Theory of Condensed Matter Group Scientific Meeting

University of Warwick, Thursday 7th June 2018

10.30 Arrival and Coffee

11.00 **Alexandra Olaya-Castro**, UCL
Bridging quantum science and biology

11.50 **Bartomeu Monserrat**, Cambridge
Hot materials: first principles calculations at room temperature

12.40 Lunch

13.40 **Silke Henkes,** Aberdeen
Polar and nematic active materials in curved geometries

14.20 Presentation of the Sam Edwards Thesis Prize

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

16.10 **Curt von Keyserlingk**, Birmingham
Many body Floquet phased of matter: Time crystals and SPTs

17.00 Close

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

Organised by Andrew Morris and Hannah Price, *Birmingham,* Bonnie Tsim, *Manchester,* Nicholas d'Ambrumenil, *Warwick*

Registration + further details: theory.warwick.ac.uk/events/iop2018

IOP Institute of Physics
Theory of Condensed Matter Group

WARWICK
THE UNIVERSITY OF WARWICK

Posters

1. Ab-initio theory of magnetic ordering in Mn3A (A=Sn, Pt, Ga, Ge): pair- and multi-spin interactions from fluctuating local moments, Eduardo Mendive Tapia and Julie B Staunton, *Warwick*

2. From Single-Particle Excitations to Sound Waves in a Box-Trapped Atomic BEC, S. J. Garratt, C. Eigen, J. Zhang, P. Turzak, R. Lopes, R. P. Smith, Z. Hadzibabic and N. Navon, *Oxford*

3. A preconditioning scheme for Minimum Energy Path finding methods, Stela Makri, James Kermode, and Christoph Ortner, *Warwick*,
In transition state theory, the study of thermally activated transi- tions between energy minima is achieved by finding minimum energy paths connecting the minima. These paths provide information on the energy barrier and reaction rates of the system without going through long and expensive simulations. To find them, current techniques use steepest descent-like minimisation to relax a discretised initial guess. However, steepest descent typically gives slow convergence rates in the presence of ill-conditioned potentials. I am presenting a precondition- ing scheme that reduces the condition number of the potential of a system in order to improve the convergence speed and robustness of minimum energy path finding methods. The key assumption is that the cost of constructing a preconditioner is much smaller than the cost of computing the potential; for density functional theory the cost of single point evaluations is much more expensive than the computation of a preconditioner and thus the proposed approach improves comput- ing times significantly. We have developed a preconditioning scheme, where the preconditioner acts as a coordinate transformation of the discrete images along the path to aid the ill-conditioning in the trans- verse direction and currently in development it is a preconditioning scheme that considers the interactions between the images as well.

4. Time-reversal symmetry breaking in superconductors through loop Josephson-current order, Sudeep Kumar Ghosh, James F. Annett and Jorge Quintanilla, *Kent*
Recent muon-spin relaxation experiments have found broken time-reversal symmetry (TRS) in a number of superconductors which from other points of view (such as specific heat, penetration depth, sensitivity to impurities etc.) appear to be conventional. We propose a novel superconducting ground state where Josephson currents flow spontaneously between distinct, but symmetry-related, sites within a unit cell. Such Loop Josephson Currents (LJC) break TRS without the need for triplet, inter-site, or inter-orbital pairing i.e. they are compatible with a conventional BCS-type pairing mechanism. The Josephson currents result from a non-trivial phase difference between the on-site pairing potentials on different sites appearing spontaneously at the superconducting critical temperature. We show explicitly how such instability emerges in the Ginzburg-Landau theory of a simple toy model. We estimate the size of the resulting spontaneous magnetization and find it to be consistent with many existing experiments. We discuss the crystal symmetry requirements and apply our theory to the recently discovered family of TRS-breaking, but otherwise seemingly conventional, family of superconductors Re6X (X=Zr, Hf, Ti), showing the possibility of a LJC instability.

5. The metal-insulator transition in doped semiconductors using *ab initio* methods, Edoardo G. Carnio, Nicholas D. M. Hine, Rudolf A. Römer, *Warwick*
The Anderson metal-insulator transition (MIT) has long been studied, but there is still no agreement on its critical exponent ν when comparing experiments and theory. In this work we employ *ab initio* methods to study the MIT in a doped semiconductor. We use linear-scaling DFT to simulate prototypes of sulfur-doped silicon (Si:S). From these we build larger tight-binding models close to the critical concentration of the MIT. When the dopant concentration is increased, an impurity band forms and eventually delocalizes. We characterize the MIT via multifractal finite-size scaling, obtaining the phase diagram and estimates of ν. Our results suggest a possible resolution of the long-standing exponent puzzle due to the hybridization of conduction and impurity bands. We present initial work on the application of this approach to 2D materials, in particular to monolayer transition metal dichalcogenides.

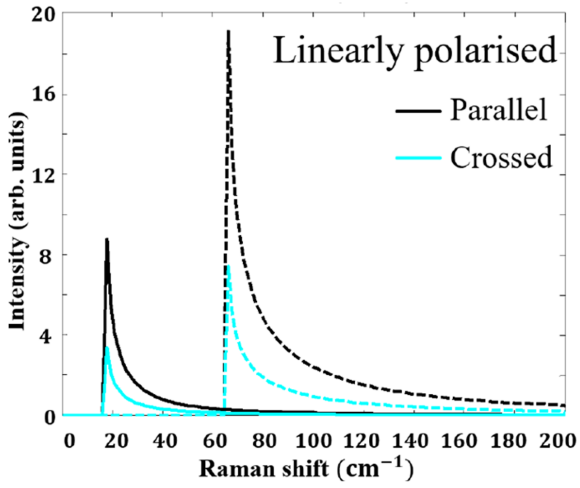
6. Exactness of Bohr-Sommerfeld Quantisation for Two Exactly Soluble Non-Central Potentials, D T S Perkins, R A Smith, *Birmingham*

We demonstrate the integrability of the Hamilton-Jacobi equa- tion for two non-central potentials in spherical polar coordinates, and present complete solutions for the classically bound orbits. We then show that the semiclassical Bohr-Sommerfeld quantisation exactly re- produces the bound state spectra of the corresponding quantum mechanical Schrodinger equations. One of these potentials has previously been analysed in parabolic coordinates; the results for the other are, to the authors' best knowledge, original.

7. Ab-initio theory of magnetic ordering in Mn3A (A=Sn, Pt, Ga, Ge): pair- and multi-spin interactions from fluctuating local moments, Eduardo Mendive Tapia and Julie B Staunton, *Warwick*

8. Superconductivity-induced features in electronic Raman spectrum of monolayer graphene, Aitor Garcia-Ruiz Fuentes, Marcin Mucha-Kruvczynski, Vladimir Fal'ko, *Bath*

Here, we study the Raman spectral features due to electronic excitations in doped monolayer graphene in the presence of superconducting ordering induced, for example, by the proximity effect. We consider an *s*-wave order parameter, with symmetries either A_{1g} or B_{2u} in the D_{6h} group, corresponding to spin singlet and spin triplet, respectively. The opening of a superconducting gap Δ at the Fermi level gives rise to a peak at a Raman shift $\omega \sim \Delta$ with the strength of the signal proportional to the value of the chemical potential as well as Δ, and also depending on the polarization of the incident and detected light. The shape of the peak is the same for both of the symmetry phases and reflects the density of states in the vicinity of the gap (Figure).



9. Modelling Liquid-Ordered Inclusions in Lamellar Bodies, C. C. Lakey and M. S. Turner, *Warwick*

10. Genetic Algorithm-Molecular Dynamics based sampling methodology for positional disordered multicomponent materials,

G. Anand[1,2*], R. Goodall[1], and Colin L. Freeman[1], [1]*Sheffield*, [2]*Warwick*

The sampling of positional-disordered materials poses a significant challenge as the random sampling is not a feasible option as the number of components and size of the system being simulated increases. In view of this, present work presents a hybrid Genetic Algorithm-Molecular Dynamics based methodology for sampling positional-disordered systems. In this work, we have shown that such scheme can be employed along with statistical mechanics based framework for calculation of thermodynamic properties such as configurational entropy of such materials. This work uses a new class of multicomponent substitutional alloys with simple crystal crystal structures (usually BCC or FCC), also known as 'High-Entropy Alloys (HEAs)' as case-studies. We have shown that configurational entropy plays significant role in the phase selection in such positional-disordered alloys. In this work, we have been able to compare the configurational entropies of BCC and FCC form of CoCrFeNi, $Al_{0.5}$CoCrFeNi, AlCoCrFeNi and CoCrFeNiTi HEAs. Additionally, we have been able to point out the entropy stabilisation mechanism as function of temperature in such HEAs.

11. Regulation of structure and functional properties of the 1D nanowires via confinement within single-walled carbon nanotubes, A. Vasylenko, S. Marks, J. M. Wynn, P. V. C. Medeiros, A. Morris, J. Sloan, D. Quigley, *Warwick*

12. An exact power series representation of the Baker-Campbell-Hausdorff formula, Jordan C. Moodie & Martin W. Long, *Birmingham*

13. Time reversal of the overdamped Langevin equation and its application to polymer diffusion, O T Dyer and R C Ball, *Warwick*

14. Topology of quantum systems out of equilibrium, Max McGinley and Nigel Cooper, *Cambridge*

15. Exchange-mediated dynamic screening in the integer quantum Hall effect regime", Rudolf Roemer, *Warwick*

16. Hidden charge order of interacting Dirac fermions on the honeycomb lattice, Elliot Christou, Bruno Uchoa, Frank Kruger, *UCL*

17. Nucleation Rates Via Seeding Methods, Craig Devonport, D Quigley, *Warwick*

18. p-Orbital Superfluid with S5 Manifold, Simon Lieu[1], Andrew F. Ho[2], Derek K. K. Lee[1] and Piers Coleman[3,2,1], [1]*Imperial*, [2] *Royal Holloway UL*, [3] *Rutgers*

19. Spin transport and filtering in the presence of disorder, Leonardo Benini, *Warwick*

20. Sign reversing quantum oscillations in thermopower and enhanced Nernst response in type-II semi-metallic WTe2, asil K. Dejene, G. Rana, N. Kumar, C. Rajimati, K. Sklare, C. Felser and S. S. P. Parkin, *Loughborough*

21. Renormalisation Group Study of the Integer Quantum Hall Effect with Geometric Structural Disorder, Benoit Assi, *Warwick*

22. Mott Point Distribution of a Single Electron, Manjinder Kainth, Martin Long, *Birmingham*

23. Hybrid QM/MM study of the effect of plasma components on dislocation glide and core structure in tungsten, Petr Grigorev, James Kermode, *Warwick*

24. Hydrodynamic instabilities in membrane tubes, Sami C Al-Izzi, Pierre Sens and Matthew S Turner, *Warwick*