth. The model consists on a two-dimensional colloidal suspension where colloidal particles are slowly deposited on a one-dimensional substrate due to the influence of an external field. The particles interact with each other through a short-range pair interaction potential. Once the particles are deposited on the substrate they can laterally diffuse on it forming islands. We consider isotropic and anisotropic interactions for the homoepitaxy and heteroepitaxy cases. The time evolution of the system is described in terms of the densities of islands and monomers. The capture zone distribution (CZD) and the island size distribution (ISD) are also used to describe the growth properties of the system. The numerical results obtained from simulations based on molecular dynamics are compared with those of an analytical model based on an approximate description of the island formation on the substrate. We found that in spite of the low diffusion rates colloidal systems allow the formation of very well controlled structures. For this reason, the use of colloids in epitaxial growth is a promising alternative for growth of structures with size and shape control.

Amphiphilic star-like polymers in linear shear flow

JARAMILLO-CANO, Diego Felipe [1]; LIKOS, Christos N. [1]; CAMARGO, Manuel A. [2]

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[2] CICBA, Universidad Antonio Nariño, Cali, Colombia

Telechelic star polymers (TPSs) are macromolecules formed by a number of amphiphilic diblock copolymers (arms) anchored to a common central core, being the internal monomers solvophilic and the end monomers solvophobic. Very recent studies have demonstrated that TPS constitute self-assembling building blocks with specific softness, fictionalization, shape and flexibility: depending on different physical and chemical parameters, e.g. number of arms (functionality), solvophobic-to-solvophilic ratio (amphiphilicity), temperature, and solvent quality. In equilibrium, the geometrical conformation of TSPs features a well defined number of attractive spot on their surface and therefore they can be considered as very tunable soft-patchy colloids, which can lead to the formation of well-controlled ordered and disordered phases in soft condensed matter systems.

We systematically analyze the behavior of one isolated TSP under linear shear flow by means of a hybrid simulation scheme, which employs Multi-Particle Collision Dynamics (MPCD) for the solvent and standard Molecular Dynamics (MD) for the monomers forming the polymer. We evaluate shape descriptors of the star and distinctive features of the assembled patches per star as a function of the shear rate for a wide range of control parameters. We study how shear rate affects the number and the size of the patches depending on the amphiphilicity and the solvent quality. Since the conformation of a single TSP is expected to be preserved in low-density bulk phases, the presented results are a first step in understanding and predicting the rheological properties of semi-dilute suspensions of this kind of polymers.

The jellium model for systems of charged colloids

ALVAREZ, Carlos [1]

[1] Universidad del Rosario

Colloidal systems of charged particles appear in a wide range of both natural and artificial systems of great scientific and technological importance, like protein suspensions and paints. For this reason they have been studied extensively, starting with the DLVO theory for the stability of liophobic colloids in the decade of the 40s. In this talk I will present some recent work on the mean field jellium theory for systems of charged colloids and its comparison to molecular simulation data. The numerical methods used for solving the equations of the mean field theory and for carrying out the simulations will be presented as well.

Oral contributions Friday Afternoon – September 1st 2017

Ensamble de Estructuras a Nivel Mesoscópico: Formación de Fibras

ARANGO RESTREPO, Andrés [1]; BARRAGÁN, Daniel [1]

[1] Universidad Nacional de Colombia

Los procesos de auto-ensamble se encuentran en la naturaleza y en aplicaciones tecnológicas. Estos procesos tienen lugar en sistemas a escala molecular elemental hasta escala cosmológica, los cuales se llevan a cabo fuera del equilibrio termodinámico, formando estructuras a partir de bloques fundamentales discretos.

Sin embargo, se conoce muy poco sobre estos procesos y se carece de teoría basada en el ensamble de componentes discretos (bloques) para describir el fenómeno de auto-ensamble. Por ende se desea entender un poco más el fenómeno de auto-ensamble de estructuras mediante el formalismo de la termodinámica mesoscópica de no-equilibrio (MNET, siglas en inglés), en el cual las estructuras se ensamblan de manera secuencial. En particular, se desea estudiar en un sistema molecular fundamental isotérmico la dinámica de la formación de fibras lineales.

Mediante el formalismo de la MNET, se obtiene un sistema de ecuaciones tipo Fokker-Planck acopladas. Al resolver el sistema se obtiene la densidad de probabilidad de encontrar una estructura compuesta por n bloques, brindando información sobre el comportamiento dinámico del ensamble de las estructuras. Además a partir de estos resultados se calcula el tamaño promedio de las fibras ensambladas y el número de estructuras con n bloques por unidad de volumen

Adicionalmente, si se consideran variables independientes como la orientación de las fibras respecto a un eje perpendicular u otras coordenadas de proceso describiendo procesos paralelos en cada paso del ensamble, podría dilucidarse un poco más sobre la micro-arquitectura interna de las estructuras ensambladas.

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