IOP Theory of Condensed Matter Group Scientific Meeting and AGM

University of Warwick, Thursday 18 December 2008

10.30 Arrival and Coffee

11.00 **Christian Ruegg,** UCL
Controlling Quantum and Thermal Melting in Magnets

11.50 **Jorge Kurchan,** PMMH, Ecole Supérieure PCI, Paris
Jamming versus Glass Transitions

12.40 Lunch

13.30 IoP Condensed Matter Theory Group AGM.
There will be an election to fill any vacancies arising on the committee of the IOP TCM group. Nominations, along with any items for discussion, should be sent to the Group Secretary Dr Derek Lee (Department of Physics, Imperial College, London SW7 2AZ, UK. Email: dkk.lee@imperial.ac.uk.

13.50 **Daan Frenkel**, Cambridge
Dense Packing and Beyond

14.40 Posters (including student poster prize) with tea at 15.30

16.00 **Igor Lerner**, Birmingham, *Jumps in current-voltage characteristics in 2D structures near a superconductor-insulator transition*

16.50 Close

The meeting will be held in the Warwick Physics Building.
The ordering of speakers is subject to revision.
Organised by Nicholas d'Ambrumenil, *Warwick,* and Chris Hooley, *St Andrews*

Registration + further details: theory.warwick.ac.uk/events/iop2008

THE UNIVERSITY OF WARWICK

MIDLANDS PHYSICS ALLIANCE GraduateSchool

ABSTRACTS

Jamming versus Glass Transitions, Jorge Kurchan, *PMMH Paris*

The traditional way to introduce the glass transition is to imagine (super)-cooling a liquid at slower and slower rates. In the limit of infinitely slow cooling, one conjectures there is an 'ideal glass' temperature at which the system freezes into a true equilibrium solid, with permanent, though aperiodic, density modulations. At the ideal glass transition, certain correlations, whose nature we do not fully understand, diverge. A completely different approach originates in the statics of frictionless spherical particles. Such a system is in 'isostatic' equilibrium, meaning that every single contact is necessary for its stability. The marginality of such an arrangement leads to diverging susceptibilities and lengths. The question is then, are these diverging lengths related at all with the ideal glassy order?

Jumps in current-voltage characteristics in 2D structures near a superconductor-insulator transition, Igor Lerner, *Birmingham*

We argue that giant jumps of current at finite voltages observed in disordered films of InO, TiN and YSi manifest a bistability caused by the overheating of electrons. The jumps occur between an overheated low-resistive state and an almost-at-equilibrium high-resistive state, which are stable at the same voltage. Such a bistability exists provided that (i) cooling of electrons is inefficient and (ii) the temperature dependence of the equilibrium resistance, R(T), is steep enough. Taking the experimental R(T) and assuming a phonon mechanism for the cooling with allowance for its strong suppression by disorder, we describe the I-V characteristics without involving adjustable parameters and reach a quantitative agreement with experiment

In collaboration with V E Kravtsov (ICTP), B L Althsuler and I L Aleiner (Columbia NY)

POSTERS

1. **Novel Soluble Potentials Related to the Harmonic and Isotonic Oscillators**,
   Jonathan Fellows, *Birmingham*

2. **Full counting statistics as geometry**,
   Y Sherkunov, A. Pratap, J. Zhang, N. d'Ambrumenil, B. Muzykantskii, *Warwick*

3. **Classical to quantum mappings for geometrically frustrated systems**,
   Stephen Powell and J. T. Chalker, *Oxford*

4. **Fractal Weyl Law in Mixed Phase Space**,
   Marten Kopp, Henning Schomerus, *Lancaster*

5. **Classical Diffusion of a Particle in a One Dimensional Random Potential**
   Gareth Woods, *Birmingham*

6. **A diagrammatic route to fundamental measure theory for hard spheres**
   Gavin Leithall and Matthias Schmidt, *Bristol*

7. **Monte Carlo Simulation of Discotic Liquid Crystals**,
   Paul A. O'Brien, Michael P. Allen, David L. Cheung, *Warwick*

8. **Transient shear banding in models with a monotonic constitutive curve**,
   JM Adams (*Cambridge)*, SM Fielding (*Manchester*) & PD Olmsted (*Leeds*)

9. **Inhomogeneous magnetic phases: a LOFF-like phase in Sr3Ru2O7**
   A.M. Berridge, A.G. Green, S.A. Grigera, B.D. Simons, *Cambridge*

10. **Two dimensional frustrated magnets in high magnetic field**,
    Luis Seabra, Nic Shannon, P. Sindzingre, T. Momoi, B. Schmidt and P. Thalmeier, *Bristol & Dresden*

11. **Magnetic surface reconstruction in frustrated magnets**
    Melanie Hopper, Martin Long (*Birmingham*), Dr Jorge Quintanilla (*RAL*)

12. **Quantum Quenches in Extended Systems**,
    Spyros Sotiriadis, John Cardy, *Oxford*

13. **Theoretical modelling for exchange interactions in organic molecules**,
    Wei Wu, Andrew Fisher, Tony Harker, Marshall Stoneham (*UCL*), Nicolas Harrison (*Imperial*)

    Here we present Green's function perturbation theory and Density function theory calculations for exchange interactions in organic molecules including Copper-Phthalocyanines (CuPc) [1, 2] and di-radical-spin coupler system [3]. These calculations also represent different methods to control the exchange interactions between or within molecules; we can either control the inter-molecule exchange interactions by changing structures or electronically control the exchange interaction within the molecule.
    The Green's function perturbation theory calculation and DFT calculation for CuPc share a consistent trend with experiments which show the exchange interaction is strongly dependent on the stacking angle of molecules. Especially DFT calculations are in a remarkably good quantitative agreement with magnetic measurements [1].
    We also calculate the exchange interactions within di-radical-spin coupler systems: optically excited Di-Phenyl-Anthracene (DPA) and Coronene. Our theoretical results for the exchange interaction in DPA are consistent with time-resolved Electron Paramagnetic Resonance (TREPR) experiments on DPA in which

an optically controlled magnetic switching is observed and demonstrated [3]. The trend of exchange interaction as varying the dihedral angle is also found through DFT calculations. For Coronene the exchange interaction is much stronger than DPA as expected, but has different sign.

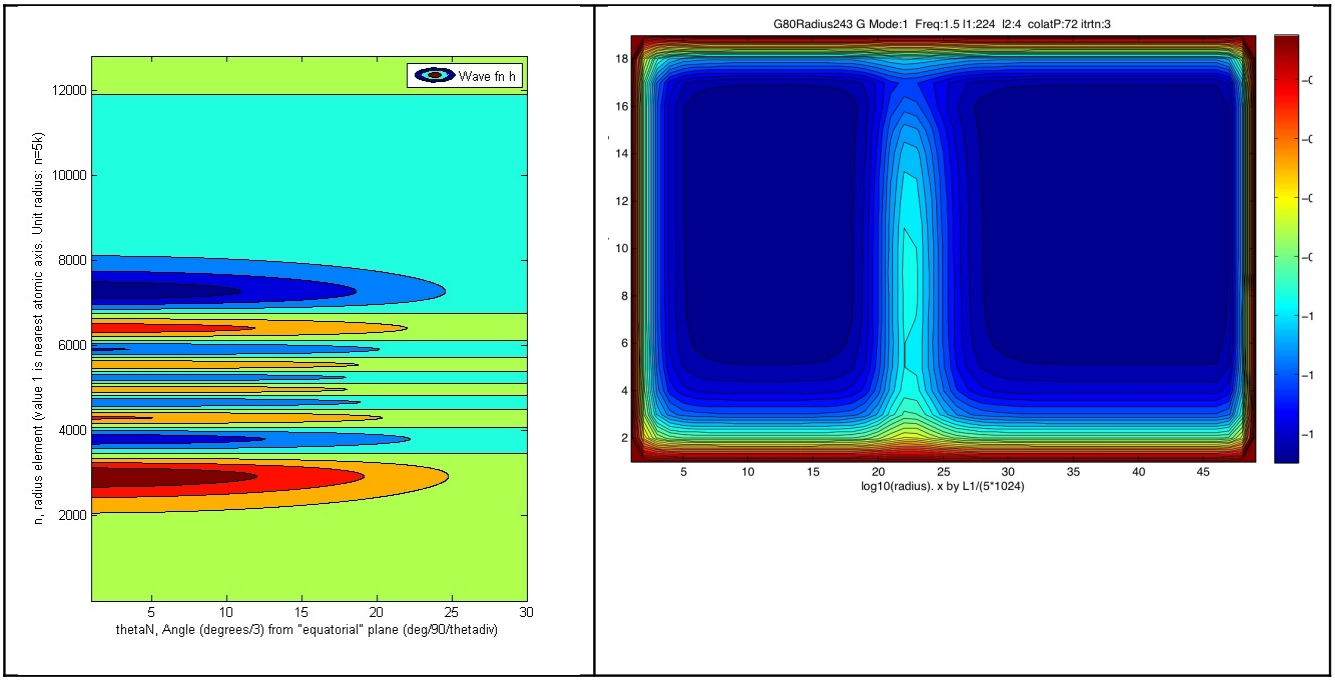
[1] Wei Wu, A. Kerridge, A. H. Harker, and A. J. Fisher, Phys. Rev. B 77 184403 (2008).
[2] S. Heutz, C. Mitra, Wei Wu, A. J. Fisher, A. Kerridge, A.M. Stoneham, A. H. Harker, J. Gardener, H.-H. Tseng, T. S. Jones, C. Renner, and G. Aeppli, Advanced Materials 19 3618 (2007).
[3] Y. Teki, M. Nakatsuji, and Y. Miura, Molecular Physics 100 1385 (2002).

14. CdSe Nanocrystals under pressure by metadynamics,
Giorgia Fugallo,Clive Bealing, Roman Martonak, Carla Molteni, *KCL*

CdSe is an interesting material because of its efficient room temperature electro-luminescence and nano-electric device applications. In particular CdSe nanocrystals exhibit a range of interestig properties that can be tuned with their size: from the colours they fluoresce with to the way they change structure under pressure. By using and adapting the metadynamics method, which is able to accelerate rare events and to explore the free energy surface of complex systems, we have simulated structural transformations in CdSe nanocrystals close to the transition pressure, without the need to overpressurize the systems typical of conventional constant pressure molecular dynamics. Results for CdSe nanocrystals of different size and shapes will be presented.

15. Quantum Criticality in Itinerant Ferromagnetic Materials,
Martin Lawley, *Birmingham*

16. Closed Causal Wave Modelling of Bound Electrons,
Christopher Johns, *Warwick Engineering*



17. Possible Orbital Ordering in the Metallic Manganites,
Matthew Brammall, *Birmingham*

18. Monte Carlo simulation of lattice peptides near surfaces,
Adam Swetnam, *Warwick*

19. **Adsorption of a Colloidal Particle at Planar Fluid-Interfaces**,
P. Hopkins, A. J. Archer and R. Evans, *Bristol*

20. **Singlet-Triplet Transitions in Multilevel Quantum Dots**,
Chris Wright and Martin Galpin, *Oxford*

21. **A Riemann-Hilbert Approach to the Non-Equilibrium Kondo Problem**,
James Baldwin, Birmingham

22. **The non-zero temperature statistics of the charge transport in quantum pumps**,
Amitesh Pratap and N. d'Ambrumenil, *Warwick*

23. **Finite Temperature Dynamical Structure Factor of the two-leg Spin-1/2 Heisenberg Ladder**,
W. D. Goetze, U. Karahasanovic, F. H. L. Essler, *Oxford*

24. **Soft quantum matter: a recipe,**
Jorge Quintanilla (1), Sam T. Carr (2), Joseph J. Betouras (3) (1) ISIS Facility, STFC Rutherford Appleton Laboratory (2) School of Physics & Astronomy, University of Birmingham (3) School of Physics & Astronomy, University of St. Andrews

Strongly correlated quantum matter (from high-temperature superconductors, through oxides and heavy fermions to quantum Hall devices) remains an outstanding scientific challenge. In it, electron itineracy survives in spite of strong interactions. A general framework was proposed for its understanding by Kivelson, Fradkin and Emery in 1998. It rests on liquid crystalline phases intervening between the Fermi gas and the Wigner crystal or Mott insulator as the strength of correlations increases. In this work we propose an alternative realisation of the relevant physics in an ultra-cold atomic gas. It exploits optical lattices and dipolar interactions to realise a particularly simple model which can be tuned systematically. We analyze theoretically the system and discover that three phase transitions compete: a meta-nematic, quasi-1D to 2D transition, where inter-chain interaction leads to the closing of the Fermi surface; a transition into a striped phase; and crystallisation of the fermions into a `checkerboard' pattern.

25. **Spin dynamics in geometrically frustrated Heisenberg models**,
P.H Conlon and J.T Chalker, *Oxford*

26. **Elementary Events of Electron Transfer in a Varying-Potential Quantum Point Contact**,
Jin Zhang, Yury Sherkunov, N. d'Ambrumenil, *Warwick*

27. **Spontaneous Breakdown of Unitarity in the Thermodynamic Limit**,
J van Wezel, *Cambridge*

28. **Exciton storage in nano-scale Aharonov-Bohm rings with electric field tuning**
Andrea Fischer (*Warwick*), Vivaldo L. Campo Jr. (*São Carlos*), Mikhail E. Portnoi (*Exeter*) and Rudolf A. Römer (*Warwick*)

We study analytically the optical properties of a simple model for an electron-hole pair on a ring subjected to perpendicular magnetic flux and in-plane electric field. We show how to tune this excitonic system from optically active to optically dark as a function of these external fields. Our results offer a simple mechanism for exciton storage and read-out.

29. **Multiparticle Interference in Electronic Mach-Zehnder Interferometers**, D. Kovrizhin and J.T. Chalker, *Oxford*

30. **Population imbalanced atomic Fermi gas ferromagnetism**,

GJ Conduit and BD Simons, *Cambridge*

We investigate ferromagnetic ordering in an itinerant ultracold atomic Fermi gas with repulsive interactions and population imbalance. In a spatially uniform system, we show that at zero temperature, the transition to the itinerant magnetic phase is first order into a fully-magnetized state. Drawing on these results, we elucidate the phases present in a trapped geometry, finding three characteristic types of system with increasing population imbalance. Finally, we outline the potential experimental implications of the work.

31. Probability Density Function at the 3D Anderson Transition,
A. Rodriguez, L. Vasquez and R. Roemer, *Warwick*

The probability density function (PDF) for the wavefunction amplitudes is studied at the metal-insulator transition of the 3D Anderson model, for very large systems up to $L^3 = 240^3$. The implications of the multifractal nature of the state upon the PDF are presented in detail. A formal expression between the PDF and the singularity spectrum $f(\alpha)$ is given. The PDF can be easily used to carry out a numerical multifractal analysis and it appears as a valid alternative to the more usual approach based on the scaling law of the general inverse participation rations.

32. A simple model for the magnetic structure of nanoclusters near a surface,
M. dos Santos Dias and J.B. Staunton, *Warwick*
A simple model is presented that allows one to derive the magnetic structure of arbitrary nanoclusters near a surface. This is done in the context of multiple scattering theory, which provides a suitable way of expressing the interaction between the atoms of the cluster, via the so-called Lloyd's formula. The relativistic treatment of the scattering processes between the atoms of the cluster reveals the magnetic anisotropy energy. This allows one to access the angular dependence of the energy via its analytical derivatives with respect to arbitrary rotations of the cluster magnetic moments. The model aims at a qualitative description of these systems, so the atoms are modelled by standard spin-dependent atomic potentials, and are embedded in a free electron gas terminated by a perfectly reflecting surface. Fully self-consistent materials-specific ab-initio calculations can be found elsewhere, and are referred to for the purpose of discussion of their qualitative features.

33. Triple Quantum Dots: Frustration and Phase Transitions,
Andrew Mitchell and Thomas Jarrold, *Oxford*

34. DNA charge transport and bioinformatics,
S.A. Wells, R. Romer, C.T. Shih, *Warwick*

35. A simple theory of the invar effect in iron-nickel alloys,
F. Liot and C. Hooley, *St Andrews*

36. Sensitivity of protein rigidity analysis to small structural variations: a large-scale comparative analysis

S.A. Wells, J E Jimenez-Roldan, R.A. Roemer, *Warwick*

Rigidity analysis using the "pebble game" can usefully be applied to protein crystal structures to obtain information on protein folding, assembly and the structure-function relationship. However, previous work using this technique has not made clear how sensitive rigidity analysis is to small structural variations. We present a comparative study in which rigidity analysis is applied to multiple structures, derived from different organisms and different conditions of crystallisation, for each of several different proteins. We find that rigidity analysis is best used as a comparative tool to highlight the effects of structural variation. Our use of multiple protein structures brings out a previously unnoticed peculiarity in the rigidity of trypsin.

37. Orbital moment of the chiral superconductor Sr_2RuO_4,

JF Annett (*Bristol*), B. Gyorffy (*Bristol*), K.I. Wysokinski (*M. Cure University, Lublin*)

The existence and magnitude of a bulk orbital angular momentum of the condensate chiral a phase in superfluid helium-3 is a longstanding matter of controversy. The analogous problem in a chiral p-wave superconducting material is the existence of a finite orbital magnetic moment in the bulk. In Sr_2RuO_4 the existence of such an orbital moment is strongly suggested by experimental evidence for spontaneously time reversal symmetry breaking (TRSB) in the superconducting state, but the theories disagree on the expected magnitude of this moment. We show that a non-zero orbital magnetization density arises natually in a realistic band model for Sr_2RuO_4, and its temperature dependence is qualitatively similar to those of the muSr and Kerr effect experimental results. The simplest model which leads to the orbital moment requires at minimum two degenerate atomic orbitals per Ru, which correspond to the Ru d xz and d yz states. This is in contrast to the theories of orbital angular momentum in the isotropic superfluid 3-He, or models of orbital moment in Sr_2RuO_4 which assume only a single band at the Fermi level. The implications of this surprising result are explored.

38. A Relationship of Mean-Field Theory for a Driven Lattice Gas to an Exact Equilibrium Density Functional, W.S. Brams Dwandaru and Matthias Schmidt, Bristol

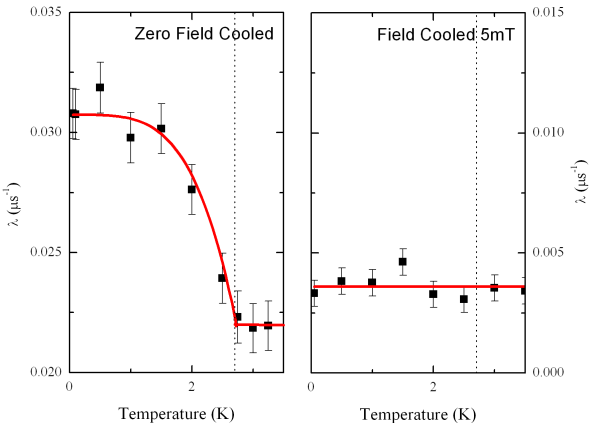
We consider the totally asymmetric exclusion process (TASEP) of particles on a one-dimensional lattice that interact with site exclusion and are driven into one direction only. The mean-field approximation of the dynamical equation for the one-particle density of this model is shown to be equivalent to the exact Euler-Lagrange equations of density functional theory for the equilibrium density profiles of a binary mixture. In this mixture particles occupy one (two) lattice sites corresponding to resting (moving) particles in the TASEP. Despite the strict absence of bulk phase transitions in the equilibrium mixture, the influence of density-dependent external potentials is shown to induce abrupt changes in the one-body density that are equivalent to the exact out-of-equilibrium phase transitions between steady states in the TASEP with open boundaries. This proposed relationship suggests that one can construct systematically mean-field-approximation for other driven models by considering corresponding inhomogeneous equilibrium mixtures. Preliminary results are shown for two-dimensional versions of the TASEP and a junction of two TASEPs.

39. Experiment-theory collaboration in Harwell: broken time-reversal symmetry and non-unitary pairing in a non-centrosymmetric superconductor, A.D. Hillier, J. Quintanilla (*RAL*), and R. Cywinski (*Huddersfield*)

Symmetry breaking is a central concept of physics for which superconductivity provides a paradigm. In a conventional superconductor gauge symmetry is broken, while unconventional superfluids and superconductors break other symmetries as well. Recently, superconductivity has been discovered in a number of materials whose lattices lack inversion symmetry, with important implications for the symmetry of the superconducting state. However despite intense theoretical and experimental efforts the issue of symmetry breaking in these systems remains uncertain. One of the most direct ways of detecting an unconventional superconducting state is muon spin relaxation (μSR), as it can unambiguously establish broken time reversal symmetry (TRS).

Here we report the results of muon spin relaxation experiments on the non-centrosymmetric intermetallic superconductor $LaNiC_2$ (Tc=2.7K) and a group-theoretic analysis of the implications of the data for the pairing symmetry. We find that the onset of superconductivity coincides with the appearance of spontaneous magnetic fields, implying that in the superconducting state time reversal symmetry is broken. We find only four states compatible with this observation, all of which feature non-unitary triplet pairing i.e. they are analogous to the A1 phase of superfluid ^{3}He in an external magnetic field (though, intriguingly, no external field is required in this case). Moreover one of these possible states corresponds to triplet pairing with the full point group symmetry of the crystal, which is only possible in a non-centrosymmetric superconductor.

The left figure is the temperature dependence of the electronic relaxation rate, λ, for $LaNiC_2$ in zero-field, which clearly shows the spontaneous fields appearing at T_C=2.7 K (dotted line). The right figure is the temperature dependence of λ for an applied field of 5 mT, in which a flat temperature dependence is observed as expected if the observed fields in the absence of the field are static on the timescale of the muon. The red lines are guides to the eye.



40. Hydrogen bonding and dynamic crossover in Polyamide-66: A molecular dynamics simulation study, Paola Carbone (*Manchester*), Hossein Ali Karimi Varzaneh and Florian Müller-Plathe (*Darmstadt*)

By means of molecular dynamics simulations we study the hydrogen-bonds dynamics and thermodynamics of bulk of polyamide-66 in a broad range of temperatures (300 K to 600 K). We show that different dynamic properties (the structure relaxation time, the orientational time correlation function of the amide groups and self diffusion coefficient) of unentangled polyamide-66 undertake a crossover transition in the same small temperature range (~ 413 K) above the experimental glass transition temperature (350 K). The data can be fitted to a Vogel-Fulcher-Tammann law for T> 413 K and to an Arrhenius equation for T< 413 K. Our results show that the global dynamics of polyamide-66 is intimately related to the relaxation of the hydrogen-bond network formed among the amide groups. The presence of a dynamic crossover at a temperature slightly higher than the glass transition one is in agreement with the more recent experimental data and glass theories.

41. **Feshbach interacting 40K atoms in a deep 1D optical lattice**. Tanja Duric, Derek K. K. Lee (*Imperial*), and Andrew F. Ho (*RHUL*)