DY 44: Poster: Statistical Physics

Time: Thursday 13:00–16:00 Location: P1

DY 44.1 Thu 13:00 P1

Understanding probability and irreversibility in the Mori-Zwanzig projection operator formalism — •Michael te Vrugt — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Center for Soft Nanoscience, Philosophisches Seminar, 48149 Münster, Germany

Explaining the emergence of stochastic irreversible macroscopic dynamics from time-reversible deterministic microscopic dynamics is one of the key problems in philosophy of physics. The Mori-Zwanzig (MZ) projection operator formalism, which is one of the most important methods of modern nonequilibrium statistical mechanics, allows for a systematic derivation of irreversible transport equations from reversible microdynamics and thus provides a useful framework for understanding this issue. However, discussions of the MZ formalism in philosophy of physics tend to focus on simple variants rather than on the more sophisticated ones used in modern physical research. In this work [1], I will close this gap by studying the problems of probability and irreversibility using the example of Grabert's time-dependent projection operator formalism. This allows to better understand how general proposals for understanding probability in statistical mechanics, namely (a) quantum approaches and (b) almost-objective probabilities, can be accomodated in the MZ formalism.

[1] European Journal for Philosophy of Science 12, 41 (2022)

DY 44.2 Thu 13:00 P1

Finite-temperature absorption spectrum of Al_2O_3 from first principles — •Angela F. Harper[1], Bartomeu Monserrat[2], and Andrew J. Morris[3] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]University of Cambridge, UK — [3]University of Birmingham, UK

Advancing the next generation of materials for solid-state devices requires an understanding of their underlying electronic structure. One such material is alumina (Al_2O_3), which is used to enhance performance in electronic devices from Li-ion batteries to perovskite solar cells and field effect transistors. By including phonon-assisted transitions within plane-wave DFT methods for calculating the X-ray absorption spectrum (XAS) we obtain the Al K-edge XAS at 300 K for two crystalline Al_2O_3 phases. The 300 K XAS reproduces the pre-edge peak for α-Al_2O_3, which is not visible at the static-lattice level of approximation. The 300 K XAS for γ-Al_2O_3 correctly describes two out of the three experimental peaks. We show that the second peak arises from 1s to mixed *s-p* transitions and is absent in the 0 K XAS. The method presented here is generalizable to any element and absorption edge, and is a feasible way to calculate finite temperature spectroscopy for any crystalline material.

DY 44.3 Thu 13:00 P1

Potts model with invisible states on a scale-free network — •Mariana Krasnytska[1,2,3] and Petro Sarkanych[1,2] — [1]ICMP, NAS of Ukraine, Lviv, Ukraine — [2]L4 Collaboration Leipzig-Lorraine-Lviv-Coventry — [3]Université de Lorraine, Nancy, France

Different models are proposed to understand magnetic phase transitions through the prism of competition between the energy and the entropy. One of such models is a (q+r)-state Potts model with invisible states. This model introduces r invisible states such that if spin lies in one of them, it does not interact with the rest. We consider such a model using the mean-field approximation on an annealed scale-free network where the probability of a randomly chosen vertex having a given degree is governed by the power law with decay exponent λ. Our results confirm that q, r and λ play a role of global parameters that influence the critical behaviour of the system. Depending on their values the phase diagram is divided into three regions with different critical behaviour. However, the topological influence, presented by the marginal value of λc(q), has proven to be dominant over the entropic one, governed by the number of invisible states r [arXiv:2211.14048].

DY 44.4 Thu 13:00 P1

Thermodynamics of $su(n)$-symmetric integrable models and their continuum limit — •Ingryd Passos and Andreas Klümper — Bergische Universität Wuppertal, Wuppertal, Germany

Traditionally the computation of the partition function of integrable quantum chains is achieved by means of the thermodynamic Bethe ansatz (TBA). On the other hand, an alternative formulation which relies on finite sets of nonlinear integral equations has been developed and successfully applied to seminal cases like for example the spin-1/2 Heisenberg chain, the supersymmetric t-J model and quantum chains with $su(3)$ and $su(4)$ invariance. This approach, known as the Quantum Transfer Matrix (QTM) method, allows for faster numerical computations and calculation of finite temperature correlation lengths. However, the derivation of these alternative equations was done in case by case studies in which by trial and error suitable auxiliary functions were identified. Another shortcoming of the QTM method is its applicability in the case of continuum integrable models. A way to circumvent this issue is to identify the proper lattice model from which the continuum model follows after a suitable scaling limit. This way, it is possible, for example, to determine the thermodynamics of multicomponent Bose gases from anisotropic spin chains. In this work we present a way to derive systematically finite sets of nonlinear integral equations for $su(n)$-symmetric integrable lattice models and discuss a scaling limit of these equations in the case of the $su(3)$-invariant anisotropic spin chain.

DY 44.5 Thu 13:00 P1

Simple-to-complex phase transition for longest increasing subsequences (Ulam's problem) — •Tammo Lentsch and Alexander K. Hartmann — Institute of Physics, University of Oldenburg, Germany

It is possible to calculate the LIS length L by efficient algorithms in polynomial time. Finding and analyzing LIS was first considered numerically in the 1950s by Stanislav Ulam. The LIS problem has applications in bioinformatics and data analysis but is also studied in mathematics and statistical physics [1].

Recently, an algorithm to count the number of LIS [2] was extended to directly sample LIS [3]. The phase space where σ are random permutations was studied by calculating the distribution $P(q)$ of overlaps, revealing a complex structure similar to Replica Symmetry Breaking.

Here we consider the effect of randomly partially presorting σ with $O(n^\alpha)$ sorting steps. For sequences up to length $n = 8192$, we analyzed the LIS length L and $P(q)$. The results indicate a phase transition at a critical value α_c from $O(n)$ to $O(\sqrt{n})$ LIS length scaling and from simple to complex phase-space structure.

[1] J. Börjes, H. Schawe, A.K. Hartmann, Phys. Rev. E **99**, 042104 (2019).
[2] P. Krabbe, H. Schawe, A.K. Hartmann, Phys. Rev. E **101**, 062109 (2020).
[3] P. Krabbe, H. Schawe, A.K. Hartmann, arXiv:2208.14955 (2022).

DY 44.6 Thu 13:00 P1

Nonergodicity of scaled fractional Brownian motion with nonliner time and space clocks — •Yingjie Liang[1,2], Wei Wang[2], Andrey G. Cherstvy[2], and Ralf Metzler[2,3] — [1]Hohai University — [2]University of Potsdam — [3]Asia Pacific Center for Theoretical Physics

Experimental evidences show that diffusion processes are not always Brownian motion. It is anomalous diffusion with the mean squared displacement (MSD) being a power law in time, ultraslow diffusion with a logarithmic law, and superfast diffusion with an exponential law. To describe different types of non-Brownion motion in heterogeneous media, this study provides scaled fractional Brownian motion (SFBM) with nonliner time and space clocks. In the Langevin system for the FBM runnning with a nonliner time clock, i.e., the time scaled FBM, the real time is a temporal function of the original times in FBM. For the FBM runnning with a nonliner space clock, i.e., the space scaled FBM, the real position is a nonlinear spatial function of the orginial positions in FBM. The nonergodicity properties of SFBM are quantified based on single particle trajectories of the fractional Brownian motion running with time and space clocks. The simulations are consistent with the general analytical results in specific values of the dominated parameters for the behaviors of the MSD, time averaged mean squared displacement (TAMSD) and aging. Potential applications of these results are encountered in diverse scientific fields, such as biophysical, soft matter and hydrology systems.

DY 44.7 Thu 13:00 P1

The Griffiths Phase: A Large Deviations Study — •Lambert

Münster[1], Martin Weigel[1], and Alexander K. Hartmann[2] — [1]Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany

For spin systems with quenched disorder, the Griffiths phase is the thermal region between the phase transition in the pure system and the corresponding transition in the disordered system. The standard example is a dilute ferromagnet, where a certain fraction of bonds is missing [1]. The physical behavior of this phase is characterized by large fluctuations in the order parameter which are visible in the tails of the distribution of the magnetic susceptibility. To directly investigate this property, we combine a large-deviation Monte Carlo sampling algorithm [2,3] with a Gaussian modified ensemble [4], thus allowing us to study the distribution of physical quantities on a much larger range of the support as compared to previous studies [5], i.e., in the region of exponential small probabilities. In addition to considering the susceptibility distribution we also study other observables such as the specific heat, thus shedding new light on this intriguing physical phenomenon.

[1] A. J. Bray, Phys. Rev. Lett. **59**, 586 (1987).
[2] A. K. Hartmann, Phys. Rev. E **65**, 056102 (2002).
[3] A. K. Hartmann, Eur. Phys. J. B **84**, 627 (2011).
[4] T. Neuhaus, J. S. Hager, Phys. Rev. E **74**, 036702 (2006).
[5] K. Hukushima, Y. Iba, J. Phys. **95**, 012005 (2008).

DY 44.8 Thu 13:00 P1

Transport Properties of Brownian Particles: Analytical Results and Computer Simulations — •Regina Rusch[1], Gerhard Jung[2], and Thomas Franosch[1] — [1]Institute for Theoretical Physics, Universität Innsbruck, Innsbruck, Austria. — [2]Laboratoire Charles Coulomb (L2C), Université de Montpellier, CNRS, 34095 Montpellier, France.

The results of computer simulations for Brownian particles can be improved by using a novel noise cancellation algorithm, with which the velocity autocorrelation function (VACF) can be measured more precisely. The algorithm is based on the fact that the Brownian noise can be stored in computer simulations and thus the noise can be subtracted from a simulated trajectory. Doing this, a reduced motion of the particle due to interactions or an external force is obtained. It could be shown that the VACF of the reduced motion is connected with the original VACF up to a cross-correlation term, which is shown to be sufficiently small. For the system of a Brownian particle in a periodic step potential the noise cancellation algorithm decreases the error of the VACF by about one order of magnitude. A power-law decay in the VACF is found by employing Monte-Carlo simulations. We also present analytical results for the probability distribution of the particle position using the Bloch theorem. This enables us to compute further correlation functions such as the intermediate scattering function which is in quantitative agreement with simulations.

DY 44.9 Thu 13:00 P1

First passage time as thermodynamical parameter — •Vasiliy Ryazanov — Institute for nuclear research NANU, Kiev, Ukraine

The first-passage time is proposed as an independent thermodynamic parameter of the statistical distribution that generalizes the Gibbs distribution. The thermodynamic parameter conjugated to the first-passage time is the same as the Laplace transform parameter of the first-passage time distribution in the partition function. The thermodynamic parameter conjugated to the first-passage time can be expressed in terms of the deviation of the entropy from the equilibrium value. Thus, all the moments of the distribution of the first passage time expressed in terms of the deviation of the entropy from its equilibrium value and the external forces acting on the system. By changing the thermodynamic forces, you can change of the first passage time.

An analogy is drawn between version of non-equilibrium thermodynamics a distribution-based containing an additional thermodynamic first-passage time parameter, nonequilibrium statistical operator method and extended irreversible thermodynamics with flows as an additional thermodynamic parameter. Various conditions for the dependence of the distribution parameters of the first-passage time on the random value of energy, the first thermodynamic parameter, are considered. Expressions are obtained for the thermodynamic parameter, the conjugate of the first passage time through the entropy change, and for the average first passage time through the flows.

DY 44.10 Thu 13:00 P1

Stochastic dynamics with multiplicative noise under resetting — •Trifce Sandev[1,2,3], Ljupco Kocarev[1,3], Ralf Metzler[2,4], and Aleksei Chechkin[2,5,6] — [1]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [2]University of Potsdam, Germany — [3]Ss. Cyril and Methodius University in Skopje, Macedonia — [4]Asia Pacific Center for Theoretical Physics, Pohang, Republic of Korea — [5]Wroclaw University of Science and Technology, Poland — [6]Akhiezer Institute for Theoretical Physic, Kharkiv, Ukraine

We analyze different stochastic processes with multiplicative noise under resetting in non-homogeneous media. We use the subordination approach, which is a powerful technique for solving various diffusion and Fokker-Planck equations, to analyze the probability density functions and the mean squared displacements. Additionally, we show that such systems under stochastic resetting reach non-equilibrium stationary states. The transition to the non-equilibrium stationary states is analyzed in terms of the large deviation function, by employing the Laplace approximation of the integral in the renewal equation for the probability density of the process with resetting events.

[1] T. Sandev, V. Domazetoski, L. Kocarev, R. Metzler, A. Chechkin, J. Phys. A: Math. Theor. 55, 074003 (2022).
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DY 44.11 Thu 13:00 P1

Quench-Probe Setup as an Analyzer of Fractionalized Entanglement Spreading — •Nicolas P. Bauer[1], Jan Carl Budich[2], Björn Trauzettel[1], and Alessio Calzona[3] — [1]Julius Maximilians Universität Würzburg, Würzburg, Germany — [2]TU Dresden, Dresden, Germany — [3]IQM Quantum Computers, München, Germany

We propose a novel spatially inhomogeneous setup for revealing quench-induced fractionalized excitations in entanglement dynamics. In this quench-probe setting, the region undergoing a quantum quench is tunnel-coupled to a static region, the probe. Subsequently, the time-dependent entanglement signatures of a tunable subset of excitations propagating to the probe are monitored. We exemplify the power of this generic approach by identifying a unique dynamical signature associated with the presence of an isolated Majorana zero mode in the post-quench Hamiltonian. In this case excitations emitted from the topological part of the system give rise to a fractionalized jump of $\log(2)/2$ in the entanglement entropy of the probe. This dynamical effect is highly sensitive to the localized nature of the Majorana zero mode, but does not require the preparation of a topological initial state.

DY 44.12 Thu 13:00 P1

Exploiting Skyrmion motion for computing — •Alessandro Pignedoli, Björn Dörschel, and Karin Everschor-Sitte — University of Duisburg-Essen, Duisburg, Germany

Brownian motion is a natural phenomenon that can be exploited for energy efficient computing. Here, an assemblage of simple parts evolves in an energetic labyrinth to a low energy state which is isomorphic to the desired solution of a computation [1]. Magnetic Skyrmions [2] are topologically stable magnetic whirls that have been shown to behave like interacting Brownian particles [3,4]. We use a Langevin model to describe and investigate the motion of Skyrmions by means of correlations and statistical observables to carry out Brownian computation. We show that besides the Brownian motion of individual Skyrmions, their interactions and external driving forces break ergodicity. This allows for a rapid convergence to the low-energy state of the system and thus solves the calculation faster.

[1] C. H. Bennett, Int. J. Theor. Phys. 21, 905 (1982) [2] K. Everschor-Sitte, J. Masell, R. M. Reeve and M. Kläui, J. Appl. Phys.124, 240901 (2018) [3]J. Zázvorka, et al. Nat. Nanotechnol. 14, 658 (2019) [4] T.Nozaki, et al Appl. Phys. Lett. 114, 012402 (2019)

DY 44.13 Thu 13:00 P1

A generalised rotational diffusion approach to modeling of the dielectric relaxation processes with resetting — •Irina Petreska[1], Ljupco Pejov[1,2], Trifce Sandev[1,3,4], Ljupco Kocarev[1,3], and Ralf Metzler[4] — [1]Ss. Cyril and Methodius University in Skopje, Macedonia — [2]University of Stavanger, Norway — [3]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [4]University of Potsdam, Germany

We consider the rotational diffusion equation with a generalised memory kernel in the context of dielectric relaxation processes in a medium composed of polar molecules. We give an overview of existing models on non-exponential relaxation and introduce an exponential resetting

dynamic in the corresponding process, providing a detailed analysis of the autocorrelation function and complex susceptibility. It is shown that stochastic resetting leads to a saturation of the autocorrelation function to a constant value, in contrast to the case without resetting, for which it decays to zero. The behaviour of the autocorrelation function, as well as the complex susceptibility in the presence of resetting, confirms that the dielectric relaxation dynamics can be tuned by an appropriate choice of the resetting rate.

[1] I. Petreska, Lj. Pejov, T. Sandev, Lj. Kocarev and R. Metzler, *Fractal Fract.* **6**, 88 (2022).

DY 44.14 Thu 13:00 P1

Dividing Active Brownian Particles — •Till Welker and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Germany.

We aim to combine active motion with cell division to answer questions like: Does nutrient input induce clustering? How does a non-uniform nutrient distribution effects population dynamics?

To include cell division and death in the model of active Brownian particles, we propose a simple rule: *in a time interval dt, each particle has a probability* $dt \cdot g(s)$ *to divide and* $dt \cdot d$ *to die.* The growth rate g depends on the nutrient concentration s at the position of the bacterium and is described by the Monod function. The nutrient diffuses with the diffusion coefficient D_N. We add a source with steady input rate S_0, in addition, each particle takes up nutrient with a rate $\gamma g(s)$.

The population dynamics strongly depends on nutrient diffusion: For large D_N, the population oscillates before reaching a steady population number N^*. For small D_N, the population is stronger damped and equilibrates quickly. N^* is independent of D_N, but the population fluctuation decreases for lower D_N due to the damping. The collective behavior is also influenced by the nutrient: First, for large D_N the swarm has a strongly asymmetric shape during the transient phase which then becomes symmetric in the steady state. Second, the swarm is less dense for larger D_N, but the relationship between spread of nutrient and bacteria is not linear.

We show that combining two key aspects of microbial life, mobility and growth, gives rise to interesting population and spatial dynamics.

DY 44.15 Thu 13:00 P1

Ornstein-Uhlenbeck process and generalizations: influence of comb geometry and stochastic resetting on the particle dynamics — •Petar Jolakoski[1], Pece Trajanovski[1], Kiril Zelenkovski[1], Alexander Iomin[2], Ljupco Kocarev[1,4], and Trifce Sandev[1,3,4] — [1]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [2]Department of Physics, Technion, Haifa, Israel — [3]University of Potsdam, Germany — [4]Ss. Cyril and Methodius University in Skopje, Macedonia

The Ornstein-Uhlenbeck (O-U) process can be interpreted as a Brownian motion in a harmonic potential. The process is an established Gauss-Markov process that has a bounded variance and admits a stationary probability distribution, in contrast to the standard Brownian motion. Over time, the process tends to drift towards its mean function: such a process is called mean-reverting. Here, we study the effects of stochastic resetting on the O-U process and its generalizations which were hitherto unexplored. In particular, we investigate the dynamics with and without resetting on comb-like structures. For the studied specific 2D comb geometry, we compute the first moment, the non-equilibrium stationary state and the mean squared displacement, and find that the global resetting hinders the particle's transport in the two dimensions. Moreover, the two divergent forces, namely the resetting and the drift towards the mean, lead to compelling results both in the case of O-U process with resetting and its generalization on a 2D comb structure.

DY 44.16 Thu 13:00 P1

Theoretical design of Geometric Brownian Information Engine: Analysis of output work — •Syed Yunus Ali, Rafna Rafeek, and Debasish Mondal — IIT Tirupati, Yerpedu, Andhrapradesh, India

We design a geometric Brownian information engine by considering overdamped Brownian particles inside a 2-D monolobal confinement with irregular width along the transport direction. Under such conditions, particles experience an effective entropic potential. We employ a feedback control protocol as an outcome of error-free position measurement.The protocol comprises three stages: measurement, feedback, and relaxation. We show that the upper bound of the achievable work shows a cross-over from $(5/3-2\ln 2)k_BT$ to $k_BT/2$ when the system changes from an entropy-dominated regime to energy dominated one. Next, we determine the benchmarks for utilizing the available information in an output work and the optimum operating requisites for best work extraction in asymmetric feedback protocol. Transverse bias force (G) tunes the entropic contribution in the effective potential and hence the equilibrium marginal probability distribution standard deviation(σ).We recognize that the amount of extracted work reaches a global maximum when $x_f = 2x_m$ with $x_m = 0.6\sigma$, irrespective of the extent of the entropic limitation.

References:

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DY 44.17 Thu 13:00 P1

Diffusion and order in mixed lattice gas of hard squares — Niklas Raake[1], •Piotr Nowakowski[2], and Ana-Sunčana Smith[1,2] — [1]Friedrich–Alexander–Universität Erlangen–Nürnberg, Erlangen, Germany — [2]Institut Ruđer Bošković, Zagreb, Croatia

We study a lattice gas composed of hard square particles of 1×1 and 2×2 size (measured in lattice constant) undergoing Brownian motion on a two–dimensional square lattice. For different concentrations of both types of particles we determine numerically the diffusion coefficients and compare them with predictions of a model based on a persistent random walk with one or two step memory. Good agreement is observed only for very low and very high concentration of particles. The deviations present in between these regimes suggest that the correlations play an important role in the dynamics of the system.

Additionally, we introduce a configurational order parameter that characterizes clustering of bigger squares. This allows us to study the continuous transition between unordered liquid and ordered crystal phases.

DY 44.18 Thu 13:00 P1

Non-Markovian modeling of non-equilibrium fluctuations and dissipation in active viscoelastic biomatter — •Amir Abbasi[1], Roland R. Netz[1], and Ali Naji[2] — [1]Freie University of Berlin, Berlin, Germany — [2]Institute for Research in Fundamental Sciences (IPM), Tehran, Iran

Viscoelastic gels such as permanently or transiently cross-linked networks of semiflexible polymers are important soft biological materials. The polymeric nature of such gels is responsible for their salient rheological properties, including their frequency-dependent response to external forces.

Here, based on a Hamiltonian that incorporates the elastic coupling between a tracer and active particles, we derive a generalized Langevin model for the non-equilibrium mechanical response of active viscoelastic biomatter. Our model accounts for the power-law viscoelastic response of the embedding polymeric network as well as for the non-equilibrium energy transfer between active and tracer particles. Our analytical expressions for the frequency-dependent response function and the positional autocorrelation function agree nicely with experimental data for red blood cells and actomyosin networks with and without ATP. The fitted effective active-particle temperature, elastic constants and effective friction coefficients of our model allow straightforward physical interpretation.

DY 44.19 Thu 13:00 P1

Ornstein-Uhlenbeck process on three dimensional comb structure under stochastic resetting — •Pece Trajanovski[1], Petar Jolakoski[1], Kiril Zelenkovski[1], Alexander Iomin[2], Ljupco Kocarev[1,4], and Trifce Sandev[1,3,4] — [1]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [2]Department of Physics, Technion, Haifa, Israel — [3]University of Potsdam, Germany — [4]Ss. Cyril and Methodius University in Skopje, Macedonia

The Ornstein-Uhlenbeck (O-U) process is a generalised diffusion process, introduced as a model for the velocity of a particle undergoing a Brownian motion confined in harmonic potential. The process is a stationary, meaning that over time, it tends to drift towards its long-time mean function: such a process is called mean-reverting. Here, we investigate the influence of the three dimensional comb structure and the stochastic resetting on the particle dynamics governed by O-U processes along the backbone (x-direction) and the main fingers (y-direction) and standard Wiener process along the secondary fingers of the comb (z-direction). The explicit analytical expressions for the first moment and mean squared displacement along all three directions are calculated and confirmed numerically. The marginal probability

density functions along all directions are simulated by using coupled Langevin equations for comb geometry.

DY 44.20 Thu 13:00 P1

Generalized molecular Stokes-Einstein and Stokes-Einstein-Debye relations including temperature-dependent slip and effective radius — •Sina Zendehroud, Jan O. Daldrop, Yann von Hansen, and Roland R. Netz — Freie Universität Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

We perform molecular dynamics simulations of water at different temperatures and calculate the viscosities as well as the rotational and translational self-diffusion constants of water molecules in the lab frame and in the comoving coordinate frame of the molecules. Instead of interpreting the results as deviations from the Stokes-Einstein and Stokes-Einstein-Debye relations, we simultaneously determine the slip length and the effective hydrodynamic radius from the simulation data. We show that the viscosity dependence of the diffusion constants of water can be understood in terms of an almost constant effective radius and a pronounced temperature dependence of the slip length.

DY 44.21 Thu 13:00 P1

Energy transfer between the librational and the inter- and intramolecular vibrational modes of liquid water — •Louis Lehmann and Roland Netz — Fachbereich Physik, Freie Universität Berlin

The molecular dynamics of liquid water can be split into librational and inter- and intramolecular vibrational modes. By applying the Eckart decomposition scheme, the infrared absorption spectrum can be exactly decomposed into contributions from these different modes. The complete energy transfer network of the librational and inter- and intramolecular vibrational modes in liquid water is established based on the energy transfer rates determined from equilibrium molecular dynamics simulations with conventional and many-body force fields. The results are validated by comparison with non-equilibrium molecular dynamics simulations that mimic pump-probe experiments.

DY 44.22 Thu 13:00 P1

Domain Drift and Diffusion in Cell-Polarization Processes — •Johannes Ewald and Jürgen Vollmer — Institute of Theoretical Physics, Universität Leipzig, Brüderstr. 16, D-04103 Leipzig, Germany

Cell polarization can be driven by the formation of signaling patterns on cell membranes. They can be modeled by two species of membrane proteins that can bind to cytosolic enzymes. The enzymes drive the conversion between cell membranes. These chemical reactions drive the coarsening of domains on the cell surface. Polarization amounts to the situation where the cell surface is covered by only two domains on opposing sides of the cell. Certain aspects of the domain coarsening are reminiscent to ripening of spin-up and spin-down domains in ferromagnets. In this analogy the conversion of membrane proteins takes the role of spin flips of the magnetic system. However, there are also distinct differences in the dynamics because the conversion is driven by a dissipative chemical reaction, while spin-flips arise due to thermal fluctuations. Based on the analytical solutions for domain drift and diffusion in the two models we will discuss differences and communalities of the processes.