Theory of Condensed Matter
Group Scientific Meeting
University of Warwick, Thursday 4th June 2015

10.30	Arrival and Coffee
11.00	**Johannes Lischner**, Imperial
	Theoretical spectroscopy beyond standard
11.50	**Gene Mele,** UPenn and Loughborough,
	Twist and texture in multilayer graphene
12.40	Lunch
13.40	**Zoran Hadzibabic,** Cambridge
	Quantum gas in a box
14.40	Posters (including student poster prize) with tea at 15.30
(14:45	TCM AGM)
16.10	**Matthew Turner**, Warwick,
	Swarming
17.00	Close

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

Organised by Halim Kusumaatmaja, *Durham*, Ryan Barnett, *Imperial*, and Nicholas d'Ambrumenil, *Warwick*

Registration + further details: theory.warwick.ac.uk/events/iop2015

Talk Abstracts

Johannes Lischner, Imperial
Theoretical spectroscopy beyond standard

Spectral functions are measured in photoemission and tunneling experiments. The GW method is the state-of-the-art approach to calculate spectral functions that include many-electron interaction effects beyond density-functional theory. While GW theory has been very successful for the description of quasiparticle excitations in a wide range of physical systems including semiconductors and insulators, other systems and properties require going beyond the standard formalism.

For open-shell systems, such as magnetic molecules or magnetic defects in solids, I have developed a Green's function approach based on the GW approximation. In these systems, the poles of the self energy give rise to the characteristic multiplet structure observed in photoemission experiments. For the calculation of plasmon satellite features in spectral functions, GW plus cumulant theory cures the failure of GW theory which is known to significantly overestimate the separation of quasiparticle and satellite peaks. Finally, I present a first-principles approach to include the coupling of quasiparticles to spin fluctuations, which play an important role in metals, magnets and unconventional superconductors.

Gene Mele, UPenn and Loughborough
Twist and texture in multilayer graphene

Multilayer graphenes feature special functionalities that microscopically arise from the atomic registry when graphene sheets are stacked. These depend on relative lateral translations, rotations and layer symmetry breaking that can occur spontaneously or be induced. This talk will focus on bilayer graphenes (BLG) in which the stacking arrangement varies in space. We examine domain walls where the local stacking order switches from local AB to BA registry, and study the electronic modes at the boundary by analyzing their valley-projected four band continuum models augmented by numerical calculations on a lattice. We then consider the more general family of two dimensional strain-minimizing BLG stacking textures, showing that they are twisted textures of the interlayer displacement field. We study the interactions and composition rules for these elementary textures which permit a unified treatment of stacking point defects, domain walls and twisted graphenes.

Zoran Hadzibabic, Cambridge
Quantum gas in a box

For almost two decades harmonically-trapped ultracold atomic gases have been used with great success to study fundamental many-body physics in a flexible experimental setting. Recently, we achieved the first atomic Bose-Einstein condensate in an essentially uniform potential of an optical-box trap [1]. This opened new possibilities for closer connections with other many-body systems and the theories that rely on the translational symmetry of the system. I will give an overview of our first experiments on this new system, including the study of the (Kibble-Zurek) dynamics of spontaneous symmetry breaking in a quenched homogeneous gas [2].

References:
[1] A. L. Gaunt et al., Phys. Rev. Lett. 110, 200406 (2013) [2] N. Navon et al., Science 347, 167 (2015)

Matthew Turner, Warwick**,**
Swarming

The interactions between swarming animals are usually assumed to be local. Recent observations of orientation correlation functions in starling flocks are only local in a weak, topological sense [1]. We propose a natural "most simple" form for interactions that are consistent with the use of vision and therefore non-local [2]. Using an agent-based model we compare with experimental data on bird flocks and identify several emergent phenotypes. In an attempt to move towards a continuum model I draw an analogy with photo-thermophoretic colloids that respond to light in a way that shares some similarities with vision [3]. In our work there is a focussed external light source and the system undergoes a first order transition to a compact state that shares one of the primary organisational features seen in bird flocks [4].

References:
[1] A. Cavagna et al., Scale-free correlations in starling flocks, PNAS 107, 11865 (2010)
[2] D. J. G. Pearce, A. Miller, G. Rowlands and M. S. Turner, The Role of Projection in the Control of Bird Flocks, PNAS 111, 10422 (2014)
[3] J. A. Cohen and R. Golestanian, Emergent cometlike swarming of optically driven thermally active colloids, PRL 112, 068302 (2014)
[4] A. Tamsett, G. Rowlands and M. S. Turner, in preparation (2015)

POSTERS

1. Soft particles in confining potentials - **Austin Tomlinson**, *Birmingham*
   We numerically and analytically study systems of soft particles in confining potentials. We develop models that tell us when and how phase transitions occur, and how tuning confinement can affect the system. Typically, we parameterise these systems by the number of chains of particles that form. Transitions are usually a change in the number of chains, such as the well-studied zig-zag transition when a single chain of particles bifurcates into two chains. We study transitions for much higher numbers of chains in some systems and present the most recent results for interesting geometries.

2. First-Principles simulation of Functional Interfaces - **Ebiyibo Collins Ouserigha**, *Warwick*

3. Edge instabilities in interacting Bose gases - **Bogdan Galilo, Ryan Barnett & Derek Lee**, *Imperial*

4. Calculation of Interfacial Free Energies for Two-Phase Systems via Capillary Waves – **Michael Ambler & David** Quigley, *Warwick*

5. Curvature induced phase separation in cubic phases - **Fabien Paillusson**, *Lincoln* & **Halim Kusumaatmaja**, *Durham*

6. Polyomino tiling and two-dimensional self-assembly - **Joel Nicholls, David Quigley & Gareth Alexander**, *Warwick*

7. Order-by-disorder degeneracy lifting of interacting bosons on the dice lattice - **Matjaz Payrits & Ryan Barnett**, *Imperial*

8. Modelling the Dissipative Transport in the Quantum Hall Regime – **Poppy Asman**, *Warwick*

9. Quantum Multicriticality - **Greg Oliver**, *Birmingham*
   Several quantum critical compounds have been argued to have instabilities towards both ferro- and antiferromagnetic order. We present an analysis of a quantum multicritical point in an itinerant magnet with competition between ferro- and antiferromagnetic order, modelled using Hertz-Millis theory. We perform a one-loop renormalization group treatment of our action in the presence of multiple dynamic exponents. We conclude that in two and in three dimensions, when both quantum critical ferro- and antiferromagnetic fluctuations are present in a system, the specific heat, thermal expansion and Gr\"{u}neisen parameter obey the same laws as predicted for a ferromagnetic quantum critical point. The antiferromagnetic correlation length and boundary of the ordered phase are suppressed by the dangerously irrelevant interactions with quantum critical ferromagnetic fluctuations. We find no difference between a quantum bicritical point and a quantum tetracritical point.

10. The Local and Long-wavelength Time-Scales of Dimer Dynamics - **T. Oakes, J. P. Garrahan, and S. Powell**, *Nottingham*

    We probe the dynamics of a fully packed dimer model on the square lattice using a local dynamical evolving Monte Carlo algorithm. This allows us to study the system in different flux sectors, which are strictly independent. We confirm the predictions about the diffusive nature of the long-wavelength properties (such as static and dynamic correlations) proposed by Henley [1]. However when we look at the persistence for this model, we see that local relaxation is more cooperative than what this would suggest. This is indicated by a stretched exponential form of the persistence function and also evident by looking at the relaxation patterns which show that at higher fluxes relaxation is heterogeneous. In fact at very high flux we can define objects called "strings" which dictate the propagation of local dynamics through the system. These strings allow us to describe both the local and long-wavelength properties of the system.

    References:

    [1] Christopher L Henley. Relaxation time for a dimer covering with height representation. Journal of statistical physics, 89(3-4):483–507, 1997.

11. Occurrence of rogue waves in optical fibers - **A. Savojardo , M. Eberhard & R. Roemer**, *Warwick*

12. Non-Fermi-liquid behaviour and anomalous suppression of Landau damping in layered metals close to ferromagnetism - **S.P. Ridgway & C.A. Hooley**, *St. Andrews*

13. Machine Learning for Structure Prediction of Nanotube-Encapsulated Crystals – **Sam Brown**, *Warwick*

14. Metamagnetism in Bilayer Strontium Ruthenate Sr3Ru4O7 - **Matthew Robson**, *Birmingham*

    Bilayer Strontium Ruthenate Sr3Ru4O7 is a metal which is on the verge of ferromagnetism. It is well-known that the system undergoes a metamagnetic transition under the application of a magnetic field[1,2]. In addition, the the Fermi surface is well understood from Photoemission experiments, and is in good agreement with Density Functional Theory calculations which have been performed[3]. The electronic structure is therefore well-understood. We have modelled the electrons in the system using the standard tight-binding description together with an on-site Coulomb energy U and Hund coupling J. A mean field theory solution to the model reproduces the metamagnetic transition, and shows it is associated with the disappearance of a Fermi surface.

    References:

    [1] R. S. Perry, L. M. Galvin, S. A. Grigera, L. Capogna, A. J. Schofield, A. P. Mackenzie, M. Chiao, S. R. Julian, S. I. Ikeda, S. Nakatsuji, Y. Maeno, C. Pfleiderer, Phys. Rev. Lett. 86, 2661 (2001)

    [2] E. Omichi, Y. Yoshida, S. I. Ikeda, N. V. Mushunikov, T. Goto, T. Osada Phys. Rev. B

67 024432 (2003)
[3] A. Tamai, M. P. Allan, J. F. Mercure, W. Meevasana, R. Dunkel, D. H. Lu, R. S. Perry, A. P. Mackenzie, D. J. Singh, Z.-X. Shen, F. Baumberger Phys. Rev. Lett. 101 026407 (2008)

15. Leaf-to-leaf distances and their moments in finite and infinite m-ary tree graphs - **A. M. Goldsborough, S. A. Rautu & R. A. Römer**, *Warwick*

16. Ferromagnetic--nematic order and strongly correlated phases of fermions in optical flux lattices - **Simon C. Davenport & Nigel R. Cooper**, *Cambridge*

17. FelixSim : A new, free, open source Bloch wave simulation program - **K Evans, R Beanland, R. Roemer & A Hubbert**, *Warwick*

18. Quantum Quenches in Chern Insulators **- M. D. Caio, N. R. Cooper & M. J. Bhaseen**, *King's College London*

19. Disorder Effects in Silicene Nanoribbons - **C. D. Nunez, L. Rosales, P. Orellana, F. Dominguez-Adame & R. Roemer**, *Warwick*

20. Correlations in Stacked, Frustrated Triangular Ising systems - **Dillon T. Liu, J.T. Chalker**, *Oxford*

21. Ab initio Anderson localisation in Si:P - **E G Carnio, N D M Hine, D Quigley & R A Roemer**, *Warwick*

22. Manipulating the Lifshitz transition in bilayer graphene - **A. Varlet, M. Mucha-Kruczynski, D. Bischoff, P. Simonet, T. Taniguchi, K. Watanabe, V.I. Fal'ko, T. Ihn & K. Ensslin**, *Bath*

23. Modelling of defects around nanoparticles in nematic liquid crystals – **Anja Humpert**, *Warwick*

24. Magnetism in Rare Earth Quasicrystals: RKKY Interactions and Ordering - **Stefanie Thiem & J. T. Chalker**, *Oxford*

25. Multiscale modelling of materials chemomechanics: from catastrophic brittle fracture to stress corrosion cracking – **James Kermode**, *Warwick*
Fracture is the dominant failure process underlying many materials reliability issues. At the same time, it remains one of the most challenging 'multi-scale' modelling problems, requiring both an accurate description of the chemical processes occurring in the near tip region and the inclusion of a much larger region in the model systems. These requirements can be met simultaneously by combining a quantum mechanical description of the crack tip

with a classical atomistic model that captures the long-range elastic behaviour of the surrounding crystal matrix, using a QM/MM (quantum mechanics/molecular mechanics) approach such as the `Learn on the Fly' (LOTF) scheme [1], or more recently a novel information-efficient Machine Learning extension of LOTF, where the results of all QM calculations are stored in a database and used to predict forces on new configurations whenever possible, thus calling upon QM only when it is strictly necessary [2]. Examples of the application of these techniques to 'chemomechanical' processes, where complex and interrelated chemical and mechanical processes that originate at the atomic scale go on to determine the mechanical behaviour of a material, include low-speed dynamical fracture instabilities in silicon [3], interactions between moving cracks and material defects such as dislocations or impurities [4], very slow crack propagation via kink formation and migration, and chemically activated fracture, where cracks advance under the concerted action of stress and corrosion by chemical species such as oxygen or water [5]. Stress-corrosion cracking in silica is the subject of ongoing work, as is expansion of the approach model the mechanical properties of nickel-based superalloys.

References:
[1] G. Csányi, T. Albaret, M. Payne and A. De Vita, Phys. Rev. Lett. 93, 175503 (2004).
[2] Z. Li, J. R. Kermode and A. De Vita, Phys. Rev. Lett. 114, 096405 (2015).
[3] J. R. Kermode et al., Nature 455, 1224-1227 (2008).
[4] J. R. Kermode, et al., Nat. Commun. 4, 2441 (2013).
[5] A. Gleizer, G. Peralta, J. R. Kermode, A. De Vita and D. Sherman, Phys. Rev. Lett. 112, 115501 (2014)

26. Surveying the Free Energy Landscapes of Continuum Models: Applications to Soft Matter Systems – **Halim Kusumaatmaja**, *Durham*