Statistical Mechanics of Complex, Glassy and Non-Equilibrium Systems

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Abstracts

Spectral partitioning in random regular blockmodels
Paolo Barucca (Zurich/LIMS)
Graph partitioning problems emerge in a wide variety of complex systems, ranging from biology to finance, but can be rigorously analysed and solved only for a few graph ensembles. In this work, an ensemble of random graphs with regular block structure, also named equitable graphs, is discussed and analytically studied. In particular, the spectral density of such graphs is computed exactly for a modular, bipartite and core-periphery structure. McKay's law for random regular graphs is found analytically to apply also for regular modular and bipartite structures when blocks are homogeneous. In core-periphery structures, where blocks are intrinsically heterogeneous, a new law is found to apply for the spectral density. Exact solution to the problem of inferring the original block structure is provided for the models discussed. All analytical results show perfect agreement with numerical experiments. In the framework of equitable graphs the picture of the detectability threshold for naive spectral clustering, i.e. only using the eigenvector associated to the second largest eigenvalue of the adjacency matrix, emerges distinctly, as well as the crucial role of eigenvectorss statistics. Insights from equitable graphs could be used to develop new spectral methods based on both eigenvalues and eigenvectors properties.

Shape universality classes in the random sequential adsorption of non-spherical particles
Adrian Baule (QMUL)
Abstract: Random sequential adsorption (RSA) of particles of a particular shape is used in a large variety of contexts to model particle aggregation and jamming. A key feature of these models is the observed algebraic time dependence of the asymptotic jamming coverage $\sim t^{-\nu}$ as $t \to \infty$. However, the exact value of the critical exponent ν is not known apart from the simplest case of the RSA of monodisperse spheres adsorbed on a line (Renyi's seminal 'car parking problem'), where $\nu = 1$ can be derived analytically. Empirical simulation studies have conjectured on a case-by-case basis that for general non-spherical particles $\nu = 1/(d+\tilde{d})$, where d denotes the dimension of the domain and $\tilde{d}$ the number of orientational degrees of freedom of a particle. Here, we solve this problem analytically for the $d = 1$ case — the 'Paris car parking problem [1]. We prove in particular that the scaling exponent depends on particle shape, contrary to the original conjecture, and falls into two universality classes: (i) $\nu = 1/(1 + \tilde{d}/2)$ for smooth convex shapes with non-zero curvature, e.g., ellipsoids; (ii) $\nu = 1/(1 + \tilde{d})$ for shapes with flat sides, e.g., spherocylinders and polyhedra. The exact solution explains in particular why many empirically observed scalings fall in between these two limits.
[1] A. Baule, arXiv:1611.03034 (2016)

Free fermions and the classical compact groups
Fabio Deelan Cunden (University of Bristol)
We unveil the existence of a precise mapping between the ground state of non-interacting free fermions in a box with classical (absorbing, reflecting, and periodic) boundary conditions and the eigenvalue statistics of the classical compact groups. The associated determinantal point processes can be extended in two natural directions: i) we consider the full family of admissible quantum

boundary conditions (i.e., self-adjoint extensions) for the Laplacian on a bounded interval, and the corresponding projection correlation kernels; ii) we construct the grand canonical extensions at finite temperature of the projection kernels, interpolating from Poisson to random matrix eigenvalue statistics. The scaling limits in the bulk and at the edges are studied in a unified framework, and the question of universality is addressed. Whether the finite temperature determinantal processes correspond to the eigenvalue statistics of some matrix models is, a priori, not obvious. We complete the picture by constructing a finite temperature extension of the Haar measure on the classical compact groups. The eigenvalue statistics of the resulting (Poissonized) matrix models corresponds exactly to the grand canonical measure of non-interacting free fermions with classical boundary conditions.

Phase separation dynamics of polydisperse colloids: a mean-field lattice-gas theory
Pablo de Castro and Peter Sollich
New insights into liquid-gas phase separation in colloidal suspensions are provided via a new dynamical mean-field theory based on the Polydisperse Lattice-Gas model, for an arbitrary number of species, and for an arbitrary overall composition. The results for the early-time spinodal dynamics show qualitative changes as one crosses a "quenched" spinodal that excludes fractionation, allowing only density fluctuations at fixed composition. This effect occurs for dense systems, in agreement with a conjecture by Warren that at high density fractionation is generically slow because it requires inter-diffusion of particles. The rich behaviour beyond the spinodal regime is examined, where we find that the evaporation of gas bubbles with strongly fractionated interfaces causes long-lived composition heterogeneities in the liquid phase when direct particle-particle swaps are not allowed.

Isolation statistics in temporal spatial networks
Carl Dettmann
Many networks are spatial in that the nodes are located in physical space, with a link probability that depends on the mutual distance. If the node locations can be considered fixed, as for example in wireless ad-hoc networks subject to fast fading, each node is isolated with a probability that depends on the locations of the other nodes. We give a mostly analytical approach for calculating the distribution of isolation probabilities for both short and long ranged connection functions. In the short ranged case, many nodes are either almost always isolated or almost never isolated, whilst in the long ranged case, most have isolation probabilities closer to the mean. We apply these results to temporal networks with links that are uncorrelated and correlated in time.

From non-ergodic eigenvectors to local resolvent statistics and back: a random matrix perspective
Davide Facoetti (KCL)
Abstract: The phenomenon of many-body localisation (MBL) has attracted considerable interest in recent years in the study of non-equilibrium quantum sytems. A feature that is not well understood is the existence of an intermediate extended non-ergodic bad metal phase between the localised and extended ones. To help the debate about the existence and role of extended, non-ergodic phases in MBL and the related problem of Anderson localisation on the Bethe lattice, we study such a phase in the simpler setting of the generalised Rosenzweig-Porter random matrix model. We confirm previous results about the multifractality of the eigenstates, and show that the intermediate phase can be characterised studying the local resolvent in a non-standard scaling limit.
DF, P. Vivo, G. Biroli, EPL 115 (2016) 47003, arXiv:1607.05942

Front propagation and bulk relaxation in the melting dynamics of a kinetically constrained model of stable glasses
Ricardo Gutiérrez and Juan P. Garrahan (Nottingham)

Kinetically constrained models (KCMs) are typically formulated in terms of mesoscopic variables that represent a coarse-grained density field. Such systems evolve according to dynamic facilitation rules from which glassy relaxation emerges. The study of KCMs in physically relevant configurations can shed light on the dynamics of stable glasses, i.e. systems prepared by physical vapour deposition at a temperature slightly below the glass transition temperature, which have been shown to possess very high kinetic and thermodynamic stabilities as compared to ordinary glasses prepared by cooling a supercooled liquid. One of the key distinguishing features of stable glasses is the heterogeneous melting behaviour they display. By exploring the dynamics emerging in a soft KCM, we are able to replicate and elucidate the competition between bulk relaxation and front propagation that is observed experimentally, and to probe those mechanisms separately, thus clarifying the origin of the crossover length that has puzzled experimentalists. In agreement with recent findings, the bulk relaxation is found to follow an Avrami equation, which can be generalised so as to include a propagating front.

Cell reprogramming modelled as transitions in a hierarchy of cell cycles

Ryan Hannam

We construct a minimal model for cell reprogramming which builds on key elements of cell biology viz. cell cycles and cell lineages. Although reprogramming has been demonstrated experimentally, much of the underlying processes governing cell fate decisions remain unknown. This work aims to bridge this gap, using a complex systems approch to model cell types as a set of hierarchically related dynamical attractors that represent cell cycles. Stages of each cell cycle are characterised by the configuration of gene expression levels, and reprogramming corresponds to triggering transitions between such configurations. Two mechanisms were found for reprogramming in a two level hierarchy: cycle specific perturbations and a noise-induced switching. These reprogramming protocols were found to be effective in large regimes of the parameter space and make specific predictions concerning reprogramming dynamics which are broadly in line with experimental findings.

Breaking detailed balance accelerates convergence of Markov chains to their steady states

Rob Jack (Bath)

Several recent results indicate that Markov chains which obey detailed balance are the slowest to converge to their steady states. We present two geometrical constructions which explain some of these results. For diffusive systems on the hydrodynamic scale, we describe a decomposition of the particle current into three orthogonal contributions [1], two of which vanish in the reversible case. For general Markov chains, the geometry is based on a non-linear relationship between probability currents and their conjugate forces. In both cases, the rate of convergence to the steady state is characterised in terms of large deviations at level 2 and level 2.5, which are related to the relevant geometries.

[1] M Kaiser, RL Jack and J Zimmer, arXiv:1611.06509.

Computing the Initial Weights of a Learning Network from the Phase Transition Region in its Error Landscape

Julius Julius (KCL)

Next generation deep neural networks for classification hosted on embedded platforms will rely on fast, efficient, and accurate learning algorithms. Initialization of weights in learning networks has a great impact on the classification accuracy. In this paper we focus on deriving good initial weights by modeling the error function of a deep neural network as a high-dimensional landscape. We observe that due to the inherent complexity in its algebraic structure, such an error function may conform to general results of the statistics of large systems. To this end we apply some results from Random Matrix Theory to analyse these functions. We model the error function in terms of a Hamiltonian in N-dimensions and derive some theoretical results about its general behavior. These results are further used to make better initial guesses of weights for the learning algorithm.

Universal coarsening kinetics and interface fluctuations in motility-induced phase separation

Chiu Fan Lee (Imperial)

Minimal models of self-propelled particles with short-range volume exclusion interactions have been shown to exhibit signatures of phase separation. By modelling the microscopic dynamics of the active particles in the interfacial region, I will show that at the onset of motility-induced phase separation (i.e., small supersaturation), the coarsening kinetics and the drop size distribution follow the Lifshitz-Slyozov universal coarsening law, and the interface fluctuations are described by the Edward-Wilkinson universality class [1]. However, if the particles speed is position dependent, then instead of coarsening, the drop size can become monodisperse [2].

[1] Lee C F (2017) Interface stability, interface fluctuations, and the Gibbs-Thomson relationship in motility-induced phase separations. Soft Matter 13, 376-85

[2] Weber C A, Lee C F and Jülicher F (2017) Droplet Ripening in Concentration Gradients. New Journal of Physics, in press

The Fractal Dimension of Interfaces in Edwards-Anderson and Long-range Ising Spin Glasses: Determining the Applicability of Different Theoretical Descriptions

M. A.Moore (Manchester)

The fractal dimension of excitations in glassy systems gives information on the critical dimension at which the droplet picture of spin glasses changes to a description based on replica symmetry breaking where the interfaces are space filling. Here, the fractal dimension of domain-wall interfaces is studied using the strong-disorder renormalization group method pioneered by Monthus both for the Edwards-Anderson spin-glass model in up to eight space dimensions, as well as for the one-dimensional long-ranged Ising spin-glass with power-law interactions. Analyzing the fractal dimension of domain walls, we find that replica symmetry is broken in high-enough space dimensions. Because our results for high-dimensional hypercubic lattices are limited by their small size, we have also studied the behavior of the one-dimensional long-range Ising spin-glass with power-law interactions. For the regime where the power of the decay of the spin-spin interactions with their separation distance corresponds to 6 and higher effective space dimensions, we find again the broken replica symmetry result of space filling excitations. This is not the case for smaller effective space dimensions. These results show that the dimensionality of the spin glass determines which theoretical description is appropriate. Our results will also be of relevance to the Gardner transition of structural glasses.

Consensus formation times in anisotropic societies

Juan Neirotti (Aston)

We developed a statistical mechanics model to study the emergence of a consensus in societies of adapting, interacting agents constrained by a social rule B. In the mean field approximation we find that if the agents' interaction H_0 is weak, all agents adapt to the social rule B, with which they form a consensus; but if the interaction is sufficiently strong a consensus is built against the established *status quo*. We observed that, after a transient time α_t, agents asymptotically approach complete consensus by following a path where they neglect their neighbours' opinions on socially neutral issues (i.e. issues for which the society as a whole has no opinion). α_t is found to be finite for most values of the inter-agent interaction H_0 and temperature T, with exception of the values $H_0 = 1$, $T \to \infty$ and the region determined by the inequalities $\beta < 2$ and $2\beta H_0 < 1 + \beta - \sqrt{1 + 2\beta - \beta^2}$, for which consensus, with respect to B, is never reached.

Dynamical large deviations of fully packed dimers

Tom Oakes (Nottingham)

We study the phase diagram of the quantum dimer model on the square lattice, using stochastic dynamics of the corresponding classical model, by identifying the deformed stochastic master operator with the quantum Hamiltonian. In order to sample the resulting activity-weighted ensemble of classical trajectories, we introduce a new method based on the exact Doob transformation for a related but computationally simpler problem. The resulting dynamical process, implemented using standard transition path sampling methods, allows the ensemble to be sampled with significantly enhanced efficiency. From various dynamical properties of the trajectories, we identify a possible dynamical phase transition.

Current fluctuations in classical and quantum systems far from equilibrium

Carlos Pérez-Espigares (Nottingham)

In this talk we will present some results derived from the study of current fluctuations in non-equilibrium diffusive systems. We will explain how by applying the Macroscopic Fluctuation Theory, interesting properties such as dynamical phase transitions can be described. In addition, we will show how the dynamics of a class of open quantum systems can be described in terms of fluctuating hydrodynamics, where fermionic open chains display a dynamical phase transition similar to that of classical exclusion processes with open boundaries. This transition is manifested in a singular change in the structure of trajectories: while typical trajectories are diffusive, rare trajectories associated to atypical currents are ballistic and hyperuniform in their spatial structure.

Faster and stronger stochastic oscillations induced by network interference

Tim Rogers (Bath)

Stochastic oscillations arising from demographic noise are known to affect a wide range of models in biology, ecology and epidemiology. For the sake of tractability, these models typically encompass only a small subset of all of the interacting elements present in the wider physical setting. In this talk I will show how this subsampling can lead to underestimation of the dominant frequency and amplitude of stochastic oscillation. The effect is explained using a random matrix theory analysis of the repulsion between the oscillation spectra of subsystems and that the bulk, which obeys a universal "quarter-circle" distribution.

Metastability in open quantum systems

Dominic Rose (Nottingham)

We apply a recently developed theory for metastability in open quantum systems to two systems; a dissipative quantum Ising model and a quantum generalization of the East model. These exhibit strongly intermittent emission dynamics characteristic of systems with competing dynamical phases. We show that for appropriate parameters these systems dynamics display pronounced metastability, i.e., the system relaxes first to long-lived metastable states, before eventual relaxation to the true stationary state. From the spectral properties of the quantum master operator we characterise the low-dimensional manifold of metastable states for these models. We also show that the long time dynamics can be approximated by a classical stochastic dynamics between the metastable phases, directly related to the intermittent dynamics observed in quantum trajectories. In particular we demonstrate that the effective dynamics between the metastable states of the quantum East model is simply an adjustment of the long-time dynamics of the classical East model.

Open quantum generalisation of Hopfield neural networks

Pietro Rotondo (Nottingham)

Abstract: We propose a new framework to understand how quantum effects may impact on the dynamics of neural networks [1]. We implement the dynamics of neural networks in terms of

Markovian open quantum systems, which allows us to treat thermal and quantum coherent effects on the same footing. In particular, we propose an open quantum generalisation of the Hopfi eld neural network [2], the simplest toy model of associative memory. We determine its phase diagram and show that quantum fluctuations give rise to a qualitatively new non-equilibrium phase. This novel phase is characterised by limit cycles corresponding to high-dimensional stationary manifolds whose interpretation from the statistical learning theory viewpoint is not clear and calls for further investigations.

[1] P. Rotondo, M. Marcuzzi, J. P. Garrahan, I. Lesanovsky, M. Muller, arXiv:1701.01727 (2017);
[2] J. J. Hopfield, PNAS, 79, 2554 (1982).

Optimising Spreading Processes

Andrey Y. Lokhov and D. Saad (Aston)

The modern world can be best described as interlinked networks, of individuals, computing devices and social networks; where information and opinions propagate through their edges in a probabilistic or deterministic manner via interactions between individual constituents. These interactions can take the form of political discussions between friends, gossiping about movies, or the transmission of computer viruses. Winners are those who maximise the impact of scarce resource such as political activists or advertisements, or by applying resource to the most influential available nodes at the right time. We developed an analytical framework, motivated by and based on statistical physics tools, for impact maximisation in probabilistic information propagation on networks; to better understand the optimisation process macroscopically, its limitations and potential, and devise computationally efficient methods to maximise impact (an objective function) in specific instances. The research questions we have addressed relate to the manner in which one could maximise the impact of information propagation by providing inputs at the right time to the most effective nodes in the particular network examined, where the impact is observed at some later time. It is based on a statistical physics inspired analysis, Dynamical Message Passing that calculates the probability of propagation to a node at a given time, combined with a variational optimisation process. We address the following questions: 1) Given a graph, a budget and a propagation/infection process, which nodes are best to infect to maximise the spreading? 2) Maximising the impact on a subset of particular nodes at given times, by accessing a limited number of given nodes. 3) Identify the most appropriate vaccination targets to isolate a spreading disease through containment of the epidemic. We also point to potential applications.

Lokhov A.Y. and Saad D., Optimal Deployment of Resources for Maximizing Impact in Spreading Processes, arXiv:1608.08278 (2016)

Transmission via a simple mode on a chaotic background

Dmitry Savin (Brunel)

Scattering on a resonant state coupled to a complicated background is a typical problem for mesoscopic quantum many-body systems as well as for wave propagation in the presence of a complex environment. On average, the coupling to background states leads to an effective damping of such a simple mode, expressed by the so-called "spreading" width. This talk will formulate and discuss a non-perturbative approach to study fluctuations in scattering, taking into account also finite dissipation in the background. Modelling the latter by random matrix theory, we employ the formalism of strength functions, adopted from nuclear physics, to derive exact expressions for the distribution functions of transmission and reflection. In particular, we discuss a sharp disappearance of the established transmission signal when the spreading width exceeds the natural width of the simple mode. Potential applications in the context of reverberation chambers and microwave communications are also briefly discussed. [Based on recent work reported in arXiv:1704.08677.]

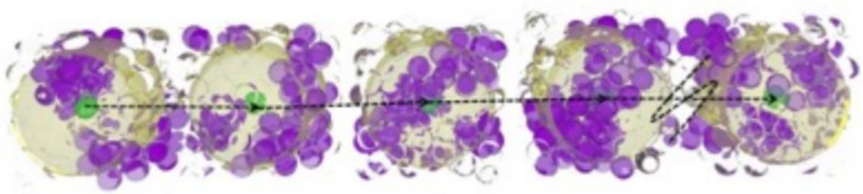
The distribution of first hitting times and last hitting times of random walks on Erdős-Rényi networks

Ido Tishby (HUJ Jerusalem)

Analytical results for the distributions of first hitting times and last hitting times of random walks (RWs) on ErdsRnyi networks will be presented. Starting from a random initial node, a random walker hops between adjacent nodes until it hits a node which it has already visited before. At this point, the path terminates. The number of steps until termination is called first hitting time (FHT). To obtain the distribution of last hitting times (LHT) we replace the RW by a self avoiding walker (SAW), which actively avoids retracing its own path. In this case the path terminates only when the walker becomes trapped in a "dead-end" node, which is completely surrounded by previously visited nodes. It is found that the FHTs follow the discrete Rayleigh distribution while the LHTs follow the Gompertz distribution. The results will be discussed, pointing out connections to reliability theory, survival analysis and the distribution of life expectancies.

Understanding phase transitions in trajectory space: theory and experiments on glass formers

Francesco Turci (Bristol)



Particles in locally favoured structures (purple) around a selected particle (green) at different time frames.

When liquids are rapidly cooled, their dynamics changes dramatically: the particle motion becomes heterogenous and cooperative, and the relaxation times rapidly exceed any human timescale. Whether a genuine thermodynamic phase transition lies behind such a phenomenology is unknown. However, when computing time-integrated quantities, a measurable, well-defined transition in the space of multiple realisations of the liquid dynamics (trajectories) naturally emerges. Employing the concepts of locally favoured structures and large deviations of time-integrated observables, we show that such dynamical phase transition corresponds to the existence of two (stable and metastable) liquid states of a model atomistic glass-former, separated by a free energy barrier that vanishes as we lower the temperature. Extrapolation indicates a finite, non-zero temperature at which the metastable, low-energy, structure-rich phase would become stable. To complement this scenario, a first experimental evidence of the same dynamical transition is also provided in a supersaturated mixture of poly-disperse colloidal hard-spheres, suggesting that the phenomenology is common to glass-formers of different interactions and fragilities.

Convergent Chaos

Michael Wilkinson (The Open University)

Chaos is widely understood as being a consequence of sensitive dependence upon initial conditions. Despite their overall intrinsic instability, trajectories may be very strongly convergent in phase space over extremely long periods, as revealed by our investigation of a simple chaotic system (a realistic model for small bodies in a turbulent flow). We establish that this strong convergence is a multi-facetted phenomenon, in which the clustering is intense, widespread and balanced by lacunarity of other regions. Power laws, indicative of scale-free features, characterise the distribution of particles in the system. We use large-deviation and extreme-value statistics to explain the effect. Our results show that the interpretation of the 'butterfly effect' needs to be carefully qualified.

This notion of convergent chaos, which implies the existence of conditions for which uncertainties are unexpectedly small, may also be relevant to the valuation of insurance and futures contracts.