Oxford Condensed Matter Theory Programme Grant, 1998-2002: IGR Report

Background/Context

The proposal for this Grant was originally submitted as a renewal of the Oxford Condensed Matter Theory Rolling Grant, which had been in existence for some years. After the proposal was submitted we were informed that the Rolling Grant would not be continued, but that the proposal would be considered for a four-year Programme Grant, with a suitably revised budget to cover all four years. This Report is on that Grant. Because the original proposal was divided into projects put forward by each individual investigator, it seems proper to adhere to that division in describing the results. Nevertheless, in carrying out the individual projects, we endeavoured to integrate them as much as was feasible into a coherent programme, especially in respect of the PDRA appointments. Each PDRA was assigned to a particular investigator and to specific projects, although in several cases they also carried out work related to other projects in the programme. The individual reports of the PDRAs (available as an Annex) show that most of them successfully carried out a broad range of projects.

By all measures, the grant has been successful. Investigators and PDRAs together produced over 250 publications during the grant period, of which 32 were in *Physical Review Letters*, and most of the rest in other leading journals.

Investigators and PDRAs have all presented their work at international meetings. With the exception of a few of the more difficult and speculative topics, all the projects originally proposed have been attacked with a large degree of success, and further work has taken place in response to emerging developments in the field. It is one of the advantages of having a Programme Grant to allow us this flexibility. All of the PDRAs formerly employed on the Grant have moved into other research posts, in some cases remaining in Oxford in longer-term postdoctoral positions.

Reports of Investigators

D B Abraham

I continued work on the dynamics of complete wetting, in particular, on the formation and structure of the precursor film as revealed by experimental studies. It is now accepted that the correct mechanism for such a phenomenon is by evaporation from the reservoir into a supernatant, low density gas phase located directly above the precursor. There is also the *dual* mechanism of hole creation at the precursor edge. The 3-d Ising lattice gas simulations, as well as showing a precursor film with the correct diffusive growth law, showed that all particle motion is essentially restricted to the immediate vicinity of the reservoir surface. This suggested the idea that the entire set-up could be replaced by a pair of planar Ising models, one above the other, with a boundary condition at one end designed to simulate the reservoir boundary and feed in particles. The lower lattice represents the precursor and the upper one, the supernatant gas. This model confirms the exponent $\frac{1}{2}$ for the universal growth law. Detailed examination of typical configurations in the simulations shows a few supernatant particles and a few holes diffusing around independently. This suggests a separate diffusive model for each species with a moving boundary representing the advancing edge of the precursor. This can be solved for the spatially averaged precursor location confirming the above universal law. This work was done with PDRA E. Moro and with R. Cuerno, supported by British Council funding.

Joint work with P.J. Upton, then an EPSRC Advanced Fellow, examined the orientation dependent of surface critical exponents in planar Ising antiferromagnets by an exact calculation. New techniques were developed and the interpretation of the results was facilitated by reference to the droplet model, a topic on which Dr. Upton and I did much earlier joint work. We also came up with the idea that incremental thermodynamics, associated with pinning-depinning phenomena and notoriously difficult to get at because of swamping by bulk effects, could be determined from correlation lengths found from diffraction experiments designed to extract surface pair correlation functions.

J L Cardy

I have mostly been active in the areas of quenched random systems, percolation and self-avoiding walks. With my student J.-L. Jacobsen I completed an extensive numerical study of the effect of quenched random impurities on first-order transitions, confirming our earlier theoretical predictions. This has inspired many papers on this subject. I showed, with my EPSRC-funded student T. Davis, how multiscaling and logarithmic correlations arise generically in quenched random systems, and was able to give some analytic formulas for multiscaling exponents near a random fractal boundary. In percolation, I derived a number of new exact formulas, for example for the mean number of clusters crossing a given sample. This is related, via a mapping worked out in collaboration with co-investigator J. T. Chalker and my EPSRC-funded student E. Beamond, to the mean conductance in the spin quantum Hall effect. In fact this mapping is quite general and this paper is likely to be the first of a series. In SAWs I derived an exact scaling function describing the collapse of two-dimensional vesicles, the first example of an exact non-trivial scaling function of two thermodynamic variables in an isotropic system. With former EPSRC-funded PDRAs G. Delfino and G. Barkema, as well as A. Sokal (supported by an EPSRC Visiting Fellowship), I worked on amplitude ratios and other aspects of Potts models, making many analytic predictions and comparing them with simulations. PDRA F. Colaiori and I established a very general connection between the unsolved problem of directed percolation and so-called friendly walkers. Partly finished and ongoing projects with other PDRAs include understanding the asymptotic behaviour of multiscaling exponents (R. Narayanan), a new approach to directed percolation (S. Krishnamurthy), the role of logarithms in percolation (V. Gurarie), and non-equilibrium models of brain function (A. Hanke).

J T Chalker

My work under this grant can be described under three headings.
Geometrically frustrated antiferromagnets. Studying Heisenberg antiferromagnets on lattices such as the kagome and pyrochlore, R. Moessner and I arrived at a reasonably general understanding of low-temperature properties in the classical limit. These systems have highly degenerate ground states, and we established the circumstances under which such degeneracy results in a classical spin-liquid. We also developed a theory for the dynamics of this state, explaining the T^{-1} dependence of relaxation rates observed in a number of experiments. Interactions additional to nearest-neighbour exchange generally select ordered ground states and, in work with S. Palmer, I showed how dipolar interactions can lead to commensurate or incommensurate long-range order. Conversely, quantum fluctuations

promote disorder, and we added a new example to the rather short list of two-dimensional quantum spin models with magnetically-disordered ground states.

Localisation. The existence of a series of novel localisation problems has been recognised recently. They arise, for example, in the study of quasiparticle dynamics in disordered superconductors, and also in the investigation of random operators in classical statistical physics. With a range of collaborators, I have shown how analogues of the quantum Hall effect are possible in some of these systems, have determined the associated phase diagrams, and have set out links with classical random walks and with the two-dimensional random-bond Ising model. Separately, I have developed techniques for calculating spectral properties of non-Hermitian random operators, and applied these techniques to classical advection and to random matrix theory. In another development, I have shown how a universal form to the low-frequency density of states appears for normal modes or bosonic excitations in certain random systems.

Quantum Hall systems. I have developed, with collaborators, a detailed theory for the properties of the chiral metal, formed by hybridisation of edge-states in a multilayer quantum Hall system. The resulting understanding, particularly of mesoscopic effects, has been crucial in the interpretation of experiments by the UCSB group. I have also been concerned with a variety of interaction effects in conventional, single-layer quantum Hall systems. Most importantly, with S. Rapsch and D.K.K. Lee, I have investigated impurity effects in quantum Hall ferromagnets, showing how competition between screening and exchange may result in ferromagnetic or spin glass order.

R J Elliott

*(Note that Prof. Elliott, while included on the grant, was not allocated any PDRA support.)*The main research effort during this period was concentrated on the properties of magnetic tunnel junctions in collaboration with former student C. Heide. His activities led to a closer collaboration with a Russian group headed by Prof. Zilberman. Earlier work studying the exchange interaction between layers across a junction was extended to include the situation where the system was in a non equilibrium steady state where a current passed across the junction. This not only affected the range and properties of the exchange interaction but introduced a new coupling which was closely related to the spin current through the system. In appropriate circumstances this effect dominates and can be used to switch the relative polarisation of the magnetic layers. More recently, inspired by certain experimental results, we investigated the effects of domains in the magnetic systems. A general interest in the properties of excitations in disordered systems has been maintained. Earlier work established how the coherent potential approximation could be extended to treat weighted two particle response functions and was used to treat the properties of excitons in alloys. There are many other systems where such two particle Greens functions are relevant, for example in particle diffusion. However our work concentrated, with a student A-C. Uldry, on the use of these methods in the Hubbard model of an electron system. Hubbard's initial treatment had well known drawbacks and we attempted to circumvent these by devising an interpolation between the mean field Stoner (VCA) treatment and the Hubbard alloy analogy (CPA) method. Another area of interest which developed during this period was the study of the states of small symmetrical magnetic clusters and in particular the way in which these evolved as the size of the spins was increased from the quantum to the classical case.

D Sherrington

Spin glass related systems with disordered and frustrated direct interactions between microscopic constituents. Within this context we have concentrated mainly on 5 sub-topics: (i) possible glassiness in quasi-ferromagnetic states in systems with biased exchange distributions, $p > 2$ spin glass plus r- spin ferromagnetic, spherical and Ising, static and dynamic, models, solved analytically. We obtained new phase diagrams, several types of replica symmetry breaking (RSB) and exponents and demonstrated the crucial relevance of r with respect to p. In particular, in contrast to suggestions elsewhere, we have shown that for $p = r$, relevant to error-correcting codes, MPM retrieval on the Nishimori line is non-glassy; (ii) we devised a novel modulated form of RSB for antiferromagnetic spin glasses and investigated its consequences, arguing for its preference in certain cases; (iii) fermionic spin glass with Hubbard and SK spin glass interactions: we examined the magnetic and electronic properties (density of states and propagators), exactly within RSB and then explicitly to fourth order with careful extrapolation to infinite order, with novel predictions; (iv) coupled dynamics of sequence selection and compactification in mean-field hetero-polymers as an idealised model of protein selection: we solved for coupled fast folding dynamics and slow genetic sequence selection in ensembles of Mattis-like heteropolymers; (v) we demonstrated the absence of RSB in a region of the phase diagram of a binary interaction spin glass.
Glassy behaviour due to constrained dynamics. We showed how two-time dynamical macro-behaviour characteristic of real glasses can arise from constrained micro-dynamics even without Hamiltonian interaction. We studied a series of increasingly simplified minimalist models (topological foams, lattice analogues, 'backgammon' models) to demonstrate universality. Simulations were backed by explanatory novel annihilation-diffusion concepts and fits based on RG theory of asymptotic non-equilibrium dynamics.
Statistical physics of the minority game. This problem considers an ensemble of agents with diverse quenched individual strategies responding to common information and making decisions, while attempting to be in the minority. It was stimulated by consideration of an idealized speculative stock market, but poses fundamental issues for statistical physics, since it demonstrates novel complex cooperative behaviour, including ergodic-nonergodic phase transitions. We introduced stochasticity of action, showed that noise can lower variance and behaves differently for additive and multiplicative noise. It both provides quantification and understanding for a problem of economic relevance and also poses fundamental challenges for statistical physics. We developed an effective microscopic continuous dynamics formulation with unusual features compared with normal systems, and employed a generating functional method to derive an effective non-Markovian one- particle dynamics, soluble in principle and solved so far in the asymptotic limit of the ergodic region and for the first few steps of the non-ergodic region. Several subtleties were exposed.

R B Stinchcombe

The area of most activity was stochastic non-equilibrium systems. An updated review on this area was published in the "jubilee edition" of Advances in Physics. This contains a number of previously unpublished results, particularly on developments of operator algebra techniques and consequent exact results for lattice based 'exclusion' models. Another review-type contribution, on non-equilibrium stochastic jamming models, was one of seven overviews in the book *Jamming and Rheology* resulting from a half-year Santa Barbara workshop. This includes an outline of original work done with a student (M. Depken) on a model for glassy dynamics. A significant advance, with EPSRC student T. Hanney, was the development of a direct scaling approach to dynamic and steady-state properties of the lattice-based collective models for non-equilibrium behaviour. This powerful and accurate approach opens up a number of proposed investigations. In particular it has already been shown to be applicable to geometrically and kinetically constrained models for glassy dynamics and to generalise to the disordered non-equilibrium models. Exact results for auto correlation functions of an important collective stochastic model (the symmetric hard core hopping process) were obtained for general disorder and particularly dilution (with M.D. Grynberg). Preliminary results for a variety of disordered exclusion processes were obtained using analytic and simulation procedures (with M.D. Grynberg and K. Kaski together with EPSRC student R. Harris).

Work on random spin systems also continued, especially with S. de Queiroz on distribution functions for correlation functions and free energies and magnetisations principally in the random field Ising model, by analytic and numerical strip scaling methods. Dynamics and scaling was also studied, in correlated random field systems and in an alternating Ising model.

Recent work with PDRA S. Krishnamurthy has focussed on models with slow dynamics and on models for fragmentation and aggregation. In the first class, one model has been proposed and analysed which exhibits coarsening on three different length scales, despite only involving diffusion and a local deposition process. With another PDRA (D. Challet) preliminary work on stochastic models of financial markets has resulted in two publications, the first on the analysis and modelling of an order-driven market, and the second on trends and overdiffusion in such markets. The resulting model is a form of stochastic lattice-based non-equilibrium model, amenable to standard techniques, and it has been adopted by other prominent groups (including that at the Santa Fe Institute).

A M Tsvelik

(*Note that Prof. Tsvelik left the group in September 2000. This report covers work he did on the grant before then.*) During this period Tsvelik co-authored one large monograph and wrote over 35 papers.

Quasi-one-dimensional Strongly Interacting Systems: In collaboration with F. H. L. Essler, an EPSRC-funded postdoc, Tsvelik made important progress on the understanding of systems in a regime intermediate between purely one-dimensional and isotropic three-dimensional behaviour. These quasi-1D systems were shown to possess instabilities related to interchain couplings, and were solved using a mixture of exact methods and RPA approximations in the series of papers. Further results on correlation functions of those systems were done in collaboration with G. Delfino, also EPSRC-funded.

Conformal Theories for Disordered Systems: Together with J.-S. Caux, I. Kogan, A. Lewis and M. J. Bhaseen (both EPSRC students), he studied a model of disordered fermions and showed that the theory is a logarithmic CFT. This was solved using three different approaches, and shed important new light on the proper structure and understanding of these exotic CFTs. Earlier, he solved an important theoretical puzzle concerning the multifractal spectrum of these theories. In addition, Prof. Tsvelik maintained ongoing collaborations with A. Nersesyan (EPSRC-funded visitor), PDRA C. Pepin (giving a physical example of Haldane's exclusion statistics), and with his students D. G. Shelton, C. Hooley and E. Papa (all EPSRC-funded).

J M Yeomans

Prof. J.M. Yeomans and her group have continued to investigate the self-assembly and rheological properties of complex fluids. Work on phase ordering in binary fluids gave the first evidence of non-universality and has led to further research by several groups investigating the surprising complexity of this problem. More recently the effect of local pinning centres on phase ordering has been elucidated.

With EPSRC PDRA Dr C. Denniston a numerical approach was pioneered which is able to treat the hydrodynamics of isotropic and nematic liquid crystals in a very general way. This led to results on the effect of hydrodynamics on the ordering of the nematic phase and on the motion of topological defects. Of particular excitement are the applications to liquid crystal devices which are being pursued in new collaborations with scientists at Sharp and Hewlett-Packard and with Dr S. Elston (Engineering, Oxford) and Dr. N. Mottram (Maths, Strathclyde). Results so far include elucidation of switching in bistable devices and an explanation of anisotropic domain growth in the switching cycle.

Building on the expertise of EPSRC PDRA Dr. A. Malevanets a hybrid mesoscale algorithm aimed at exploring polymer hydrodynamics was developed. This was used to show that hydrodynamics significantly increases the speed of the polymer collapse transition. Simple models were used to investigate the extent to which similar hydrodynamic interactions between different parts of a protein molecule could be expected to be important in the folding process. We investigated the effects of oscillatory shear on binary and polymer mixtures, and found that localised ordering, even in the mixed phase, can result as a consequence of viscous drag between the fluid components.

The first lattice Boltzmann algorithm for acoustic streaming was written and applied to investigate acoustic-enhanced flow in porous media. This work is of interest to Unilever and has led to us being involved in the network 'Development of ultrasonic standing wave systems for life science applications' recently funded by EPSRC.

Mesoscale simulations are particularly suited to modelling flow in microfluidic devices and capabilities in this direction were recently developed in collaboration with Prof. Anna Balazs (Univ. of Pittsburgh). We showed that modifying the wetting properties of the substrate can generate local mixing and switching stations in microchannels carrying binary fluids. Dr. D. Bucknall (Materials, Oxford) is currently initiating an experimental programme based on this work. The research was backed up by algorithm development which introduces wetting into a liquid-gas lattice Boltzmann model in a way that reproduces Cahn theory. This led to an understanding of how the contact line singularity is resolved within the simulation approach. New algorithms were developed which allow simulation of a two-phase liquid gas system where the two phases have significantly different density, helping to resolve a long-standing difficulty in the field. As a result of our involvement in this area we have received PDRA funding as a partner in IMAGE-IN, a EU project aimed at better understanding the fundamental science behind ink-jet printing.