

## Progress in Non-equilibrium Green's Functions (PNGF VI)

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## Foreword

The sixth interdisciplinary conference 'Progress in Non-equilibrium Green's Functions' (PNGF6) took place at Lund University, Sweden, on 17-21 August 2015. The conference was attended by 60 scientists, from Europe and overseas, sharing an interest in Green's function methods and/or non-equilibrium phenomena. At the conference, 34 invited and contributed talks were given, together with a poster session with 17 contributions. As its predecessors (Rostock 1999, Dresden 2002, Kiel 2005, Glasgow 2009, Jyväskylä 2012) the conference succeeded in gathering different communities for exchange of recent developments and results.

Among the topics of the conference, we mention approaches for strongly correlated systems, improvements of existing perturbative many-body schemes, electron-phonon/-photon interactions in time-dependent treatments, numerical scalability of NEGF approaches, connections with other non-equilibrium methods and concrete physical applications. For the latter, we mention quantum transport, semiconductor kinetics, multiply excited states in atoms and ions, nuclear reactions, high energy physics, quantum cascade lasers, strongly correlated model systems, graphene-nanostructures, optoelectronics, superconductors, spin-dynamics, photovoltaics, excitations in atoms and ions, and time-resolved spectroscopy.

The present volume contains 20 articles from participants to PNGF6, devoted to these topics. Compared to previous conferences, a completely novel and successful aspect of PNGF6 was the participation of experimentalists among the invited speakers, to establish a connection between emerging experimental techniques (for example, time-dependent spectroscopies) and the theoretical NEGF community. As at the previous PNGF conferences, the atmosphere was friendly and exciting at the same time, favoring vivid and stimulating discussions among experienced scientists, young researchers and students.

The conference would not have been possible without financial support from the Swedish Research Council and from the Christian-Albrechts-Universität-Kiel via Kiel Nano, Surface and Interface Science (KiNSIS). Particular thanks go to Katarina Lindqvist, the administrator at the division of Mathematical Physics in Lund, who provided assistance in many different matters, particularly in making the conference to unfold very smoothly. We also acknowledge the contributors to this volume for their papers and all the referees of the manuscripts.

Finally, we are glad to announce that the seventh conference 'Progress in Nonequilibrium Green's Functions' (PNGF7) is organized by Andrea Marini and Gianluca Stefanucci, and it will take place in August 2018 in Rome, Italy. *Arrivederci in Roma!*

Claudio Verdozzi, Andreas Wacker, Carl-Olof Almbladh,  
*Lund, February 2016*

Michael Bonitz,  
*Kiel, February 2016*





## Leo Kadanoff - Obituary

*By the Editors of PNGF6*



Two months after the PNGF6 conference, the condensed matter and many-body physics communities were saddened by the death of Leo Kadanoff. Kadanoff was an outstanding physicist and teacher, with seminal work in several areas of Physics. His most prominent contribution and legacy arguably remains the introduction and use of the scaling technique in statistical physics; however, for those involved in non-equilibrium Green's function techniques, his name is indissolubly tied to two fundamental, pioneering contributions to the subject, namely one article [1] and one book [2] together with Gordon Baym, both published in the early sixties. These works belong to the very early production of Kadanoff, when he and Baym both were postdoctoral researchers in Copenhagen, investigating conservation laws in theories of transport within the Martin-Schwinger Green's function formalism, and approximations fulfilling such laws. The results, published in a joint paper, were further expanded in a book entitled "Quantum statistical mechanics", where a main topic is the derivation of generalized Boltzmann's equations from Green's functions-based conserving approximations: since then, this short monograph has become a truly classic reference source in the field of non-equilibrium quantum phenomena. It is perhaps worth to add that further advances on conserving  $\Phi$ -derivable approximations came from subsequent work by Gordon Baym, and that at the same time, largely independently, progress in the same area was being obtained by soviet scientists, primarily by Leonid Keldysh. In a landmark paper, where the notion of round trip contour explicitly plays the central role [3], Keldysh extended the equilibrium standard Feynman-Dyson perturbation (diagrammatic) expansion technique to describe systems far away from equilibrium. It is appropriate to say that by then, the most basic elements of the so-called Martin-Schwinger-Kadanoff-Baym-Keldysh technique for non-equilibrium phenomena, as we know it today, were all in place. These and other historical facts are vividly recollected in the papers by Paul Martin, Gordon Baym, Alexey Abrikosov and Leonid Keldysh, published in the 1st and 2nd volume of the PNGF6 conferences-proceeding series [4,5].

It is interesting to note how Kadanoff himself largely moved away from the topic of NGF for the rest of his career; and yet, in one of his very last papers, he came back one last time to the subject, with a thorough scrutiny of the concept of entropy in non-equilibrium situations and the role played by entanglement ("Entropy is in Flux" arXiv:1403.6162 (2014)). As said before, Kadanoff's contributions cover several different fields; many of these, including

his deep involvement in teaching and mentoring, are mentioned in an article that originally appeared in UChicagoNews after his death, and reproduced here in abridged form by kind permission of the author, Steve Koppes. By us, the Editors of these proceedings, and the rest of the NGF community, Leo Kadanoff will be deeply missed, and remembered as one of the key figures in the beautiful and challenging field of non-equilibrium many-body physics.

## **Leo Kadanoff, leading figure in theoretical physics, 1937-2015**

*Adapted from the article published in UChicagoNews by Steve Koppes [6].*

Theoretical physicist Leo Kadanoff, who transformed theory and practice across scientific disciplines, died of respiratory failure on October 26 in Chicago. He was 78. “Leo was a prodigious scientist”, said his longtime UChicago colleague Sidney Nagel, the Stein-Freiler Distinguished Service Professor in Physics. “His work on statistical mechanics is one of the great achievements of 20th-century theoretical physics. It laid the conceptual and mathematical foundations for some of the most insightful and effective tools on which our modern understanding of nature is based”.

Kadanoffs work has applications throughout physics, ranging from condensed matter (liquids and solids) to elementary particles, Nagel said, with the reach of his work extending to mathematics and other sciences. Kadanoff received the 1999 National Medal of Science, the nation’s highest science honor, from President Bill Clinton in a White House ceremony. Kadanoff was cited “for leadership in fundamental theoretical research in statistical, solid-state and nonlinear physics, which has led to numerous and important applications in engineering, urban planning, computer science, hydrodynamics, biology, applied mathematics and geophysics.”

In 2013, UChicago received a \$3.5 million gift from anonymous donors to support the Leo Kadanoff Center for Theoretical Physics. The center brings together physicists who ordinarily work in a specialty such as particle physics, relativity theory or condensed matter theory and encourages them to work on problems of interest in all of those areas.

In the 1960s, Kadanoff made innovative and original contributions to the understanding of phase changes, such as the change of water from liquid to ice. In later years, working in collaboration with students, junior scientists and colleagues, he helped construct a new field of knowledge called soft condensed matter physics, which deals with such phenomena as the flow of fluids and the behavior of granular materials.

Kadanoff was especially interested in how complexity arises from simple phenomena, such as avalanches forming from the forces that are transmitted between grains of sand. A skilled teacher of colleagues, graduate students and undergraduates, one of his contributions was to use and to show others how to use computer models and simplified conceptual models for better understanding the world.

### **CURATOR AND CULTIVATOR**

Kadanoff had been active at the James Franck Institute until a few weeks before his death. One of his particularly important contributions there in his final years was to lead the long-running Computations in Science seminars. “This was easily the most influential seminar connected with the physics department,” said longtime UChicago colleague Thomas Witten, the Homer J. Livingston Professor Emeritus in Physics. “Its strategy was to scout actively for the most promising topics that would attract many disciplines, from math and physics to chemistry and geology. Its success was due to Leo’s persistent search for the most exciting topics and speakers. He evolved gracefully from his series of landmark discoveries in statistical physics to his last role of curator and cultivator.”

Nagel also commented on Kadanoff’s ability to attract the attention of scientists from

multiple disciplines.

"Here at the University, he was the center of so much activity that it is difficult to imagine the campus without him," Nagel said. "He had an extraordinary breadth of interests with a keen eye and appreciation for novel and imaginative science of all kinds." Kadanoff championed that work to his colleagues and was central to the culture of collaboration in the Physical Sciences Division. "When he saw an opportunity, he brought many of us together to attack a problem from different perspectives," Nagel noted. "The Leo I knew was all about developing people," Witten said.

Born January 14, 1937 in New York City, Kadanoff received his bachelor's, master's and doctoral degrees from Harvard University. After completing his doctorate in 1960, Kadanoff conducted postdoctoral research at the Bohr Institute for Theoretical Studies in Copenhagen. He joined the faculty of the University of Illinois at Urbana-Champaign in 1962, where he remained until joining the Brown University faculty in 1969.

#### **DISTINGUISHED PROFESSORSHIP**

Kadanoff became a professor of physics at UChicago in 1978 and was named the John D. and Catherine T. MacArthur Distinguished Service Professor of Physics and Mathematics in 1982. He directed UChicago's Materials Research Center from 1981 to 1984 and from 1994 to 1997. He also had served as a visiting professor at Cambridge University in 1965, and as the Lorentz Professor at the University of Leiden in The Netherlands in 2003. He retired as professor emeritus in 2003 but remained professionally active, serving as president of the American Physical Society in 2007.

Kadanoff had received many honors during his career. These included the Wolf Foundation Prize in Physics, the Grande Medaille d'Or of the Académie des Sciences de l'Institut de France, the American Physical Society's Onsager and Buckley prizes, the Franklin Institute's Elliott Cresson Medal, the Boltzmann Medal of the International Union of Pure and Applied Physics, and the Lorentz Medal of the Royal Dutch Academy of Sciences. He also was a member of the National Academy of Sciences and a fellow of the American Academy of Arts and Sciences, the American Association for the Advancement of Science, of the American Physical Society, and of the Alfred P. Sloan Foundation.

Kadanoff was further recognized for his undergraduate teaching. At UChicago he designed a new undergraduate course, "Chaos, Computers and Physics". Nominated by his students, he received the University's prestigious Quantrell Award for Excellence in Undergraduate Teaching in 1990.

#### **References**

- [1] Conservation Laws and Correlation Functions, G. Baym and L.P. Kadanoff, Phys. Rev. 124, 237 (1961).
- [2] Quantum Statistical Mechanics, G. Baym and L.P. Kadanoff, (New York, W.A. Benjamin, 1962).
- [3] Diagram technique for non-equilibrium processes, L. V. Keldysh, Zh. Eksp. Teor. Fiz. 47, 1515 (1964); Sov. Phys. JETP 20, 1018 (1965).
- [4] Progress in Nonequilibrium Green's functions, M. Bonitz (Ed.) (World Scientific, Singapore, 2000).
- [5] Progress in Nonequilibrium Green's functions II, M. Bonitz and D. Semkat (Eds.) (World Scientific, Singapore, 2003).
- [6] <http://news.uchicago.edu/source/steve-koppes>

## General Information

**International Advisory Board:** M. Bonitz, P. Danielewicz, F. Jahnke, A.-P. Jahuo, R. van Leeuwen.

**Organising Committee:** C. Verdozzi (Chair), A. Wacker, C.-O. Almbladh.

**Conference Secretary:** Katarina Lindqvist.

**Support:** The organisers acknowledge support from the Swedish Research Council and from the Christian-Albrechts-Universität-Kiel via Kiel Nano, Surface and Interface Science (KiN-SIS).

**Workshop Venue:** The Department of Physics, University of Lund  
Postal address: Box 118, 221 00 LUND, Sweden

## List of Talks

I=Invited talk, C= Contributed talk

**A. P. Jauho,**

*Green's function techniques applied to large scale nanostructuring of graphene* (I)

**M. Galperin,**

*Transport and optical response in a nanoscale device* (I)

**T. Kubis,**

*Contact self-energies: More than simple boundary conditions* (I)

**M. Garny,**

*Renormalization out of equilibrium in relativistic quantum field theory* (I)

**P. Danielewicz,**

*Progress in Application of Nonequilibrium Green's Functions to Nuclear Reactions* (I)

**K. Thygesen,**

*Many-body GW calculations for molecular transport junctions* (I)

**M. Schüler,**

*Time propagation of coupled fermionic-bosonic Kadanoff-Baym equations for plasmon-assisted double photoemission* (C)

**M. Sentef,**

*Theoretical investigations of laser-driven superconductivity* (C)

**S. Ristinmaa Sørensen,**

*Double ionization: investigating mechanisms and time scales* (I)

**L. Reining,**

*A direct approach to the calculation of many-body Green's functions* (I)

**I. Knezevic,**

*Coupling Electrons, Phonons, and Photons at the Nanoscale: Challenges in Nonequilibrium Transport Simulation* (I)

**H. S. Köhler,**

*Nuclear Response Functions by two-time Green's functions* (C)

**R. van Leeuwen,**

*Kadanoff-Baym equations for time-dependent coupled electron-boson systems* (I)

**P. Lipavský,**

*Formation of superconducting condensate under non-equilibrium conditions* (I)

**D. Winge,**

*Second Harmonic Generation in Quantum Cascade Lasers Simulated using Green's Functions* (C)

**M. Hopjan,**

*Real-time dynamics of Hubbard-type model systems via a combination of the Kadanoff-Baym formalism with adiabatic DFT* (C)

**A. L'Huillier,**

*Ultrafast Atomic Physics using Attosecond Pulses* (I)

**S. Hermanns,**

*Nonequilibrium Green's functions - Going beyond standard approximations for extended systems with state-of-the-art computing* (I)

**K. Balzer,**

*Solving the Kadanoff-Baym equations via the auxiliary Hamiltonian representation: method and applications* (I)

**M. Pereira,**

*Nonequilibrium Green's Functions Theory for Transport and Optics of TERA-MIR Materials*

*and Devices* (I)

**R. Citro,**

*Spin pumping through an interacting quantum dot* (I)

**P. Werner,**

*Nonequilibrium dynamics of electron-phonon systems*

**M. Potthoff,**

*Non-equilibrium self-energy-functional theory* (I)

**E. Arrigoni,**

*Steady-state dynamical mean-field theory within an auxiliary master equation approach* (C)

**H. Strand,**

*Real-time dynamics of lattice bosons in high dimensions from nonequilibrium dynamical mean-field theory* (C)

**E. Lindroth,**

*Study of attosecond dynamics in atomic many-body systems using complex scaling* (I)

**E. K. U. Gross,**

*Some thoughts on the electron-phonon interaction* (I)

**G. Stefanucci,**

*NEGF approach to pump-probe photoabsorption spectroscopy* (I)

**J. Wang,**

*Current conserving theory on shot noise* (I)

**F. Jahnke,**

*Semiconductor nanolaser with superradiant light emission connecting carrier and photon correlations* (I)

**K. Kaasbjerg,**

*Non-equilibrium Green's function approach to light emission from plasmonic contacts* (C)

**N. Schlünzen,**

*Nonequilibrium Green's functions approach to transport and diffusion in strongly coupled finite quantum systems* (C)

**U. Aeberhard,**

*Nonequilibrium Green's function theory of nanostructure solar cells* (I)

**Y. Pavlyukh,**

*Non-equilibrium approach to scattering theory and to plasmon losses in photoemission* (I)

## List of Posters

BAUCH, Sebastian

*The time-dependent generalized-active-space configuration interaction approach to correlated ionization dynamics*

BONITZ, Michael

*Path integral Monte Carlo for correlated fermions - ways around the sign problem*

BOSTRÖM, Emil

*Time-Resolved Spectroscopy and Dissociation Dynamics of Atoms at Surfaces: Insight from a Model-System Approach*

DAMTIE, Fikeraddis Ahmed

*Time dependent study of multiple exciton generation (MEG) in nanocrystal QDS*

DORDA, Antonius

*Spectral and transport properties of the nonequilibrium Anderson impurity model: auxiliary master equation approach within matrix product states*

FRANCKIE, Martin

*Non-Equilibrium Green's Functions as a Validation Tool for QCL Modeling*

HERRMANN, Andreas

*Non-Equilibrium Dynamical Cluster Approximation of the Falicov-Kimball Model*

HINZ, Christopher

*Towards a Unified Numerical Framework for Quantum Mechanical Simulations*

HYRKÄS, Markku

*Computing Exact Self-Energies with Polynomial Expansion*

KARLSSON, Daniel

*NEGF for studying strongly interacting systems in quantum transport*

LANI, Giovanna

*The SCE functional in the time domain: insights into its formal properties*

RIDLEY, Michael

*Generalised Theory of Current Noise for an Arbitrary Time-Dependent Bias*

SHAHID, Nazish

*Different forms of the Kadanoff-Baym equations in quantum statistical mechanics*

TANG, Gaomin

*Full-counting statistics of charge and spin transport in the transient regime*

TITVINIDZE, Irakli

*Non-equilibrium inhomogeneous DMFT for correlated Heterostructures*

TUOVINEN, Riku

*Extending the time-dependent Landauer-Büttiker formalism to superconducting junctions and arbitrary temperatures*

YANG, Kaike

*Dynamical correction of thermoelectric coefficients for strongly interacting electrons in the Coulomb blockade regime*

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## Conference Photographs



Visit at Kulturen in Lund. From the left: Frank Jahnke, Angus MacKinnon, Andreas Wacker, Gaomin Tang, Jian Wang, Miroslav Hopjan, Eva Lindroth, Gianluca Stefanucci, Lucia Reining, Kaike Yang, Carl-Olof Almbladh, Pawel Danielewicz, Hardy Gross, Daniel Karlsson, Markku Hyrkäs, Claudio Verdozzi, Robert van Leeuwen, Giovanna Lani, Karsten Balzer



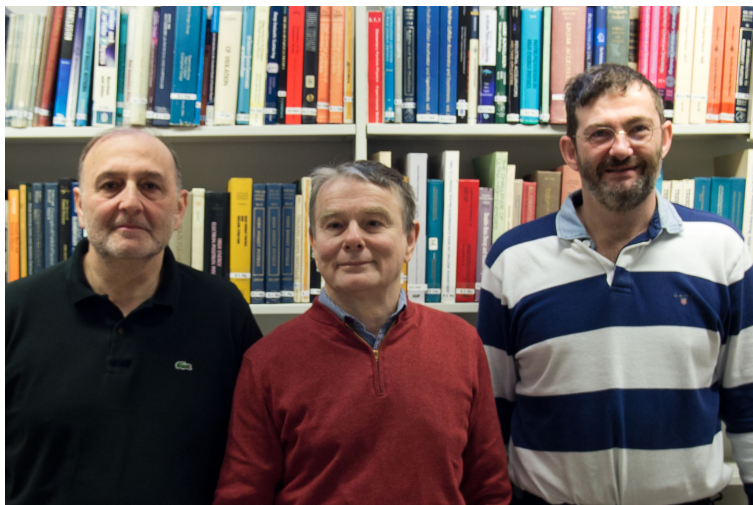
Visit at Kulturen in Lund. From the left: Andreas Wacker, Michael Galperin, Emil Boström, Yaroslav Pavlyukh, Claudio Verdozzi, Daniel Karlsson, Lucia Reining, Karsten Balzer, Eva Lindroth, Nazish Shahid, Hardy Gross, Angus MacKinnon, Michael Ridley.



Poster Session: Kaike Yang (left), Riku Tuovinen (center), Pawel Danielewicz (right)

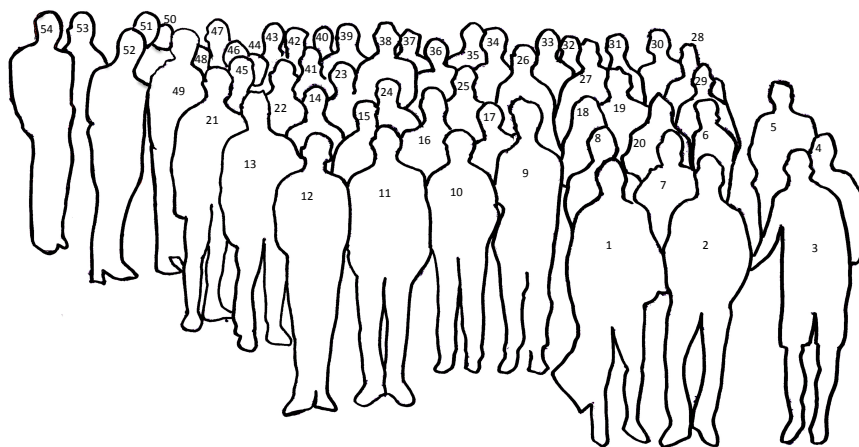
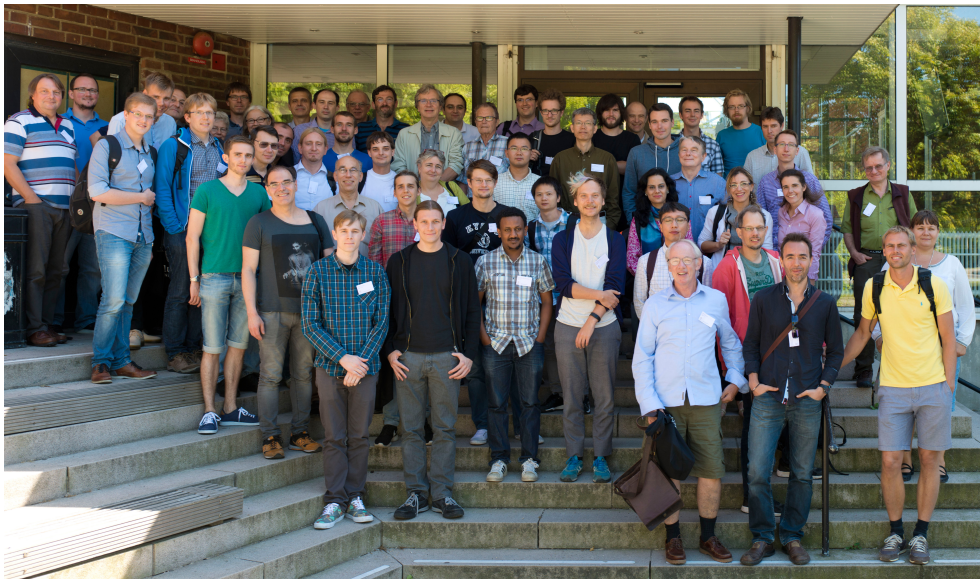


Poster Session: Hardy Gross (left ) and Robert van Leeuwen (right)



The PNGF6 organizers. From the left: Claudio Verdozzi, Carl-Olof Almbladh, Andreas Wacker





### Conference Photo Legend

(1) U. von Barth; (2) G. Stefanucci; (3) K. Thygesen; (4) K. Lindqvist; (5) P. Danielewicz; (6) G. Lani; (7) R. van Leeuwen; (8) G. Lee; (9) E. Boström; (10) F. A. Damtie; (11) A. Herrmann; (12) R. Tuovinen; (13) M. Pereira; (14) E. Gross; (15) M. Franckić; (16) H. Strand; (17) K. Yang; (18) N. Shahid; (19) C.-O. Almbladh; (20) R. Citro; (21) F. Brange; (22) K. Balzer; (23) C. Hinz; (24) L. Reining; (25) G. Tang; (26) J. Wang; (27) A. Dorda; (28) U. Aeberhard; (29) M. Schüler; (30) M. Hyrkäs; (31) D. Karlsson; (32) E. Arrigoni; (33) M. Ridley; (34) F. Hofmann; (35) S. Hermanns; (36) S. Köhler; (37) T. Kubis; (38) A.-P. Jauho; (39) A. Wacker; (40) A. Mackinnon; (41) M. Hopjan; (42) Y. Pavlyukh; (43) F. Jahnke; (44) I. Titvinidze; (45) M. Galperin; (46) E. Lindroth; (47) M. Potthoff; (48) A. L'Huillier; (49) S. Bauch; (50) C. Verdozzi; (51) D. Winge; (52) N. Schlünzen; (53) M. Sentef; (54) P. Lipavsky.