

PROGRESS IN  
NON-EQUILIBRIUM  
GREEN'S FUNCTIONS IV  
Programme



University of Glasgow, Glasgow, Scotland, UK

17<sup>th</sup> – 21<sup>st</sup> August, 2009

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## **General Information**

**Workshop Venue:** the University of Glasgow, Glasgow G12 8QQ, Scotland, UK: the Western Infirmary Lecture Theatre (WILT) complex.

**Telephone:** +44 (0) 141 330 5218

**Fax:** +44 (0) 141 330 4907

**Talks:** in the Western Infirmary Lecture Theatre (WILT).  
(see map at end of booklet)

**Internet Access:** will be available by wi-fi in the meeting room area.

**Posters:** to be displayed in the meeting area of the WILT. Posters can be put up at 1 p.m. on Monday, and remain on display until Wednesday at 12.45 p.m.

**Breakfast:** free coffee, tea and juice plus pastries and fruit will be available from 8:30 a.m. each day at the WILT meeting place.

**Breaks:** There will be a 20 minute break after the second morning talk. There will be a 20 minute break each afternoon. There will be free coffee, tea and juice in front of the lecture theatre.

**Conference desk:** located in the Western Infirmary Lecture Theatre complex.

**Excursions:** Details at the Conference Desk.

**Information and Updates:** These will be posted on a poster board in front of the Lecture Theatre.

## **Workshop Format**

The workshop continues the tradition of the previous meetings held in Rostock, Germany, Dresden, Germany and Kiel, Germany. The main intention is to provide an inter-disciplinary and informal gathering of theorists for discussion of theoretical concepts across many fields of discipline.

This fourth meeting provides ample time for discussions and will be underpinned by broadly understandable invited review (R) talks (40 minutes plus 10 minutes discussion). A range of invited (I) talks addresses topics in specific fields (30 minutes plus 5 minutes discussion). Contributed talks (C) are allocated 20 minutes plus 5 minutes discussion time. Sessions are chaired by experts/moderators and they may give short introductory remarks or comments. Discussions should be lively; interrupting speakers (in a friendly and polite way, of course) will be encouraged.

Equally important are the posters, for which an afternoon session is provided. All abstracts (talks, posters) will be included in the workshop Abstract booklet (separate). Poster area: 1 m<sup>2</sup> for each poster.

Facilities will be available for PowerPoint or similar presentations via Data Projector. Overhead projection facilities will also be available.

# Workshop Programme, Sunday, August 16<sup>th</sup>, 2009.

## Arrival

**Registration:** 18:00 – 21:00 Western Infirmary Lecture Theatre (Foyer)

**Drinks:** 19:00-21:00 Western Infirmary Lecture Theatre (Foyer)

# Workshop Programme, Monday, 17<sup>th</sup> August

**08:30** Registration (Western Infirmary Lecture Theatre)

**09:00** Welcome and Opening

## Session I: Nuclear and High Energy Physics (A)

**09:15-10:05** Gordon Baym, University of Illinois at Urbana-Champaign  
(R) *Connections between quark-gluon plasmas and cold atom physics*

**10:05-10:40** Kimmo Kainulainen, University of Jyväskylä  
(I) *Extended Quasiparticle Approximation and nonlocal coherence*

**10:40-11:00** **Break**

## Session II: Quantum Transport (A)

**11:00-11:50** Gerry Mahan, Pennsylvania State University  
(R) *Energy Bands and Electron transport in Periodic Arrays of Quantum Dots*

**11:50-12:25** Bedrich Velicky, A. Kalvova and V. Spicka  
Charles University of Prague  
(I) *Fast transients in mesoscopic systems.*

**12:25-14:15** **Lunch Break**, Ad Hoc Sessions (individual)

## Poster Session

**14:15-17:45** **5 minute preview from all contributors**

**Coffee during session**

## List of Posters (Monday 14:15-17:45)

Andreas Alvermann<sup>1</sup>, David M. Edwards<sup>2</sup>, Holger Fehske<sup>1</sup>,

1 Institute of Physics, Ernst-Moritz-Arndt Universität,

2 Department of Mathematics, Imperial College, London SW7 2BZ, United Kingdom

*Calculation of Drude weight for a correlated quantum transport process*

Sebastian Bauch, Karsten Balzer, Christian Henning, David Hochstuhl  
and Michael Bonitz,

Institut für Theoretische Physik und Astrophysik,

Christian-Albrechts- Universität Kiel,

*Quantum Breathing Mode for Fermions and Bosons at Arbitrary Coupling*

C.A. Paz de Araujo, K. Xue, J. Zelinska, and C. McWilliams,

University of Colorado

*Quantum Transport in Nanoscale Fine Tuned Transition Metal Oxide Random Access Memories*

V.S. Filinov<sup>1</sup>, M. Bonitz<sup>2</sup>, Y.B. Ivanov, V.V. Skokov,

P.R. Levashov<sup>1</sup>, V.E. Fortov<sup>1</sup>

1 Joint Institute for High Temperatures, Russian Academy of Sciences, Izhorskaya

Moscow, 2 Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-

Universität Kiel, 3 Gesellschaft für Schwerionenforschung, Darmstadt,

4 Russian Research Center “Kurchatov Institute”, Moscow,

5 Bogoliubov Lab. of Theoretical Physics, Joint Institute for Nuclear Research, Dubna,

*Equation of state of strongly coupled quark–gluon plasma –Path integral Monte Carlo results*

A.V. Glushkov, S.V. Malinovskaya, A.A. Svinarenko, N.V. Mudraya,

Odessa University, and Russian Academy of Sciences,

*Optimized Quasiparticle Dirac-Kohn-Sham DFT Theory and its Application to Autoionization and Electron- $\beta$ -Nuclear Processes*

A.V. Glushkov, S.V. Malinovskaya, G.P. Prepelitsa,

Odessa University, and Russian Academy of Sciences,

*Energy approach to photon-plasmon transitions in positronium and diagnostics of the astrophysical plasma*

M. Heimsoth, D. Hochstuhl and M. Bonitz,

Institute for Theoretical Physics and Astrophysics,

Kiel University,

*Time-dependent unrestricted Hartree-Fock approximation for strongly correlated mesoscopic Bose systems*

Olga Yu Khetselius, Odessa University  
*QED Many Body Perturbation Theory:  
Atomic Parity Non-Conservation in Heavy atoms*

O.Yu.Khetseliusa, A.V. Glushkov , T.A. Florko, I.N. Serka  
Odessa University  
*Green's Function of the Dirac Equation with Complex Energy ad Central Non-Singular Fermi-Model Potential*

T. Koch<sup>1</sup>, J. Loos<sup>2</sup>, A. Alvermann<sup>1</sup>, H. Fehske<sup>1</sup>,  
1 Institute of Physics, Ernst-Moritz-Arndt Universität, Greifswald,  
2 Institute of Physics, Academy of Sciences of the Czech Republic, Prague,  
*Transport through a vibrating quantum dot: Polaronic effects*

Petri Myohanen<sup>1</sup>, Anna-Maija Uimonen<sup>1</sup>  
Gianluca Stefanucci<sup>2</sup>, Robert van Leeuwen,  
1 University of Jyväskylä, 2 University of Rome  
*Time-dependent quantum transport with the Kadanoff-Baym equations*

Marat Myrzakhmet and Bagdat Shagirbaev  
Eurasian National University,  
*Green function study of electronic excitations  
migration in crystals*

Arnau Rios, University of Surrey  
*Self-Consistent Green's Functions in equilibrium:  
the ladder approximation and nuclear matter*

Sebastian Schmitt, Technische Universitaet Dortmund  
*Single impurity Anderson model out of equilibrium – a comparative study*

Zhandos Seksembayev, Marat Myrzakhmet,  
Eurasian National University  
*Correlation of electrons in electron beam in a path trajectory of free-electron laser*

D. Semkat, F. Richter, D. Kremp, G. Manzke, W.-D. Kraeft, and K. Henneberger  
Universität Rostock,  
*Ionization equilibrium in electron-hole plasmas: Mott effect vs. Bose-Einstein  
condensation*

S. A. Smolyansky<sup>1</sup>, A. V. Tarakanov<sup>1</sup> and M. Bonitz<sup>2</sup>  
1 Saratov State University, 2 Universität Kiel  
*Vacuum Particle Creation: Analogy with the Interband Transitions in Solid State  
Physics*

Claudio Verdozzi  
Division of Mathematical Physics and ETSF  
Lund University, 22 100 Lund – Sweden  
*TDDFT and the Hubbard model*

## Workshop Programme, Tuesday 18<sup>th</sup> August, 2009

09:00-09:15 Announcements

### Session III: Plasmas

09:15-09:40 Wolf Dietrich Kraeft, University of Rostock  
(C) *Thermodynamics of Strongly Coupled Plasmas*

09:40-10:15 Dirk Gericke, K. Wünsch and J. Vorberger  
University of Warwick  
(I) *Structural Properties of Warm Dense Matter*

10:15-10:40 J. Vorberger<sup>1</sup>, D.O. Gericke<sup>1</sup>, Th. Bornath<sup>2</sup>, M. Schlanges<sup>3</sup>  
1 University of Warwick, 2 Universität Rostock, E.-M.-  
Arndt-Universität Greifswald  
(C) *Energy Transfer Rates & Relaxation in Dense Two-  
Temperature Plasmas*

10:40-11:00 **Break**

### Session IV: Excitonic Systems and Collective Effects

11:00-11:35 Dietrich Kremp, D. Semkat, and K.Henneberger,  
Universität Rostock,  
(I) *BEC-BCS transition in excitonic systems*

11:35-12:10 C. Gies, S. Ritter, P. Gartner, and F. Jahnke  
University of Bremen  
(I) *Photon statistics of semiconductor microcavity lasers and  
its connection to carrier correlations*

12:10-12:35 Felix Richter, D. Semkat, and K. Henneberger  
University of Rostock  
(C) *The photon Green's function for bounded media: Splitting  
property and nonequilibrium radiation laws*

12:35-14:00 **Lunch and Ad Hoc Sessions.**

## Session V: Quantum Transport (B)

- 14:15-14:50** Antti-Pekka Jauho, Technical University of Denmark, and Helsinki University of Technology,  
(I) *Ab initio calculations of phonons and vibrations in nonequilibrium nanowire*
- 14:50-15:15** Tomi Ruokola<sup>1</sup>, Teemu Ojanen<sup>2</sup>, and Antti-Pekka Jauho<sup>1,3</sup>  
1 Helsinki University of Technology,  
2 Freie Universität Berlin  
3 Technical University of Denmark  
(C) *Radiative heat transport in quantum circuits*
- 15:15-15:40** Peter Kleinert, Paul-Drude-Institut für Festkörperelektronik  
(C) *Unified theory of double-time quantum transport and quantum diffusion*
- 15:40-16:00** **Break**

## Session VI: Quantum Transport (C)

- 16:00-16:35** Stefano Sanvito  
Trinity College, Dublin  
(I) *Ab initio electronic transport in macro-molecules from first principles*
- 16:35-17:10** Petri Myöhänen,<sup>1</sup> Adrian Stan,<sup>1</sup> Gianluca Stefanucci,<sup>2,3</sup>  
and Robert van Leeuwen<sup>1,3</sup>  
1 University of Jyväskylä, 2 Università di Roma  
3 European Theoretical Spectroscopy Facility (ETSF)  
(I) *Kadanoff-Baym approach to quantum transport through interacting nanoscale systems: From the transient to the steady-state regime*
- 17:10-17:35** Gianluca Stefanucci, University of Rome  
(C) *Time-dependent quantum transport in nanoscopic Josephson junctions: A NEGF approach*

# Workshop Programme, Wednesday 19<sup>th</sup> August, 2009

09:00-09:15 Announcements

## Session VII: Graphene and Correlated Systems (A)

09:15-10:05 David. K. Ferry<sup>1,2</sup>, Liang Huang<sup>1</sup>, R. Akis<sup>1</sup>, Y.-C. Lai<sup>3</sup>, J. P. Bird<sup>4</sup>, N. Aoki<sup>5</sup>, Y. Ujie<sup>5</sup>, S. Motooka<sup>5</sup>, T. Morimoto<sup>5</sup>, Y. Ochiai<sup>5</sup>, R. Brunner<sup>6</sup>, R. Meisels<sup>6</sup>, and F. Kuchar<sup>6</sup>  
<sup>1</sup>Department of Electrical Engineering, Arizona State University, Tempe, AZ 85287  
<sup>2</sup>Dept. of Physics, Arizona State University, Tempe, AZ 85287  
<sup>3</sup>Dept. of Mathematics, Arizona State University, Tempe, AZ 85287  
<sup>4</sup>Dept. of Electrical Engineering, University at Buffalo, Buffalo, NY 14260  
<sup>5</sup>Dept. of Materials Science, Chiba University, Chiba, Japan  
<sup>6</sup>Institute for Physics, Montanuniversität, Leoben, Austria  
*(R) Open Quantum Dots in Bilayer Graphene: Study of Conductance Fluctuations with Recursive Green's Functions*

10:05-10:40 Peter Schmitteckert, Universität Karlsruhe  
*(I) Non-equilibrium transport calculations within DMRG*

10:40-11:00 **Break**

## Session VIII: Graphene and Correlated Systems (B)

11:00-11:35 Matthew Gilbert, University of Illinois at Urbana-Champaign  
*(I) Probing the existence and the stability of the Superfluid Phase of Bilayer Graphene*

11:35-12:10 Barry Dunietz, University of Michigan  
*(I) A spectroscopic analysis of electron transport dynamics through molecular junctions*

12:10-12:45 John McGrady and Vihar Georgiev, University of Glasgow  
*(I) Electron transport through 'molecular wires': establishing a link between ground-state electronic structure and conductivity.*

12:45-14:00 **Lunch and Ad Hoc Sessions.**

14:00 **Excursion(s)**

## Workshop Programme, Thursday 20<sup>th</sup> August, 2009

09:00-09:15 Announcements

### Session IX: Numerical Methods for NEGF

09:15-09:50 Karsten Balzer, D. Hochstuhl, S. Bauch, and M. Bonitz  
Christian-Albrechts-Universität, Kiel  
(I) *Efficient grid-based method in non-equilibrium Green's function calculations for inhomogeneous systems*

09:50-10:15 Anna-Maija Uimonen, P. Myohanen, A. Stan, R. van Leeuwen  
University of Jyväskylä,  
(C) *Kadanoff-Baym approach to density and current bistability in quantum transport*

10:15-10:40 Peter Schmitteckert, Karlsruhe Institute of Technology  
(C) *Calculating Green's function from finite systems*

10:40-11:00 **Break**

### Session X: Nuclear and High Energy Physics (B)

11:00-11:35 Pawel Danielewicz<sup>1</sup> and Arnau Rios<sup>2</sup>,  
1 Michigan State University, 2 University of Surrey  
(I) *Towards Application of Green's Functions to Nonequilibrium Processes in Nuclear Systems*

11:35-12:00 Arnau Rios<sup>1</sup>, Pawel Danielewicz<sup>2</sup> and Brent Barker<sup>3</sup>,  
1 University of Surrey, 2 Michigan State University  
(C) *Time-dependent Green's Functions Approach to Nuclear Reactions*

12:00-14:00 **Lunch and Ad Hoc Sessions.**

### Session XI: Alternative Computational Methods

14:15-14:50 Kris van Houcke and Nikolay Prokofev, University of Massachusetts, Amherst, USA and University of Ghent, Belgium  
(I) *Diagrammatic Monte Carlo: what happens to the sign-problem?*

14:50-15:25 Frithjof Anders, University of Dortmund  
(I) *Quantum transport through nano-devices: A scattering-states numerical renormalization group approach to open quantum systems*

- 15:25-15:50**      David Hochstuhl, S. Bauch, K. Balzer and M. Bonitz  
Christian-Albrechts-Universität, Kiel  
(C) *Time-dependent photo-ionization of atoms-Non-equilibrium Green's functions versus Multi-Configuration Hartree-Fock*
- 15:50-16:15**      **Break**
- Session XII: Quantum Transport (D)**
- 16:15-16:50**      Marc Puig von Friesen, Claudio Verdozzi,  
and Carl-Olof Almbladh, Lund University  
(I) *Off-equilibrium dynamics of Hubbard Clusters*
- 16:50-17:25**      Antonio Martinez, Natalia Seoane, Andrew Brown,  
John Barker and Asen Asenov, University of Glasgow  
(I) *Dopants and Roughness induced Resonances in thin Si Nanowire transistors: A self-consistent NEGF-Poisson study*
- 17:25-17:50**      Christian Brouder, Institut de Minéralogie et de Physique des  
Milieux Condensés, Paris  
(C) *Nonequilibrium Green's functions for degenerate systems*
- 19:00**              **Banquet**
- Melville Room, University Main Building**

# Workshop Programme, Friday 21<sup>st</sup> August, 2009

**09:00** Announcements

## **Session XIII: Laser/Matter Interaction, Transport**

**09:15-09:40** Sebastian Bauch, D. Hochstuhl, K. Balzer, and M. Bonitz  
Christian-Albrechts-Universität, Kiel  
*(C) Quantum kinetic approach to time-resolved photoionization of multi-electron atoms*

**09:40-10:05** Alexander Glushkov, Odessa University  
*(C) Energy Approach and QED Lines Moments Technique for Atoms and Nuclei in a Strong Laser Field*

**10:05-10:40** John Barker, University of Glasgow  
*(I) NEGF quantum transport phase space formalism with compact support*

**10:40** **Closing Remarks**

**Coffee**

# Committees

## Programme Committee

A. Abrikosov (Argonne),  
C-O. Almladh (Lund),  
J. R. Barker (Glasgow),  
G. Baym (Illinois),  
M. Bonitz (Kiel), CHAIR  
P. Danielewicz (Michigan),  
D. Ferry (ASU),  
F. Jahnke (Bremen),  
A.P. Jauho (Lyngby),  
J. Knoll (GSI Darmstadt ),  
L.V. Keldysh (Moscow),  
P.C. Martin (Harvard),  
R. van Leeuwen (Groningen),  
B. Velicky (Prague).

## Organising Committee

J.R. Barker (Glasgow) CHAIR, S. Roy (Glasgow) CO-CHAIR,  
J. Ayubi-Moak (Glasgow), A. Brown (Glasgow), K. Kalna (Glasgow), A. Martinez,  
(Glasgow), C. Millar (Glasgow), G. Roy (Glasgow), J. Watling (Glasgow).

## Support

The organisers acknowledge support from:

The University of Glasgow vice-Chancellors Fund

Deutsche Forschungsgemeinschaft, support via SFB-TR 24

## **Publication and manuscript preparation**

Please bring your draft manuscripts to the Workshop and hand them in at the Registration desk. Manuscripts may also be submitted after the meeting.

It is planned to referee the manuscripts during the conference.

The deadline for final submission of accepted revised manuscripts is October 1<sup>st</sup>, 2009.

Final versions of accepted manuscripts will be published in the Journal of Physics Conference Series.

**Please submit final accepted manuscripts** (Word or Latex , plus pdf copy) in the first instance to:

John Barker ([jbarker@elec.gla.ac.uk](mailto:jbarker@elec.gla.ac.uk))

or

Michael Bonitz ([bonitz@physik.uni-kiel.de](mailto:bonitz@physik.uni-kiel.de))

**Format:** see the IOP web site for the correct Word or Latex templates:

<http://www.iop.org/EJ/journal/-page=extra.3/1742-6596>

### **Manuscript limitations**

Review Papers: 20 pages

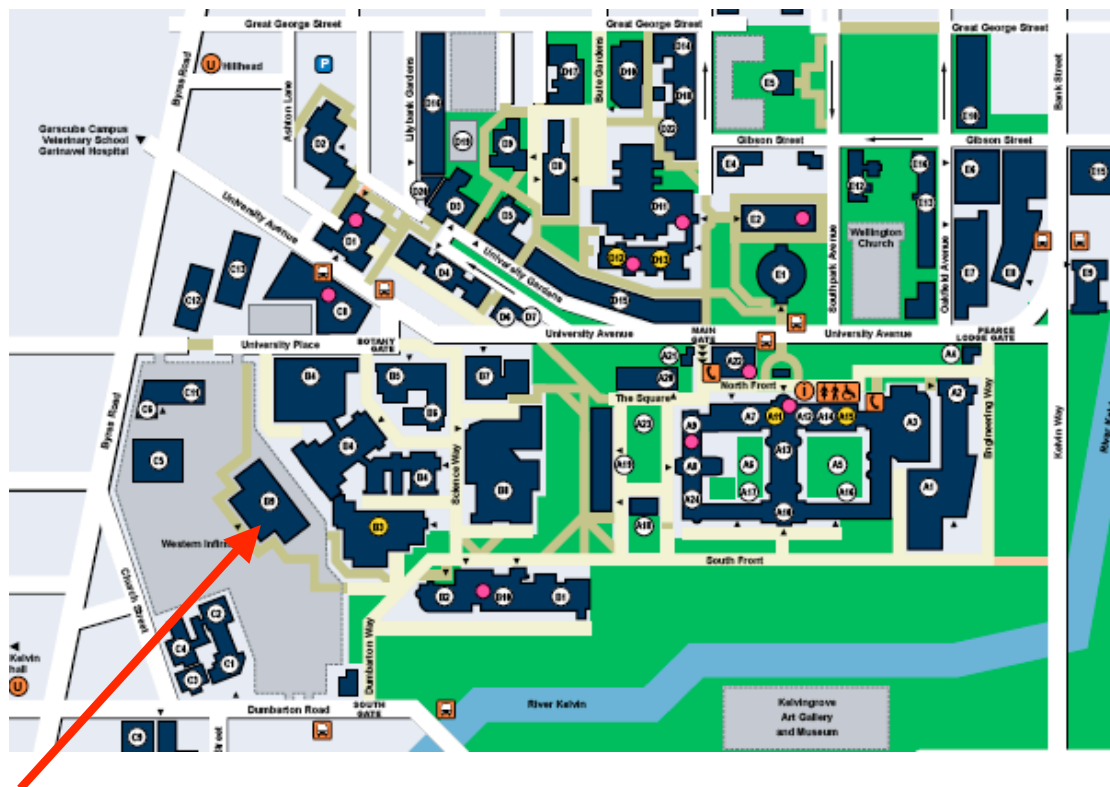
Invited Papers: 15 pages

Contributed Papers/Poster papers: 10 pages

# Maps

## University and environs

<http://www.gla.ac.uk/about/locationmapsandtravel/>



Location of meeting rooms (talks, posters): Western Infirmary Lecture Theatre

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