# Theory of Condensed Matter Group Scientific Meeting

University of Warwick, Thursday 13th June 2019

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| 10.30 | Arrival and Coffee |
| 11.00 | Andela Šarić, UCL,<br>*Toy models of biological nanomachines* |
| 11.50 | Chris Pickard, Cambridge,<br>*New Directions in Random Search* |
| 12.40 | Lunch |
| 13.40 | Presentation of the Sam Edwards Thesis Prize |
| 13.45 | Sid Parameswaran, Oxford<br>*Topology, Symmetry, and Anomalies in Quantum Hall nematic Domain Walls* |
| 14.35 | Posters (including student poster prize) with tea at 15.30 |
| 16.20 | Shiladitya Banerjee, UCL<br>*Living Tissue as Adaptive Soft Materials* |
| 17.10 | Close |

The meeting will be held off the Warwick Science Concourse.
The ordering of speakers is subject to revision.

Organised by Ryan Barnett (Imperial), Buddhapriya Chakrabarti (Sheffield), and Nicholas d'Ambrumenil (Warwick)

Registration + further details: theory.warwick.ac.uk/events/iop2019

# Posters

1. 2D Statistical Mechanics corresponds to 1D Quantum Mechanics: An explicit construction, Jordan C. Moodie, M. W. Long, *Birmingham*
2. Understanding the Tip Tracking Mechanism of End-Binding Proteins on Microtubules, Lewis Mosby, Daniel Roth, Anne Straube, Marco Polin, *Warwick*
3. Semiclassical dynamics in weakly coupled quasicrystals, Stephen Spurrier and Nigel Cooper, *Cambridge*
4. Fluctuation Spectroscopy in Superconducting Granular Boron-doped Diamond Films, D. T. S. Perkins, R. A. Smith, G. M. Klemencic, J. M. Fellows, *Birmingham*
5. Stark many-body localization, Chris Hooley, Maximilian Schulz, Roderich Moessner, and Frank Pollmann, *St Andrews*
6. Bend Geometry in Liquid Crystals, Joseph Pollard, Jack Binysh & Gareth Alexander, *Warwick*
7. Quantum Simulations Using Photonics, Chris Oliver, Hannah Price, *Birmingham*
8. Strong-coupling Polarons in 1D Bose Condensates, Jonas Jager, Ryan Barnett, *Imperial*, Michael Fleischhauer, Martin Will, *Kaiserslautern*
   We discuss the interaction of a mobile impurity with a surrounding BE condensate forming a Bose polaron. For high BEC-impurity couplings, the standard approach of expanding around a homogeneous condensate does not account adequately for condensate deformatins and thus becomes inappropriate. We present an alternative approach taking into account the condensate deformation already on the mean-field level, for which analytic solutions can be obtained in 1D. The calculated ploaron energy and condensate deplection show excellent agreement with quantum MC simulations and improves on approaches based on expansions around an undepleted BEC. Finally we discuss potential problems in the calculation of a proper polarion mass.
9. Statistics-dependent three-particle quantum walks in 1D lattices, Xiaoming Cai, *Warwick*
10. Truncation of the Active Nematic Lengthscale, Rian Hughes, Jerome Hardouin, Amin Doostmohammadi, Justine Laurent, Teresa Lopez-Leon, Julia M Yeomans, Jordi Ignes-Mullol, Francesc Sagues, *Oxford*
11. Dynamical quantum phase transitions and many-body localization in spin chains with quasiperiodic fields, Leonardo Benini (*Warwick*), Piero Naldesi (*Grenoble*) Rudolf A. Roemer (*Warwick*) and Tommaso Roscilde (*Lyon*)
    We study dynamical properties of many-body localized systems through the lens of dynamical quantum phase transitions (DQPTs) theory. Exploring the quench dynamics of a one-dimensional spin system with a quasi-periodic on-site magnetic field, we show the emergence of a non-analytic structure in the return rate of the survival probability in the many-body localized phase, both close to the transition point and in the strong disorder regime. Quenching from an initially ordered Neel state, we show the appearance of a periodic structure of DQPTs deep in the MBL phase for strong values of the quasi-periodic potential. We then establish a connection between this non-equilibrium structure of peaks in the dynamical free energy and the oscillations of a well-known sensitive measure of memory effects in MBL systems, i.e. the imbalance. Our quantum quench protocols can be effectively realized in ultra-cold atoms setups, exploiting recently established quantum many-body interferometry techniques.
12. A first-principles study of the phase diagram of solid hydrogen, Alice Shipley, John Trail, Richard Needs, *Cambridge*
13. Properties of Bulk SrTiO3 and SrTiO3/LaAlO3 Heterostructures, J. Spink and R. Smith, *Birmingham*

14. A type of robust superlattice type-I Weyl semimetals with four Weyl nodes, Lijun Meng, Jiafang Wu, Jianxin Zhong and Rudolf A Roemer, *Warwick*
We investigate the topological properties of the Janus superlattices WTeS and WTeSe by first-principles methods and Wannier-based tight-binding Hamiltonians. The thermal stability of the Janus structures is checked by first-principles molecular dynamics. The topological properties are identified through node chirality, surface states and surface Fermi arcs. Our calculations reveal that both WTeS and WTeSe are Type-I Weyl semimetals with only four Weyl nodes in the Brillouin zone, which is a minimal number in a time reversal symmetry system. This small number of Weyl nodes makes them an excellent platform to study their topological properties experimentally. The Weyl nodes are located in four different quadrants of the Brillouin zone and consequently the separation of Weyl points in reciprocal space, and the length of Fermi arc, is of the order of the magnitude of the reciprocal lattice vector |Gz| as might be easily observed in experiment. The Weyl nodes have approximately the same energy below the Fermi level and are hence accessible by conventional ARPES. In addition, under external strain, the Weyl semimetal state is more robust than the sister compounds Td-WTe2/MoTe2. Our findings are important to explore Weyl fermion physics and useful for realizing possible applications of Weyl semimetal materials in future topological electronic devices.

15. Magnetic properties of Ni19, Laia Delgado Callicó, Kevin Rossi, Francesca Baletto, *KCL*

16. Grassmannization of the 3D Ising Model , E. Martello, G. G. N. Angilella, L. Pollet, *Birmingham*

17. Truncation of the Active Nematic Lengthscale, Rian Hughes, Jerome Hardouin, Amin Doostmohammadi, Justine Laurent, Teresa Lopez-Leon, Julia M Yeomans, Jordi Ignes-Mullol, Francesc Sagues, *Oxford*

18. Analyses on Representations of Materials for Machine Learning, James Brixey and James Kermode, *Warwick*

19. Long-range Coulomb interactions and non-hydrodynamic behaviour in thermal quenches in spin ice, Oliver Hart, Marianne Haroche and Claudio Castelnovo, *Cambridge*

20. Operator spreading in Hamiltonian systems without symmetries, Ewan McCulloch, *Birmingham*

21. Topological states in chiral active matter: dynamic blue phases and active half-skyrmions, Luuk Metselaar, Amin Doostmohammadi, and Julia M. Yeomans, *Oxford*
Motivated by the common occurrence of chirality in biological systems, we numerically explore pattern formation in active chiral liquid crystals. We show that introducing contractile activity results in stabilised blue phases, while small extensile activity generates ordered but dynamic blue phases characterised by coherently moving half-skyrmions and disclinations. Increasing extensile activity above a threshold leads to the dissociation of the half-skyrmions and active turbulence. We also analyse isolated active half-skyrmions in an isotropic background and compare the activity-induced velocity fields in simulations to an analytical prediction of the flow. Finally, we show that confining an active blue phase can give rise to a system-wide circulation, in which half-skyrmions and disclinations rotate together.

22. Building a Multiscale Model of Crack Propagation in Diamond, Berk Onat and James Kermode, *Warwick*

23. Population simulation methods for parallel computing, Martin Weigel, *Coventry*
We discuss a range of methods based on population annealing, a generalized simulation scheme initially proposed for Monte Carlo sampling of systems with complex free-energy landscapes by Hukushima and Iba. Similarly to parallel tempering, this method, that is formally a sequential Monte Carlo sampling technique, allows to dramatically improve the sampling of systems with many metastable states. Unlike parallel tempering, however, it permits one to naturally make use of an essentially unlimited number of parallel resources, and it is found to scale extremely well up to many thousand cores. In population annealing, a population of independent copies of the studied system are simulated in parallel while sweeping through an external control parameter (typically temperature)

over the range of interest. At each step the population is resampled according to the relative weight of configurations and the changed values of the control parameter. As it is shown here, the method is an extremely flexible meta heuristic that can be combined with Monte Carlo in a range of different ensembles as well as with molecular dynamics. A number of intrinsic features of the approach include the possibility to estimate free energies and the density of states, and a range of natural extensions that make the approach self-adaptive by choosing the temperature, sweep and population protocols in a self-adaptive fashion. We present a detailed analysis of the dependence of bias and statistical errors on the parameters of the approach, in particular the population size as well as the sweep and temperature protocols. A number of applications are discussed, including the sampling of the density of states of frustrated spin systems such as disorder samples from the D-Wave quantum annealer as well as the simulation of biopolymers with population annealing molecular dynamics.

24. Neighbour Correlations and Long Range Interactions in Flocking Models, A E B T King, M S Turner, *Warwick*

25. Edge Distribution of a 1-D Bose Gas, Michael Clark, *Birmingham*
We consider the probability distribution of the last particle in a 1-D harmonically trapped Bose gas. A phenomenon related to the emptiness formation probability. By considering two different interaction regimes we investigate how this distribution changes with interaction strength and hypothesize a link between the two regimes.

26. An Ising Transition of Chessboard Tilings in a Honeycomb Liquid Crystal, William S. Fall, Constance Nürnberger, Xiangbing Zeng, Feng Liu, Stephen J. Kearney, Gillian A. Gehring, Carsten Tschierske and Goran Ungar, *Sheffield*

27. A Rigorous Demonstration of Superconductivity in a Repulsive Hubbard Model, Manjinder Kainth, M.W. Long, *Birmingham*

28. Dynamics of Passive and Active Membrane Tubes , S C Al-Izzi, M S Turner, P Sens & S Komura, *Warwick*

29. Embedded mean-field theory in the linear scaling density functional theory code ONETEP, Joseph C.A. Prentice, Robert J. Charlton, Arash A. Mostofi, Peter D. Haynes, *Imperial*

30. Transport of Bosons in One Dimension, Rory Whelan, *Birmingham*

31. Catastrophic and Defective: Active Flows of Nematic Defect Pairs, Alexander Houston and Gareth Alexander, *Warwick*

32. Goldstone Modes in the Emergent Gauge Fields of a Frustrated Magnet, S. J. Garratt and J. T. Chalker, *Oxford*
The Heisenberg antiferromagnet with uniform nearest-neighbour exchange on the pyrochlore lattice has a ground state that is macroscopically degenerate in the classical limit, and the degrees of freedom within the ground state manifold form an emergent gauge field. Weak exchange randomness lifts this ground state degeneracy and leads to spin glass freezing at a temperature scale set by the disorder. We discuss the low-energy excitations in this frozen state. Since the frozen state spontaneously breaks symmetry under global spin rotations, these excitations are expected to be Goldstone modes. In addition, to be low energy modes, they must be excitations of the emergent gauge field, which is distinguished from the one arising in spin ice materials because it has an intrinsic dynamics inherited from the precessional dynamics of Heisenberg spins. We show how the Halperin-Saslow theory of Goldstone modes in a spin glass must be modified to describe this constrained dynamics.

33. Quantum limits to the superresolution of multiple point sources, Evangelia Bisketzi, Dominic Branford, Animesh Datta, *Warwick*
The resolution of two incoherent point sources is—from a quantum estimation point of view—a wellstudied physical problem. For realistic purposes such as microscopy more complex descriptions involvingmultiple sources will be necessitated. We find that there is a limit to the parameters which can be estimatedwhen resolving multiple point sources in a 1D configuration through the multi-parameter quantum Cramér-Rao bound.

34. Percolation in Fock space and many-body localisation, Sthitadhi Roy, *Oxford*

35. Nucleation rate calculations from seeding methods, Craig Devonport, *Warwick*

36. Swimmers in Smectics, C C Lakey and M S Turner, *Warwick*