Preface

The fifth interdisciplinary conference “Progress in Nonequilibrium Green’s Functions” (PNGF5) was held at the University of Jyväskylä, Finland, on August 27th — 31st, 2012. The conference continued the successful tradition of its predecessors (Rostock 1999, Dresden 2002, Kiel 2005 and Glasgow 2009) to bring together different communities for an interdisciplinary exchange of recent results and theoretical concepts.

The conference focused on recent developments, current challenges and future perspectives in nonequilibrium Green’s functions theory in various fields of physics but included also other many-body methods. Roughly 20 invited talks were given by some of the top scientists in the field, accompanied by 10 contributed talks.\(^1\) Also a poster session was set up to enhance scientific discussions, building up new collaborations and enriching views and ideas. As at the previous meetings, the atmosphere was interactive and stimulating, benefiting both experienced scientists and young researchers and students.

The present volume contains 14 articles based on works presented at this conference. The articles partly have review character so they should be of use for an interdisciplinary community working or interested in nonequilibrium Green’s functions. All papers were refereed according to high scientific standards.

The conference would not have been possible without financial support from the Federation of Finnish Learned Societies, Finnish Academy of Science and Letters and Nanoscience Center of the university of Jyväskylä which are greatly acknowledged. The local organizing committee is also grateful to the administration personnel, Marjut Hilskä and Riitta-Liisa Kuittinen, for assistance. We further thank professor Antti-Pekka Jauho for invaluable help and advice during the organization of the conference.

The editors of the present conference proceedings acknowledge the authors for their excellent papers and all the referees for participating in a thorough peer-reviewing of the manuscripts. Finally, it is our pleasure to announce that the sixth conference “Progress in Nonequilibrium Green’s Functions” (PNGF6) will be held in August 2015 at the University of Lund, Sweden.

Riku Tuovinen and Robert van Leeuwen, University of Jyväskylä
Michael Bonitz, University of Kiel
February 2013

\(^1\) Slides of several presentations can be found online at www.jyu.fi/physics/pngf5.
David C. Langreth — Obituary

Antti-Pekka Jauho
Lyngby, Denmark

David C. Langreth passed away on May 27th, 2011. He was an outstanding theoretical condensed matter physicist with a large number of important contributions in many areas, such as surface physics, density-functional theory, many-body physics, and transport theory. For the community working with nonequilibrium Green’s functions his name is inseparably linked to “Langreth identities”, a set of rules which elegantly and concisely allows one to extract real-time Green’s functions from their contour-ordered counterparts. Using these rules one can very easily derive the (generalized) Baym–Kadanoff equations, or, equivalently, the Keldysh equation, which encode the standard paradigm for nonequilibrium transport phenomena. His famous lecture notes on nonequilibrium Green’s functions [NATO ASI 17, (1976)] have been the cornerstone for generations of students learning nonequilibrium techniques, until text-books relying on these very same notes became available.

David learned the nonequilibrium techniques during his stay at Illinois with Leo Kadanoff, one of the originators of the formalism. His very first published paper [D. C. Langreth and L. P. Kadanoff, Phys. Rev. 133, 1070 (1964)] on polaron mobility contains a precursor of the Langreth rules, though in equilibrium disguise. In subsequent works he developed these concepts further, and one can see the contours of the modern theory already in his paper from 1967 [D. C. Langreth, Phys. Rev. 159, 717 (1967)], which addresses finite temperature effects on the polaron problem. His monumental 39-page long paper on spin resonance in magnetic alloys together with John Wilkins [D. C. Langreth and J. W. Wilkins, Phys. Rev. B 6, 3189 (1972)] is even today perhaps the most complete application of the Kadanoff–Baym equations to a problem involving both continuous (space, time) and discontinuous (spin) variables: all the key concepts such as gradient expansion, nonequilibrium analytic continuation, and spin-sums are carefully explained and elaborated. In later years he used the nonequilibrium techniques from time to time, for example in studies of the out-of-equilibrium Kondo effect [R. Aguado and D. C. Langreth, Phys. Rev. Lett. 85, 1946 (2000)]. All of his papers are examples of scholarly excellence.

The nonequilibrium Green’s function community will miss sorely David Langreth, one of the deepest thinkers in our discipline, and whose work will continue to influence our research for many years to come.
David C. Langreth — In memoriam

Ulf von Barth and Bengt Lundqvist
Lund and Göteborg, Sweden

Ulf and Bengt had the pleasure of getting to know David Langreth very early on in their careers, i.e., in the early seventies. Ulf has had very few role models in his life and David has been one of them. And so he was for Bengt. What attracted our admiration was David’s ability to combine his excellence and his deep knowledge of fundamental physics with a modest and humble personality. His integrity was unquestionable and David never overstated his case.

In the seventies David had several occasions to visit Lund, Chalmers and Nordita in Copenhagen. He was an appreciated guest scientist. He was also an evaluator of Swedish Solid State Physics. From 1975 to 1976 he was a guest Professor at Nordita. At that time, David had a strong interest in electrons at surfaces - an interest shared by the experimental and theoretical groups at Chalmers. An important work by David from this time is his sum rule for surfaces [Phys. Rev. B 11, 2155 (1975)]. This work led on to some of the most influential parts of David’s research. In a collaboration with John Perdew, David engaged in a detailed study of the effects of electronic correlations in surfaces of varying steepness. In a series of papers from 1975 to 1985 [examples are: Phys. Rev. B 15, 2884 (1977), Phys. Rev. B 21 5469 (1980), and Phys. Rev. B 26, 2810 (1982)] David and his collaborators laid down the many-body foundation of the subsequent generalized gradient approximations within density-functional theory (DFT). In our mind, this fact is often not sufficiently appreciated by the practitioners of DFT calculations. In the later stages of this period, Ulf worked at IBM, Yorktown Heights (NY) and had the privilege to be of help to David in numerically testing the Langreth–Mehl gradient functional [Phys. Rev. B 28, 1809 (1983), Physica Scripta 32, 391 (1985)] in atoms and solids.

The groups at Chalmers and in Lund strongly benefited from David’s deep knowledge of DFT. In those days, however, the Lund group was mainly interested in the theoretical interpretation of X-ray and Auger spectra. Also in this area David had made major advances. In a famous paper from 1970 [Phys. Rev. B 1, 471] David gave a formally exact solution to the Green function of a long lived core hole in a fully interacting electron gas. Later important works in this area resulted from a collaboration with Shung, for instance Phys. Rev. B 28, 4976 (1983) and Phys. Rev. B 33, 2247 (1986).
The first picture from 1981 shows David (on the left) as faculty opponent of the thesis of Ulf's first graduate student in Lund, Günter Grossmann. The overhead picture shows the energy dependent singularity exponents calculated by Grossmann within the 'independent Fermion model' of Mahan, Nozieres, and de Dominicis.

David's connections to Chalmers and particularly his friendship with Bengt go back some forty years.

![Second picture of David in 1988 at the helm of Bengt's sailing boat in the archipelago of Bohuslän.](image)

In later years David was a visiting professor at Nordita in 1988 and at Chalmers in 1993. In 1994, David was made an honorary doctor to Chalmers University. The long time collaboration with Bengt and his group at Chalmers ("the Rutgers–Chalmers collaboration") has led to yet another very successful outcome of David's research, namely the use of the methods of DFT to treat the notoriously difficult problem of van-der-Waals interactions. The use of the non-local functionals resulting from this collaboration has been expanding very rapidly and broadly over the past ten years. Fortunately, David lived long enough to see the exponential growth of the citations to this part of his work. Examples of early works: Phys. Rev. 76, 102 (1996), Phys. Rev. Lett. 77, 2029 (1996), and Phys. Rev. B 59, 4708 (1999) and of later works: Phys. Rev. Lett. 92, 246401 (2004) and Phys. Rev. B 82, 081101 (2010).

David's research interests have been very broad but still confined to the general framework of many-body physics. And David has been successful also in areas of less interest to the authors of the present notes. As highlighted by the notes by Professor Jauho, David made major contributions within the area of non-equilibrium physics and he also spent a lot of his talent on processes like charge transfer at surfaces. [Phys. Rev. B 43, 2541 (1991)]. Yet another area with great contributions by David is Kondo physics with connections to problems at surfaces and quantum conduction. [Examples: Phys. Rev. B 43, 2541 (1991), Phys. Rev. B 61, R13341 (2000), and Phys. Rev. B 71, 165321 (2005)].
Conference participants

Arrachea, Liliana (Buenos Aires, Argentina) Kainulainen, Kimmo (Jyväskylä, Finland)
Balzer, Karsten (Hamburg, Germany) Kinnunen, Jami (Espoo, Finland)
Bonitz, Michael (Kiel, Germany) Marini, Andrea (Rome, Italy)
Brandbyge, Mads (Lyngby, Denmark) Ness, Hervé (York, UK)
Cunningham, Brian (Belfast, UK) Nozaki, Daijiro (Dresden, Germany)
Eckstein, Martin (Hamburg, Germany) Pastawski, Horacio (Córdoba, Argentina)
Garny, Mathias (Hamburg, Germany) Pavlyukh, Yaroslav (Halle, Germany)
Gomes da Rocha, Claudia (Jyväskylä, Finland) Rios, Arnau (Surrey, UK)
Guo, Hong (Montréal, Canada) Stefanucci, Gianluca (Rome, Italy)
Han, Jong (Buffalo, USA) Säkkinen, Niko (Jyväskylä, Finland)
Harju, Ari (Espoo, Finland) Tuovinen, Riku (Jyväskylä, Finland)
Hermanns, Sebastian (Kiel, Germany) Uimonen, Anna-Maija (Jyväskylä, Finland)
Hochstuhl, David (Kiel, Germany) van Leeuwen, Robert (Jyväskylä, Finland)
Hyrkäs, Markku (Jyväskylä, Finland) Verdozzi, Claudio (Lund, Sweden)
Jahnke, Frank (Bremen, Germany) Wu, Ming-Wei (Hefei, China)
Jauho, Antti-Pekka (Lyngby, Denmark)
List of talks and posters

(I) — Invited talk; (C) — Contributed talk; (P) — Poster

(I) Yaroslav Pavlyukh,
University of Halle, Germany,
ON THE INITIAL STAGE OF QUASIPARTICLE DECAY

(I) Ari Harju,
Aalto University, Finland,
ELECTRONIC TRANSPORT IN GRAPHENE STRUCTURES

(I) Kimmo Kainulainen,
University of Jyväskylä, Finland,
FLAVOURED QUANTUM TRANSPORT EQUATIONS AND THEIR APPLICATIONS IN COSMOLOGY

(I) Karsten Balzer,
University of Hamburg, Germany,
FEW-ELECTRON DYNAMICS FROM THE KADANOFF–BAYM EQUATIONS. SINGLE AND DOUBLE EXCITATIONS IN QUANTUM WELLS AND HUBBARD CHAINS

(C) David Hochstuhl,
University of Kiel, Germany,
TIME-DEPENDENT RESTRICTED ACTIVE SPACE CONFIGURATION INTERACTION CALCULATIONS FOR THE PHOTOIONIZATION OF MULTIELECTRON ATOMS

(I) Mads Brandbyge,
Technical University of Denmark,
SEMI-CLASSICAL LANGEVIN AND NEGF APPROACH TO ATOMIC DYNAMICS IN NON-EQUILIBRIUM NANOSYSTEMS

(I) Liliana Arrachea,
University of Buenos Aires, Argentina,
NONEQUILIBRIUM GREEN’S FUNCTIONS IN THE STUDY OF HEAT TRANSPORT AND COOLING IN MESOSCOPIC DEVICES AND NANOMECHANICAL SYSTEMS

(C) Martin Eckstein,
University of Hamburg, Germany,
THE HUBBARD MODEL IN STRONG ELECTRIC FIELDS

(C) Anna-Maija Uimonen,
University of Jyväskylä, Finland,
CORRELATION EFFECTS ON THE TIME-DEPENDENT QUANTUM TRANSPORT: COMPARATIVE STUDY OF MANY-BODY PERTURBATION THEORY AND TIME-DEPENDENT DENSITY FUNCTIONAL THEORY

(I) Ming-Wei Wu,
University of Science and Technology of China,
SPIN DYNAMICS IN SEMICONDUCTORS AND GRAPHENE
(I) Claudio Verdozzi,
University of Lund, Sweden,
\textit{Kadanoff–Baym dynamics for lattice model Hamiltonians: Comparative assessment of some conserving approximations to exact and TDDFT results}

(C) Claudia Gomes da Rocha,
University of Jyväskylä, Finland,
\textit{Controlling AC transport in graphene-based Fabry–Perot devices}

(C) Jami Kinnunen,
Aalto University, Finland,
\textit{Extended Brueckner theory for ultracold atomic gases}

(C) Arnau Rios,
University of Surrey, UK,
\textit{Towards a non-equilibrium Green's functions approach for nuclear reactions}

(I) Hong Guo,
McGill University, Canada,
\textit{Device modeling from atomistic first principles: theory of the nonequilibrium vertex correction}

(I) Frank Jahnke,
University of Bremen, Germany,
\textit{Configuration-picture description of carrier scattering in semiconductor quantum dots}

(I) Gianluca Stefanucci,
University of Rome “Tor Vergata”, Italy,
\textit{Wick theorem for nonequilibrium systems in general initial states}

(I) Andrea Marini,
National Research Council, Italy,
\textit{Phonon-induced dynamics of electrons and excitons in solids driven out-of-equilibrium by strong laser pulses: an ab-initio approach}

(I) Hervé Ness,
University of York, UK,
\textit{Modelling non-equilibrium and many-body effects in quantum transport through single-molecule nanodevices}

(I) Horacio Pastawski,
LaNAIS, Argentina,
\textit{Decoherent many-body interactions in quantum transport: from conducting polymers and giant magnetoresistance to quantum dynamical phase transitions in double dots and heterogeneous catalysis}
(I) Jong Han,
University at Buffalo, USA,
QUANTUM SIMULATION OF STRONGLY CORRELATED QUANTUM DOTS OUT OF EQUILIBRIUM

(C) Niko Säkkinen,
University of Jyväskylä, Finland,
DOUBLE EXCITATIONS IN FINITE SYSTEMS WITH THE KADANOFF–BAYM FORMALISM

(I) Mathias Garny,
DESY, Germany,
REnormalization of Relativistic Kadanoff–Baym Equations

(C) Daijiro Nozaki,
Technical university of Dresden, Germany,
Prediction of Quantum Interference in Molecular Junctions Using a Parabolic Diagram: Understanding the Origin of Fano and Anti-Resonances

(C) Riku Tuovinen,
University of Jyväskylä, Finland,
Transient Dynamics Without Time Propagation

(P) Michael Bonitz,
University of Kiel, Germany,
Nonequilibrium Quantum Pair Distribution Function from Nonequilibrium Greens Functions

(P) Claudia Gomes da Rocha,
University of Jyväskylä, Finland,
Manifestation of Quantum Wagon-Wheel Effect in Carbon Based Nanostructures

(P) Sebastian Hermanns,
University of Kiel, Germany,
Non-Equilibrium Green’s Function Description of Hubbard nanoClusters Within the Generalized Kadanoff–Baym Ansatz

(P) Brian Cunningham,
Queen’s university of Belfast, UK,
Non-Conservative Current-Induced Forces: The Concept of an Atomic Waterwheel

(P) David Hochstuhl,
University of Kiel, Germany,
Time-Dependent Restricted Active Space Configuration Interaction Calculations for the Photoionization of Multielectron Atoms

(P) Arnau Rios,
University of Surrey, UK,
Equilibrium Green’s Function Calculation of the Nucleon Mean-Free Path
Conference photographs

Group photo. Upper row from left to right: Hervé Ness, Liliana Arrachea, Gianluca Stefanucci, Claudio Verdozzi, Jong Han, David Hochstuhl, Michael Bonitz, Andrea Marini, Martin Eckstein, Markku Hyrkäs, Robert van Leeuwen, Yaroslav Pavlyukh, Sebastian Hermans, Frank Jahnke, Ari Harju, Ming-Wei Wu, Jami Kinnunen, Antti-Pekka Jauho, Anna-Maija Uimonen, Niko Säkkinen and Riku Tuovinen.
Lower row from left to right: Daijiro Nozaki, Mads Brandbyge, Horacio Pastorowski, Arnau Rios, Brian Cunningham, Karsten Balzer, Hong Guo and Claudia Gomes da Rocha.
Photo: Ville Kotimäki
Waiting for the ship to arrive in the Jyväskylä harbour: Brian Cunningham, Horacio Pastawski, David Hochstuhl, Sebastian Hermans, Karsten Balzer, Martin Eckstein, inter alios.

Hopping in the ship Suometar where the conference dinner was served: Claudia Gomes da Rocha and Horacio Pastawski, inter alios.
Under the Äijälänjoki bridge: Frank Jahnke, Jong Han, Antti-Pekka Jauho and Martin Eckstein.

Sunset and rainbow on the lake Päijänne: Riku Tuovinen, Michael Bonitz, Robert van Leeuwen and Yaroslav Pavlyukh.