Final Report EPSRC Grant GR/S42798/01
Symposium on the Mathematics of Quantum Systems

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October 28, 2007

1 Objectives of grant

This grant was supporting the Warwick Symposium on The Mathematics of Quantum Systems during the academic year 2004-5. The symposium was run by the Mathematics Research Centre (MRC) at Warwick. The principal organizer was Gero Friesecke (Warwick), advised by a board of national and international experts:

E Brian Davies (King's College London)
Laszlo Erdös (Georgia Institute of Technology, USA)
W Des Evans (Cardiff)
Yan Fyodorov (Brunel)
Jon Keating (Bristol)
Robert MacKay (Warwick)
Eric Séré (Paris)
Herbert Spohn (Munich)
Peter Taylor (Warwick)

The stated objectives of the grant were:

- To run a symposium of international excellence on the mathematics of quantum systems.

- To bring together top mathematicians from the UK and from abroad around the world to exchange ideas and to make progress on important problems in the field.

- To facilitate interdisciplinary interactions with applied practitioners of quantum mechanics in physics, chemistry, materials science.

- To encourage and help young researchers (graduate students, postdocs) to do research in the subject.

2 Outcomes of grant

During the academic year 2004-05, the backbone of the Warwick Symposium consisted of six Symposium workshops in different key areas which took place as follows: Large Many-body Systems (23-28 August 2004, organizers: W Des Evans, Cardiff, and G Friesecke, Warwick), Quantum Dynamics and Quantum Transport, 6-10 September 2004, organizer: G Friesecke, Warwick), Mathematical challenges in quantum chemistry (13-15 December 2004, organizers: P Taylor, Department of Chemistry, Warwick, E Séré, Paris Dauphine, and G Friesecke, Warwick), Quantum Lattice Models (15-16 March 2005, Organizers: G Friesecke, R S MacKay FRS, O Zaboronski, all Warwick), Spectral Theory (4-9 April 2005, organizers: E Brian Davies FRS, King's College London, and W Des Evans, Cardiff), Random matrices and random Schrödinger operators (11-13 April 2005, Organizers: G Friesecke, Warwick, and J Keating, Bristol). The three workshops on Large many-body systems, Mathematical Challenges in Quantum Chemistry, and Spectral theory were high-level international events which attracted leading experts, junior researchers, and research students from the UK and abroad. The three workshops on Quantum Dynamics, Quantum Lattice Models, and Random matrices/random Schrödinger operators brought to gether smaller but topically more focused groups of experts.

Throughout the year 2004-05 various workshop participants spent longer periods of time in Warwick to collaborate with local researchers or other visitors, and to participate in the weekly Symposium research seminar. An example of a particular success story was long-term visitor V Betz (August to December 2004), at the time a junior postdoc in mathematics just past his PhD. His collaboration with the Warwick group and other UK visitors turned out to be so successful that Warwick appointed him as a permanent lecturer the following academic year; Betz has hence been awarded an EPSRC Advanced Fellowship by the EPSRC Chemistry panel for his interdisciplinary research at the Mathematics/Chemistry interface which he began during the Warwick symposium. Examples like this demonstrate the success of long-term visitor programmes like those of the Warwick EPSRC Symposiums in aiding junior researchers to develop a wide perspective of their field early in their careers.

An important feature of the symposium was the strong interdisciplinarity of some of the workshops. In particular, about half the participants of the workshop on Quantum Lattice Models were from physics departments, and more than half the participants of the Mathematical Challenges in Quantum Chemistry workshop came from chemistry departments. The strong interest from these neighbouring communities, especially from chemistry, justified the idea to use some of the Symposium funds to strengthen (in the past somewhat limited) links of the UK mathematics community with chemistry. These links have since been followed up in various ways, such as via a recently submitted proposal of an interdisciplinary UK network on molecular dynamics.

2.1 Workshop on Large many-body systems

This one-week international workshop was attended by 36 participants, 20 of which were from the UK. Highlights included two series of survey lectures of four hours each by internationally leading experts,

- Rigorous results on the energy and structure of ground states of large many-body systems, by J P Solovej (Copenhagen)

- Mathematical results for Bose-Einstein condensates, by Amandine Aftalion (Paris).

In particular, Solovej surveyed classical as well as more recent results concerning stability of fermionic and bosonic matter starting from the basic many-body equations, and Aftalion - taking the Gross-Pitaevskii model for Bose-Einstein condensates as her starting point - explained novel models developed by her group which allow to explain mathematically the emergence and structure of vortices in rotating BEC's. In particular she explained results which allow to underpin the more heuristic arguments in Abrikosov's Nobel-Prize winning predictions of vortex lattice formation, as well as novel predictions concerning vortex bending, which have since been confirmed experimentally by Jean Dalibard's group at ENS Paris. Other speakers at the workshop included N Manton (Cambridge), B Schroers (Heriot-Watt), O Penrose (Heriot-Watt), J M Barbaroux (Toulouse), M Lewin (Parix IX / Copenhagen), W D Evans (Cardiff), T Dorlas (Dublin Institute of Advanced Study), C Hainzl (Vienna), M Kiessling (Rutgers), C Melcher (Minneapolis) and A Balinsky (Cardiff).

A small follow-up workshop on the topic 'Large quantum systems' was organized on the topic by Betz, Kotecky and Ueltschi (all Warwick) from 11-15 June 2007, which attracted various new participants, as well as some repeat visitors; the focus was on statistical mechanics aspects, and keynote speakers included J Yngvason (Vienna), B Nachtergaele (UC Davis), and R Seiringer (Princeton).

2.2 Workshop on Quantum Dynamics and Quantum Transport

This one-week international workshop was attended by 27 participants, 16 of which were from the UK. Three survey lecture courses of three hours each were given on

- Energy transport in weakly anharmonic dielectric crystals, H Spohn (TU Munich)

- Quantum diffusion, L Erdoes (Georgia Tech)

- Adiabatic perturbation theory in quantum dynamics, S Teufel (Warwick).

The speakers had made recent breakthroughs in their fields and the goal of these lecture series was to give them the opportunity to explain the underlying technical ideas and advances to a wider audience. Other speakers at the workshop included M Wilkinson (Open University), A Sobolev (Sussex), A Joye (Grenoble), J Marklof (Bristol), R Schubert (Bristol), C Lasser (TU Munich), A Arnold (Muenster), A Sacchetti (Modena), and C Sparber (Vienna). Despite a list of diverse applications topics, the workshop had a unifying mathematical theme, namely the search for, and mathematical justification of, simplifying models for the dynamics of complex quantum systems which capture the essential dynamics on a desired scale.

2.3 Workshop on mathematical challenges in quantum chemistry

This strongly interdisciplinary workshop was attended by 42 participants, 23 of which were from the UK. The goal of the workshop was to bring together leading mathematicians and quantum chemists to discuss current challenges and explore topics of possible joint interest between these two (traditionally not so well connected) communities. The stage for a workshop full of lively cross-community discussions was set by eminent quantum chemist Brian Sutcliffe (Brussels) in his opening lecture: "Has Dirac's 1929 claim been substantiated and is Chemistry now just a branch of applied mathematics?" Survey lecture series of three hours each were given by

- Werner Kutzelnigg (Bochum, Chemistry): 1. Rate of convergence of expansions in a Gaussian basis, 2. The partial wave expansion for atomic states, unnatural parity states, and Hund's rules, 3. The Nooijen conjecture.

- Claude LeBris (ENPC Paris, Mathematics): Mathematical and numerical analysis for ab initio computational chemistry

- Peter Taylor (Warwick, Chemistry): Wave functions and density matrices.

Other speakers were P Gill (ANU), H J Flad (MPI Leipzig), J Olsen (Aarhus), J Coleman (Queens University, Kingston, Canada), P Knowles (Cardiff), M Lewin (Copenhagen), F Manby (Bristol), H Yserentant (TU Berlin), S Teufel (Warwick), F Lodier (ENPC Paris), J Morgan III (Delaware), E Sere (Paris Dauphine), D Tozer (Durham), P A Malmqvist (Lund), and T Oestergaard Soerensen (Aalborg). This workshop initiated various interactions between mathematicians and chemists, for example between Friesecke and Gill on understanding mathematically counter-intuitive numerical observations of dimension-dependence of convergence rates of the choice of basis set (P.Gill, A.Gilbert, S.Taylor, G.Friesecke, M.Head-Gordon, Decay behaviour of least-squares coefficients in auxiliary basis expansions, J. Chem. Phys. 123, 061101, 2005).

A follow-up interdisciplinary workshop, with old and new participants, on 'Mathematical Challenges in quantum chemistry problems' was organized by Volker Betz (Warwick), Irene Burghardt (ENS Paris), Gero Friesecke (Warwick), Peter Gill (Australian National University), Andreas Savin (Paris VI) on 16-20 July 2007. Topics of particular focus were quantum dynamics near conical intersections, wave packet propagation methods, Van der Waals interactions, and high accuracy computation of electronic wavefunctions. This workshop was attended 40 participants, 21 of which were from the UK, with chemists slightly outnumbering the mathematicians and speakers included leading UK quantum chemists such as P Knowles (Cardiff), P Taylor (Royal Society Professor, Warwick), D Tozer (Durham), R Wheatley (Nottingham), A Alavi (Cambridge), F Manby (Bristol), and distinguished international speakers such as P Gill (ANU), I Burghardt (ENS Paris), P Hobza (Prague), K Szalewicz (Delaware), H Nakamura (National Institute for Molecular Science, Japan), and B Kendrick (Los Alamos National Laboratory, USA).

2.4 Workshop on Quantum Lattice Models

This 4-day workshop was attended by 21 participants, 18 of which were from the UK. Many of the participants came from UK physics departments.

The focal topics of the workshop were Hubbard and related fully quantized models, order/disorder transitions and Anderson localization, nonlinear quantum lattice models such as the discrete nonlinear Schrödinger equation and quantum Frenkel-Kontorova models, and recent applications in condensed matter and materials science such as spin electronics, optical lattices, and quantum wires.

A key theme was to what extent the rigorous results available for single-electron models can be transferred to fully quantized lattice models where the state space per site is high- or infinite-dimensional, and where a mathematical understanding of many interesting results and ideas in the physics literature is currently lacking.

From the mathematical side, B Nachtergaele (UC Davis) spoke on ferromagnetic Lieb-Mattis theorems, S Aubry (Saclay) on discrete breathers, J Keating (Bristol) on entanglement in quantum spin chains, J C Eilbeck on quantization and spectra of classical dynamics of solitons and breathers, and D Yarotsky (Dublin) on ground states of

quantizations of classical lattice systems.

From the physics side, A Alexandrov (Loughborough) spoke on molecular quantum dots, R Roemer (Warwick) on weak disorder and localizaton lengths in random Schrödinger lattice models, A Ho (Birmingham) on spin-dependent optical lattices, J Chalker (Oxford) on a statistical physics picture of quantum localisation-delocalisation transitions, F Essler (Oxford) on the continuum limit of the integrable 3 - 3^- superspin chain, D Edwards (Imperial) on the Holstein Double-Exchange Model, and M Long (Birmingham) on correlations in spin-orbital models.

2.5 Workshop on Spectral Theory

This large, one-week workshop took place during the week 4-8 April 2005, and was organized scientifically by leaders of the EPSRC funded Spectral Theory Network from outside Warwick (E Brian Davies FRS, King's College London, and W Des Evans, Cardiff). In total, the workshop was attended by 67 participants, 33 of which were from the UK.

There had been some discussion whether, in line with the 'Outreach' aims of the grant, this workshop should be held at a venue outside Warwick, but it emerged that the organizers preferred to run the workshop in Warwick and invite the various UK and international visitors there, making use of the tried and tested MRC staff, facilities and local infrastructure. For this reason some funds originally earmarked for 'Outreach' were transferred to support travel and subsistence of UK visitors at this workshop.

Spectral theory is a classical area of mathematics which has continued, for several decades, to serve as a basic theoretical foundation as well as source of tools for novel problems in quantum theory, and conversely quantum theory has inspired new and wider developments in spectral theory, e.g. concerning non-selfadjoint operators. As stated in the grant application, the aim of the workshop was to cover both aspects.

Recent progress on theoretical methods reported at the workshop included survey lecture series of three lectures each on

- Asymptotics of heat flow (M van den Berg, Bristol)

- Spectral inequalities and their applications (A Laptev, Stockholm)

- Functional model and spectral structure of non-self-adjoint operators (S Naboko, St Petersburg),

as well as one-hour lectures by W N Everitt (Birmingham), A Pushnitski (Loughborouh), M Hager (Ecole Polytechnique, Paris), L Parnovsky (UCL), K Schmidt (Cardiff), A Tyukov (Cardiff), A Shkalikov (Moscov), H Langer (Vienna), A Sobolev (Sussex), P Kurasov (Lund), G Barbatis (Ioannina), H Kovarik (Stuttgart), A Tertikas (Heraklion).

Applications of spectral theory to quantum problems presented at the meeting included new work on quantum field theory (H Siedentop, Munich, and S Vugalter, Munich), magnetic Hamiltonians (M Melgaard, Uppsala; C Förster, Stuttgart), the Dirac-Fock model for relativistic atoms (M Esteban, Paris Dauphine), Klein-Gordon equations (C Tretter, Bremen), the Fermi golden rule (A Jensen, Aalborg), non-adiabatic transitions (A Elgart, Stanford), and to the many-electron Schrödinger equation (T Hoffmann-Ostenhof, Vienna; M Hoffmann-Ostenhof, Vienna; J Fleckinger, Toulouse).

2.6 Workshop on random Schrödinger operators and random matrix theory

This small 2-day workshop took place on 11-12 April 2005 and was organized by G Friesecke (Warwick) and J Keating (Bristol). There were 25 participants, 16 of which were from the UK. The goal was to bring together the leading specialists within the UK from the two fields, as well as some selected international speakers, and to compare the latest results and techniques. Topics covered by the speakers were applications of random matrix theory in quantum mechanics (J Keating,Bristol; F Mezzadri, Bristol), localization transitions in disordered systems (S Jitomirskaya, Irvine; N Ueki, Kyoto; Y Fyodorov, Brunel), spectral statistics and level repulsion for matrices and Schrödinger operators (E Bogomolny, Orsay; L Pastur, Paris 7; E Kanzieper, Weizmann), applications of random matrix theory to Dirichlet L-functions in number theory (I Smolyarenko, Brunel), and connections between random matrix theory and more general stochastic point processes (E Strahov, Caltech).

2.7 Small Underspend on Consumables

Compared to Warwick Symposia in previous years, there was a small drop in the use of Consumables such as stationary, use of photocopying and printing facilities by the Symposium visitors. Of the allocated £ 2116, only £ 1599.56 were spent. We attribute this drop to a further increase in the already large use of electronic means of communication, data transfer, and data storage, and transferred the remaining £ 516.44 to travel.

3 Summary

The Symposium was a great success in bringing together top mathematicians from the UK and from around the world to exchange ideas and to make progress on important problems in the field. Besides the inspiration it contributed to the work of the participating leading researchers, postdocs and graduate students, it also served as a valuable forum where theoreticians in the mathematics community could connect to practicioners of quantum mechanics in neighbouring fields such as physics and chemistry.

A significant potential long-term benefit of the Symposium has been an initiation of novel links of the UK mathematics community with theoretical chemistry; first follow-up activities are currently under way, such as a recently submitted proposal for an interdisciplinary UK network on molecular dynamics.