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Editorial: 50 years of Statistical Physics in Mexico: Development, State of the Art and Perspectives

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Editorial on the Research Topic

50 years of Statistical Physics in Mexico: Development, State of the Art and Perspectives

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In the autumn of 1971, the small group of physicists then working at the Instituto Mexicano del Petróleo (IMP), in Mexico City, was expecting the visit of several distinguished scientists from abroad, who had been invited for talks and seminars on various topics of Statistical Physics. The Mexican physicists at IMP realized that it was an excellent opportunity to organize a meeting on the subject; it could be held the coming January, when most of the would-be speakers were available. Nevertheless, no formal organizing committee was appointed. Leopoldo García Colín, then director of the Applied Research Division at IMP, oversaw the whole operation, made the formal invitations and secured the financial support from IMP. The meeting itself was organized by Fernando del Río, who was assisted by his then Ph.D. student, Luis Mier y Terán, and by Sigurd Larsen, who was on sabbatical stay at the Institute.

Besides a few Mexican speakers who joined the visitors from abroad, the participants in that meeting were mostly graduate students who were working on the subject. By a combination of sheer luck and common sense, the meeting was planned to be held at Oaxtepec, a lush site about 70 km south of Mexico City that boasts a spring-like weather all year round. The meeting had no title nor name, and nobody foresaw that it would become a yearly event, nor thought to take a group photograph. Among the foreign speakers on that (first) meeting were Melville Green, Sigurd Larsen, Joel Lebowitz, Anneke Sengers, Jan V Sengers, and Robert Zwanzig. The meeting had a wide success. The talks were of the highest quality, and the ample time available and pleasant surroundings was profited by the young Mexican students, who interacted closely with the speakers. This success spurred the decision to organize a yearly event every winter. Since then, 49 meetings have been held, the last one in January 2020. This year should have seen the 50th, but it was suspended due to the Covid pandemic. The Winter Meeting on Statistical Physics (WMSP) constitute the series of physics gatherings of longest standing in Mexico, and have been a valuable asset in promoting the growth and consolidation of the discipline. In these 50 years, Statistical Physics in Mexico has grown from a single site of research and a handful of practitioners to almost twenty centers around the country and hundreds of scientists.

The present collection aims to commemorate the long standing tradition of the WMSP. It begins with a review of molecular-based equations of state. Regardless of how they are derived (experimental data or simulation results) when obtained from statistical mechanics; these equations are labeled molecular-based. In this work, a general scheme for the derivation of truly perturbed equations is presented. Two approaches are identified, Bottom-up and Top-down, and individual steps are discussed in detail along with several rules, reflecting the fundamentals of fluid physics. To exemplify these approaches, the author shows some well-established theoretical approximations, such as the Statistical Association Fluid Theory, to study the equation of state for water.

During the last decades, thermodynamic properties of model fluids have been studied using theoretical tools of Statistical Physics. As an example of the contribution of the Mexican community on the development of accurate approximations to account for the phase behavior of molecular fluids, López de Haro and Rodríguez Rivas solved the equation of state of a parabolic-well fluid combining both a second-order thermodynamic perturbation theory and molecular simulations.

Next, an investigation about the intermediate phase in glasses via a lattice gas model with a modified Hamiltonian considering different energies for cycles of connected atoms (glass with contaminants that form rigid and flexible structures) is presented. Authors study density transitions as a function of chemical potential and a parameter representing the quantity of contaminants. Finally, using hysteresis loops over these quantities they calculate the heat flow of the system, showing that the model present an intermediate phase, minimizing the non-reversing heat flow.

Statistical Physics often use the tools of Quantum Mechanics, but the converse is also true. In a macroscopic system in equilibrium, the probability for a system to occupy a given state is proportional to $\exp(-E/k_B T)$ (Boltzmann factor) where E is the energy of that state and $k_B T$ the kinetic energy. This result can be obtained by maximizing entropy while constraining the energy. On the other hand, the amplitude for a quantum system undergoing a given path is proportional to $\exp(-S/i\hbar)$ (Feynman factor) where S is the action of that path. The similarity between both factors raises the question about the quantum analog of entropy. This quantity is called "quantropy." Here, an extension of quantropy is presented in an integrated version.

Brownian particles have drawn the attention of physicists since the beginning of the last century. Recently, it has been seen that the diffusion of this type of particle is affected when the system is near a jammed state or in the presence of external potentials. This change in dynamical behavior where the particles slow down or accelerate occurs in certain time regimes. In this article, authors report experimentally and numerically different time regimes of a single, colloidal particle diffusing under the influence of a periodic optical potential. They show that the time at which a regime change occurs depends only on the height of the periodic potential.

Soft condensed matter is well represented in this volume. For instance, Vázquez-Vergara et al. investigated the relaxation dynamics of resonances in viscoelastic microfluidics. Aside from their theoretical importance as models for non-equilibrium phenomena in non-Newtonian hydrodynamics, pulsatile flows of viscoelastics have important applications in nano-fabrication and lab-on-a-chip devices. Experimental analysis of a viscoelastic zero-mean flow slug subjected to periodic pulses allow the authors to propose and validate a model for the constitutive equations. Delicate experimental measurements of the hydro-mechanical properties of DMPC/Cholesterol mixed monolayers were performed by Bañuelos-Frías et al. via Langmuir force determination and Brewster angle microscopy. Measurements were made under physiological concentration and pH conditions, leading to further advances in the understanding of why double chain lipids are better than single chain lipids to made up the cell membrane.

Structured soft condensed matter presents challenges to statistical mechanical modeling. Among these challenges, self-assembly of liquid crystals in constrained fields is relevant due to theoretical and practical reasons. The study of the nonlinear dynamical equations for coupled conserved and non-conserved fields describing nanoparticle concentration and liquid crystal order parameters under such conditions was also discussed here. The team lead by Guzmán, tackled this question by writing down these equations and solving them for bidimensional domains to determine approximate relaxation dynamics for the order parameter of the liquid crystal. Assembling dynamics are also at the center of the manuscript by Valadez-Pérez et al. Reversible aggregation of purely short-ranged attractive colloidal particles led to cluster formation with fractal-like morphology. Authors found that the fractal dimension of competing interaction fluids does depend on the second virial coefficient, as in the purely attractive case. And that the addition of repulsive forces in the potential between colloids changes the clustering morphology.

Propagation of topological defects in self-assembly liquid crystals is of particular interest in the production of metamaterials. Three-dimensional topological properties of liquid crystals had much of the attention through the two-dimensional variants are of interest from a theoretical and technological point of view. Calderon-Alcaráz et al. present molecular dynamics simulations to study strongly confined two-dimensional liquid crystals. The impact of constrained geometries on the phase diagram and the appearance of prominent topological defects are analyzed in detail.

Pattern formation and aggregation were also studied in relation to chocolate surfaces. Delgado et al. applied topography atomic force microscopy and cone-plate rheometry to experimentally characterize temperature-dependent pattern formation dynamics of melted chocolate with and without additives (sugar and lecithin), as well as 2D computer simulations of the polymorphic phase molecules under the *NVT* ensemble using a Mie-segmented coarse-grained potential. Experimental and simulation results showed agreement with the Avrami model for aggregation based on phase change kinetics. These observations led to predict sizes for chocolate grains which compare accurately with real sizes.

When colloids are confined to non-flat and closed geometries, they experience curvature effects that can induce new phenomena in the static and dynamical properties not seen typically in flat and open spaces. In the particular case of interacting colloids diffusing on a spherical surface, Ledesma-Durán et al. provide evidence that the different dynamical transitions observed at the level of the mean-square displacement can be explained in terms of the existence of an entropic potential that limits the number of accessible states to the colloids. Furthermore, colloids are a class of soft materials that also serve to understand fundamental questions in Statistical Physics. One of the latter concerns with the validity of some thermodynamic processes at the molecular level. In his contribution, Gómez-Solano reviews and describes both the operation and performance of a colloidal heat engine under finite-time Stirling cycles.

Single-file diffusion refers to transport of particles in narrow channels such that mutual passage is excluded. This degree of confinement induces a kind of anomalous diffusion as a result of the correlation between particle displacements. To further understand the diffusive behavior in quasi-one-dimensional channels, Huerta et al. report on molecular dynamic results of the collective dynamics in a system made up of hard disks. The results show that the transverse excitations obey very specific dispersion law associated to optical transverse modes, not typically seen in both $1D$ and $2D$ cases.

Since the birth of Statistical Physics, it has contributed to the development and growth of other branches of science, such as Mathematics, Chemistry and Ecology, just to mention a few examples. This fundamental aspect has brought the possibility of applying the tools and methods of the Statistical Physics in multidisciplinary problems. In his contribution, Hernández-Lemus nicely summarizes the main elements and aspects of the modern theory of random fields and discusses in detail some of its recent applications not only in Physics, but also in Biology and Data Science; applications that will serve to better understand problems of interdisciplinary character. Among the other applications of Statistical Physics is the study of how DNA compact within cells, or a biopolymer can be encapsulated. Linear chains of molecules are called semiflexible polymers, these include DNA, biopolymers, or common polymers like polyester. Castro-Villareal and Ramirez develop the theory to study semiflexible polymers in the 3-dimensional domain, applying their results via Monte Carlo simulations to the case of a an open domain, an sphere and a cube, where they observe a shape transition in the polymer for the closed domains, one state where the mean square distance from end-to-end exhibits an oscillating behavior, and the other exhibits a monotonic behavior.

Hopefully, the content of this issue will allow the reader to witness the qualitative growth, geographical expansion and maturity reached by Mexican researchers in Statistical Physics, plus the very welcome contribution from abroad. We can be confident that these Winter Meetings will continue to be held for many years ahead, for this discipline is foundational to an increasing number of fields, and young students and mature researchers alike will certainly continue profiting and enjoying the interaction with their peers from around the world.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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