

CMSP - Section Meeting

3rd to 5th of May 2023 @ Kastler lecture hall (Adriatico)

Organizers: Titas Chanda (tchanda@ictp.it), Dhanshree Pandey (dpandey@ictp.it), Zhi Li (zli@ictp.it), Gerald Fux (gflux@ictp.it), Federica Delconte (cm@ictp.it)

Schedule

3rd of May, 2023 — Wednesday

Time	Duration	Speaker	Title
14:00-14:15	15 mins	Welcome	
Chair: Uriel Morzan			
14:15-15:00	45 mins	Martina Stella	Towards accurate excitation energies in supramolecular systems: combining T-CDFT and fragments in the BigDFT code
15:00-15:45	45 mins	Roberto Verdel Aranda	Data mining in many-body physics: from critical behavior to universal dynamics
15:45-16:15	30 mins	Coffee break	
Chair: Roberto Verdel Aranda			
16:15-16:45	30 mins	Giulia Sormani	Zirconium Coordination Chemistry in presence of Hydroxymate-based chelators: Insights from Molecular Dynamics
16:45-17:15	30 mins	Zejian Li	Phase transitions in open quantum systems
17:15-17:45	30 mins	Titas Chanda	Quantized bubble nucleations

4th of May, 2023 — Thursday

Time	Duration	Speaker	Title
Chair: Giulia Sormani			
9:30-10:00	30 mins	Zhi Li	Phase diagram of pure iron at Earth's core conditions from deep learning
10:00-10:30	30 mins	Mikheil Tsitsishvili	Measurement induced transitions in partly monitored free fermion ladders
10:30-11:00	30 mins	Edward Donkar	Unsupervised Machine-Learning of Water Structure at the putative liquid-liquid critical point
11:00-11:30	30 mins	Coffee break	
11:30-12:15	45 mins	Uriel Nicolas Morzan	Turning up the heat can give us a lesson on drug discovery
12:15-12:30	15 mins	Group photo at Adriatico terrace	
12:30-14:15	1:45 hours	Lunch at Adriatico	
Chair: Colin Egan			
14:15-14:45	30 mins	Dhanshree Pandey	Cluster expansion extended to W-Ta-Vacancy Multi-component Alloy
14:45-15:15	30 mins	Nishan Ranabhat	Probing dynamical confinement in spin model with temperature
15:15-15:45	30 mins	Wen-Jin Yin	The structural evolution and CO ₂ catalytic properties of 2D Materials TMDs from first-principles study
15:45-16:15	30 mins	Coffee break	
Chair: Zhi Li			
16:15-16:45	30 mins	Anna Delmonte	The Quantum Kuramoto Model
16:45-17:15	30 mins	Solana Di Pino	Unsupervised learning of the excess proton structure in bulk water
17:15-17:30	15 mins	Debarshi Banerjee	Development of a computational toolbox to analyse first-passage times and diffusion coefficients in heterogeneous soft-matter systems

5th of May, 2023 — Friday

Time	Duration	Speaker	Title
Chair: Martina Stella			
09:30-10:00	30 mins	Anton Kutlin	Bridging the gap: a phenomenology of level repulsion in random matrices
10:00-10:30	30 mins	Khatereh Azizi	Investigating the microscopic nature of the solvation and hydrophobicity in aqueous solutions from cavity shapes
10:30-11:00	30 mins	Rajat Kumar Panda	Spectral PCA Entropy: Ising models
11:00-11:30	30 mins	Coffee break	
11:30-12:15	45 mins	Colin Egan	The Alchemist's Guide to Free Energy Decompositions
12:15-13:15	1 hour	Lunch at Adriatico	
13:15-14:00	-	Transport to Duino Castle	
14:00	-	Guided Tour @Duino Castle	

Abstracts — 3rd of May, 2023 — Wednesday

Martina Stella

Towards accurate excitation energies in supramolecular systems: combining T-CDFT and fragments in the BigDFT code

Despite the variety of available computational approaches, state-of-the-art methods for calculating excitation energies such as time-dependent density functional theory (TDDFT), are typically computationally demanding and thus limited to moderate system sizes. Thanks to a new variation of constrained DFT (CDFT), implemented in the BigDFT code and recently published by our group, we have shown to be able to robustly model both local and charge-transfer excitation energies with a comparable precision to TDDFT for local excitations, while not exhibiting the typical limits of standard TDDFT for charge-transfer states, for a computational cost close to Δ SCF. As T-CDFT is implemented within the linear scaling formalism it is naturally suited to be paired with the fragment approach already available in the BigDFT code. By properly combining these two infrastructures, one can use TCDFT to impose excitations on particular fragments in supramolecular systems. In the example of local excitations on a molecule (fragment) in a given environment, where no strong coupling with the environment is expected, the constraint could be imposed between orbitals associated with the target fragment only, while still treating the full system at DFT level. In this talk, after a brief introduction of DFT and its variations, I will show how the aforementioned approach allows the exploration of explicit environment effects on excitation energies in systems such as TADF materials, paving the way for future simulations of excited states in realistic morphologies.

Roberto Verdel Aranda

Data mining in many-body physics: from critical behavior to universal dynamics

In this talk, I will give a general introduction to the field of data mining in many-body physics, going from standard techniques such as principal component analysis to state-of-the-art non-parametric learning methods and network theory. I will then illustrate how one can use such data-driven approaches to extract and discover information in large data sets associated to many-body problems. Concretely, I will consider the unsupervised learning of phase transitions in classical Ising models and the assumption-free discovery of relevant information in experiments on dynamical properties of Bose-Einstein condensates.

Giulia Sormani

Zirconium Coordination Chemistry in presence of Hydroxamate-based chelators: Insights from Molecular Dynamics

In the last decade, there has been a growth in using Zirconium-89 (^{89}Zr) as a radionuclide in nuclear medicine for cancer diagnostic imaging and drug discovery processes. One of the most popular chelators for ^{89}Zr , is desferrioxamine (DFO) which acts as a hexadentate ligand, although numerous studies have questioned its in-vivo stability in cellular environments. The microscopic mechanisms underlying this observation has primarily been informed by DFT-based calculations which typically ignore temperature and therefore entropic and dynamic solvent effects. In our work, free energy calculations using molecular dynamics simulations, where the conformational fluctuations of both the ligand and the solvent are explicitly included, are used to compare the binding of Zr^{4+} cation with two different chelators, DFO and 4HMS, the latter of which has been recently proposed as a better chelator. We find that thermal induced disorder leads an open hexadentate chelate structure of Zr^{4+} -DFO complex, leaving the Zr^{4+} metal exposed to the solvent. A stable coordination of Zr^{4+} with 4HMS, however, is formed involving both hydroxamate groups and water molecules in a more closely packed structure.

Zejian Li

Phase transitions in open quantum systems

Phase transitions are common yet intriguing phenomena that we encounter in everyday life. For example, solid ice can melt into liquid water, which is a phase transition driven by thermal fluctuations that occurs at equilibrium. On the other hand, open quantum systems, i.e. those that are in contact with an external environment, can exhibit dissipative phase transitions that are far from equilibrium. These are known as dissipative phase transitions, whose physics is decided by the rich interplay between the quantum fluctuations and drive / dissipation from the environment. I will first present an experimental (therefore non-technical) investigation of a dissipative phase transition of photons [1], where we proposed a way to observe the effect of spatial dimension on this transition, that was confirmed by our experimentalist collaborators. I will explain why such experiment is in principle not difficult, and then briefly discuss our ongoing work on another type of phase transitions known as measurement-induced phase transitions, which are much harder to detect in experiments.

Titans Chanda

Quantized bubble nucleations

Non-equilibrium dynamics of slow quenches across continuous phase transitions have been understood very successfully under the unifying theory of the Kibble-Zurek mechanism. However, relatively less attention has been paid to the understanding of dynamics across first-order quantum phase transitions (FOQPT). In an attempt to mitigate this, here we will talk about the consequences of a slow dynamical ramp across the FOQPT transition line present in the Ising model with both transverse and longitudinal fields. The existence of a potential barrier, quintessential to the FOQPTs, gives rise to metastability in the dynamical state. We find that in the considered model, such metastability wears off by nucleating bubbles of the true ground state driven by quantum fluctuations. Specifically, we identify special resonant regions in the longitudinal field, where the metastable state can easily tunnel to nucleate bubbles of specific sizes. Further, we will describe our attempt to explain the entire non-adiabatic process under the unifying umbrella of Landau-Zener theories.

Abstracts — 4th of May, 2023 — Thursday

Zhi Li

Phase diagram of pure iron at Earth's core conditions from deep learning

Iron is considered to be the main component of the Earth's core. Substantial efforts have been made to understand its phase diagram and physical properties at extreme conditions. However, it remains debated about how the atoms in solid iron are arranged at Earth's core conditions, where possible candidates include hexagonal close-packed (hcp), body-centered cubic (bcc), and face-centered cubic (fcc) structures. As crystal structure and physical properties are closely related, there is also a significant uncertainty in the properties of Earth's core, such as elasticity, heat conductivity, and density, making the accurate interpretation of seismic observations difficult. Here we aim to study the phase stability of solid iron at Earth's core conditions. For this, a deep-learning interatomic potential was developed with ab initio accuracy but is more cost-effective. To further check the performance of such potential, we examine the elastic and plastic behaviour of hcp iron and the effects of structural defects at inner core conditions [1]. We then compute the Gibbs free energy of the bcc, fcc, hcp and liquid phases by performing large-scale molecular dynamics simulations. The calculated free energy allows for determining the phase stability of solid iron in Earth's core[2].

1. Li, Z., & Scandolo, S. (2022). Elasticity and viscosity of hcp iron at Earth's inner core conditions from machine learning-based large-scale atomistic simulations. *Geophysical Research Letters*, 49, e2022GL101161
2. Li, Z., & Scandolo, S. (2023), submitted.

Mikheil Tsitsishvili

Measurement induced transitions in partly monitored free fermion ladders

In recent years there has been great interest in the role of quantum entanglement in phase transitions of many-body systems. In this talk, I will present some results obtained on the entanglement transition that arises from unitary evolution (which builds up entanglement) and dissipative measurements that destroy coherences. In particular, I will discuss what happens when the measurements arise from a non-Markovian environment, in contrast to the Markovian case studied so far in the literature. I will briefly demonstrate the coexistence of measurement induced phase transition and non-Markovian dynamics, using the example of random unitary circuit and partly monitored free fermion ladder.

Edward Danquah Donkor

Unsupervised Machine-Learning of Water Structure at the putative liquid-liquid critical point

Hydrophobic interfaces are integral to both chemical and biological systems and are found throughout nature. Despite their importance, understanding the local structure of water near hydrophobic surfaces remains a challenge. This work uses state-of-the-art statistical techniques and unsupervised clustering methods to characterize water structure at hydrophobic interfaces and in the supercooled regime. We demonstrate that local atomic descriptors used in machine learning to describe waters' local environment differ from commonly used chemical-intuition-based order parameters like tetrahedrality. These findings have implications for understanding the nature of local structural fluctuations close to the putative second liquid-liquid critical point under supercooled conditions, highlighting the importance of non-local structures. Additionally, we identify the structural fingerprints of water near air and oil interfaces, providing a comprehensive characterization of water near hydrophobic surfaces. This approach offers a new framework for re-examining textbook notions of the physical chemistry of solvation.

Uriel Nicolas Morzan

Turning up the heat can give us a lesson on drug discovery

Allosteric drugs have the potential to revolutionize biomedicine due to their enhanced selectivity and protection against overdose. However, we need to better understand allosteric mechanisms in order to fully harness their potential in drug discovery. In this seminar I will present a molecular dynamics study, combined with unsupervised learning techniques, that investigates how increases in temperature affect allostery in imidazole glycerol phosphate synthase. Results demonstrate that temperature increase triggers a cascade of local amino acid-to-amino acid dynamics that remarkably resembles the allosteric activation that takes place upon effector binding. The differences in the allosteric response elicited by temperature increase as opposed to effector binding are conditional to the alterations of collective motions induced by either mode of activation. This work provides an atomistic picture of temperature-dependent allostery, which could be harnessed to more precisely control enzyme function.

Dhanshree Pandey

Cluster expansion extended to W-Ta-Vacancy Multi-component Alloy

Tungsten (W) is considered to be the leading plasma facing materials (PFM), with high melting temperature, low erosion rates, etc. Unfortunately the above merits are coupled with very low fracture toughness characterized by brittle failure regimes, etc. A possible way of overcoming these problems consists of the identification of alloying elements [1]. In alloys, however, the formation energy depends on the local arrangement of different atoms around the vacant sites. Hence the vacancy concentration should be a function of alloy composition. Thus, in the present study, we treat the mono-vacancies as an extra 'chemical' component of the W-based alloy. Hence, in this study, the phase diagram of W-Ta-Vacancy (WTaVac) is calculated using a combination of first-principles energy methods and Monte Carlo simulations. First-principles total-energy calculations of different ordered arrangements (more than 400 structures) of W/Ta and mono-vacancy within the bcc W host are performed. These energies are then used to parametrize a cluster expansion that describes the energy of the WTaVac system in terms of an Ising-like Hamiltonian. The structures that are actually stable at low temperature out of this large set are found by constructing the convex hull of the formation energies. A well-converged cluster expansion then used in Monte Carlo (MC) simulations to calculate thermodynamic properties.

[1] O. El-Atwani et al., *Sci. Adv.*, 5, eaav2002 (2019).

Nishan Ranabhat

Probing dynamical confinement in spin model with temperature

Confinement as observed in high energy physics clumps together quarks into hadron. A similar signature of confinement is observed in many-body quasi 1D systems (chains and ladders) where a pair of quasi-particles are confined into a bound state that typically travel slower than the free quasi-particles thus hindering the propagation of correlation in the system. Long range Ising chain is one such model where the effects of confinement in a non-equilibrium setup has been observed. In this study we probe confinement by initializing the system as non-trivial thermal states and observe the effect of confinement following a global quench. We also introduce kink density as a suitable order parameter to study such a problem and show that the variance of kink density acts as a signature showing a smooth transition from confined to de confined regimes.

Wen-Jin Yin

The structural evolution and CO₂ catalytic properties of 2D Materials TMDs from first-principles study

Abstract: The electronic property is mainly determined by the structure configuration of the materials. Thus, understanding the structural behavior such as evolution, is important. Here, taking Janus MoSSe as a representation, the evolution process from MoS₂ is systematically investigated by first-principles calculation. The simulation shows that the evolution process of the structure is related to the crystal field involved in the structure. On the other, the application of the 2D material on CO₂ reduction is also investigated. It is interesting to find that surface modification can effectively improve the product efficiency and selectivity.

Anna Delmonte

The Quantum Kuramoto Model

Spontaneous synchronization is a collective phenomenon that can be observed in many-body interacting systems across many different fields, such as physics, biology, technology, and social sciences. With the recent advancements in the field of quantum technologies, synchronization can now be observed in the quantum regime. Understanding this collective phenomenon in the quantum realm has become increasingly important, and theoretical models are still lacking. In the classical case, a prototypical example of synchronization is given by the Kuramoto Model, a model describing a system of interacting rotors. Its phase diagram supports both a dynamically disordered phase and a synchronized one. In this talk, I will introduce the phenomenon of spontaneous synchronization and discuss the classical Kuramoto model and its relevant findings. Then, I will propose a generalization of this model to the quantum realm, the Quantum Kuramoto Model. Finally, I will conclude by highlighting the differences in behavior between the classical and quantum regimes.

Solana Di Pino

Unsupervised learning of the excess proton structure in bulk water

We studied the structure of the excess proton in HCl solutions using Ab Initio molecular dynamics (AIMD) and Path Integral AIMD (PI-AIMD). In order to do so, we analyzed the local environment of all oxygen atoms in the trajectory using Smooth Overlap Atomic Positions (SOAP) descriptors. Then we combined this description with unsupervised learning clustering algorithms (Density Peaks Advanced) so as to identify different types of structures in the system. This way we were able to find protonated molecules structures and compared them to the two most common configurations proposed to describe the excess proton in water.

Debarshi Banerjee

Development of a computational toolbox to analyse first-passage times and diffusion coefficients in heterogeneous soft-matter systems

The analysis of first-passage time statistics in soft-matter systems, such as water near amino-acid crystals ¹, can be vital in understanding the dynamical complexity of their chemical and geometrical properties. From the first-passage time statistics of water molecules, it is possible to infer space-dependent diffusion coefficients in directions normal to various phase boundaries ^{1,2}. The analysis developed in the cited work is highly-nontrivial, computationally expensive, and system-dependent. Here, in an interdisciplinary collaboration between statistical physics and atomistic simulations, we developed a generic computational methodology³ which allows us to extract and analyse trajectories, obtained from molecular dynamics simulations by programs such as GROMACS or LAMMPS, to determine first passage times and spatially resolved diffusion coefficients. We parallelised the program to take advantage of high-performance computing facilities, and performed exhaustive benchmarks of our algorithm in various aqueous systems. Finally, we investigated a novel system with non-trivial behaviour (curcumin crystals), to see if our methodology could accurately predict the observed dynamics.

(1) Belousov, R.; Qaisrani, M. N.; Hassanali, A.; Roldán, É. First-Passage Fingerprints of Water Diffusion near Glutamine Surfaces. *Soft Matter* 2020, 16 (40), 9202–9216. <https://doi.org/10.1039/D0SM00541J>.

(2) Belousov, R.; Hassanali, A.; Roldán, É. Statistical Physics of Inhomogeneous Transport: Unification of Diffusion Laws and Inference from First-Passage Statistics. *Phys. Rev. E* 2022, 106 (1), 014103. <https://doi.org/10.1103/PhysRevE.106.014103>.

(3) Banerjee, D. Development of a Computational Toolbox to Analyse First- Passage Times and Diffusion Coefficients in Heterogeneous Soft-Matter System, 2022. <https://hdl.handle.net/20.500.11767/130791>.

Abstracts — 5th of May, 2023 — Friday

Anton Kutlin

Bridging the gap: a phenomenology of level repulsion in random matrices.

Dyson Brownian Motion (DBM) is the stochastic process describing the joint evolution of certain random matrix eigenvalues. While DBM was initially considered in the framework of rotationally invariant ensembles, similar equations also occur in more exotic random matrix models, such as the Rosenzweig-Porter model or the Anderson model on Random Regular Graphs. In this talk, we will discuss how DBM arises in such models and how to deduce some of their spectral characteristics without solving the corresponding stochastic equations exactly; understanding the underlying processes may enhance our understanding of many-body localization.

Khatereh Azizi

Investigating the microscopic nature of the solvation and hydrophobicity in aqueous solutions from cavity shapes

Understanding the mechanism of solvation is essential in many areas of both fundamental and applied sciences ranging from materials chemistry to biological processes such as protein folding and aggregation. Despite many decades of theoretical and experimental investigations, the ground rules that determine the thermodynamics and dynamical behavior of solvated systems still present unresolved and open questions. The first step for solvation is the creation of a cavity to host the solute molecule. Using computer simulations and data science tools, we are able to characterize the cavities around the solute in aqueous solutions. In this talk, I will show two main results of how the cavities give insights into thermodynamic properties by providing a microscopic picture of those observables. First, I show the cavities around polymers in the unfolded and folded state. We find that the cavities around the folded polymers are extremely rough, with branches that can extend up to over 1 nm away from the polymer. These branches disappear, and the voids start resembling the quasi-spherical shape predicted by dewetting theory only when they surround particles with a radius of around 1 nm, well above the size occupied by a folded hydrophobic polymer. Second, I will show the cavities around the 20 amino acids. We find that all the free energy of solvation, entropy, enthalpy, and the hydrophobicity of amino acids in water, can be explained solely by the shapes of the cavities around them if one also considers the branchiness of those shapes. A simple linear regression model can link the cavity shapes (density fluctuations) and the solvation and provides a clear insight into the microscopic nature of solvation and hydrophobicity.

Rajat Kumar Panda

Spectral PCA Entropy: Ising models

In recent times, learning phases of matter through machine learning techniques has attracted a lot of attention. We apply unsupervised machine learning techniques, mainly principal component analysis (PCA), to compare and contrast the phase behavior and phase transitions in 2D and 3D Ising model. We use techniques inspired by quantum statistical mechanics to define an entropy measure for our data set based on spectral properties, such as Shannon entropy.

Colin Egan

The Alchemist's Guide to Free Energy Decompositions

We (gently) outline a free energy decomposition framework which combines a coarse-grained cluster expansion with the potential distribution theorem (Zwanzig's relationship). Applying this approach to study the thermodynamics of surfactant interfacial adsorption processes illuminates the role of collective effects. We show how the method of computational alchemy allows one to decompose these collective effects into contributions due to cavity formation, van der Waals stabilization, and electrostatics, and explain the consequences of each effect.