

$$\begin{aligned}
 & \langle \psi | H | \psi \rangle = 0 \\
 & \frac{d}{dt} \int \psi^* \psi d^3r \\
 & \langle \psi_n | v_{\text{ext}} | \psi_n \rangle = 0 \\
 & \mathcal{L}(r) \langle \psi(r) | \psi(r) \rangle \\
 & \int n(r) \epsilon_{xc}(n(r)) dr \\
 & \frac{\delta E_{xc}}{\delta n(r)} = v_{xc}(r)
 \end{aligned}$$

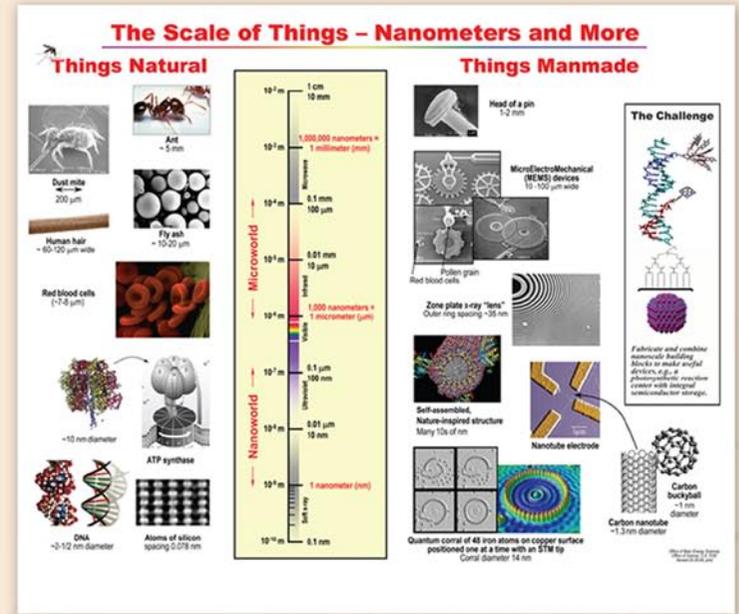
Theoretical condensed matter physics

Theoreticians at the Division of Mathematical Physics are working to understand and predict the quantum mechanical properties of matter on the subatomic, atomic, and nanometre scales.

Our knowledge of materials

One of the great challenges in physics is to understand, control, and exploit the properties of materials in novel ways. This requires an accurate, and preferably predictive, theoretical description of materials.

This is not easy for several reasons, e.g. some materials have a highly complex structure, or it may be necessary to consider several length- and time-scales simultaneously to predict the functional properties of interest. Furthermore, novel properties often emerge when the interactions among electrons and between electrons and lattice vibrations play an important role.

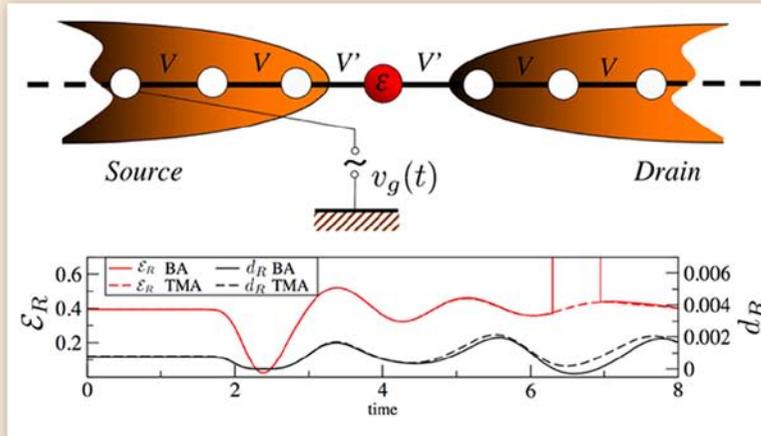


Time-dependent fields

Carl-Olof Almladh has worked on combining advanced theories related to relevant experiments. His main areas of interest include self-energies and excitation energies, density functional theory and various forms of spectroscopy and, more recently, systems with strong correlations, nanoscale systems and systems in external time-dependent fields.



Correlated nanosystems

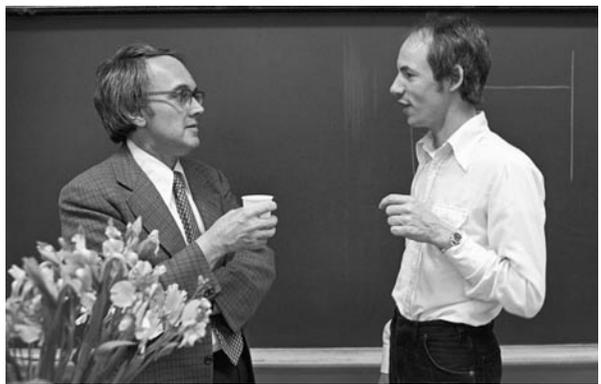
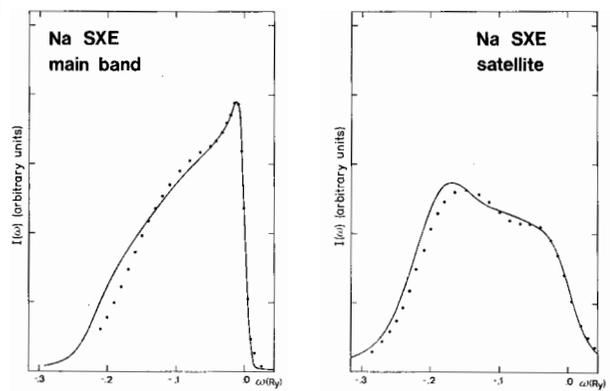


Double occupation in a nanoscopic scale conductor, according to the work of Puig von Friesen, Verdozzi, and Almladh in 2011.

A key experiment in nanophysics is quantum transport, where current flows through a nanoscopic system (e.g. a molecule) connected to external electrodes.

Stefanucci and Almladh have developed a theory in which the system is studied when it is disturbed from its equilibrium state by externally applied, possibly time-dependent, fields and voltages at the electrodes. Work on this has been continued by Almladh and Verdozzi and their students through the development of theories and detailed calculations of strongly correlated nanosystems.

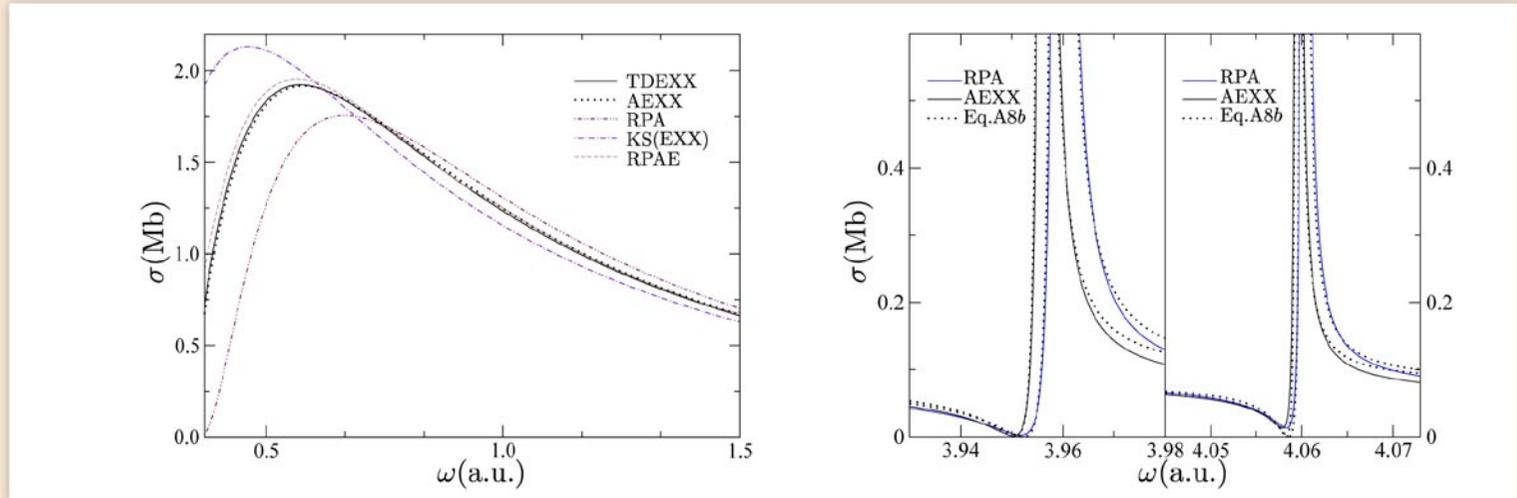
The final-state rule



Ulf von Barth in conversation with Günter Grossmann's examiner, Professor David C Langreth.

Ulf von Barth's first PhD student, Günter Grossmann, obtained his PhD in 1981. His work included the numerical evaluation of a model describing X-ray and Auger electron spectra. The model reproduced the shape of the X-ray edges well. Most importantly, the model provided theoretical support for *The Final-State Rule*. This rule explains, for example, why we see no effects of the inner-shell tail in X-ray emission, while it is seen in the corresponding satellite spectrum or why KLV Auger spectra are strongly affected by the vacancy, while KVV spectra are not.

Time-dependent density functional theory



Top left: Photoionization cross section for Be after the first ionization threshold.

Top right: First two Fano resonances resulting from the $1s \rightarrow 2p$ and $1s \rightarrow 3p$ transitions.

Density functional theory (DFT) provides a way of simplifying the complicated many-body problem to a single-body problem. Ulf von Barth has devoted a great deal of his research to the DFT, and was one of the world's leading experts in the field. Amongst other things, von Barth showed that the eigenvalues predicted by the theory do not describe the band gaps in semiconductors. An early paper by von Barth and Lars Hedin, generalizing the theory to magnetic material, has about 5 000 citations.

In more recent years, von Barth has been working on a time-dependent variant of DFT (TDDFT), which allows calculations of excitations. One of von Barth's PhD students, Maria Hellgren, showed that a certain approximation worked well for low-energy spectra.

The electronic structure of strongly correlated compounds

Approximate practical methods of applying quantum mechanics should be developed which can lead to an explanation of the main features of complex atomic systems without too much computation.

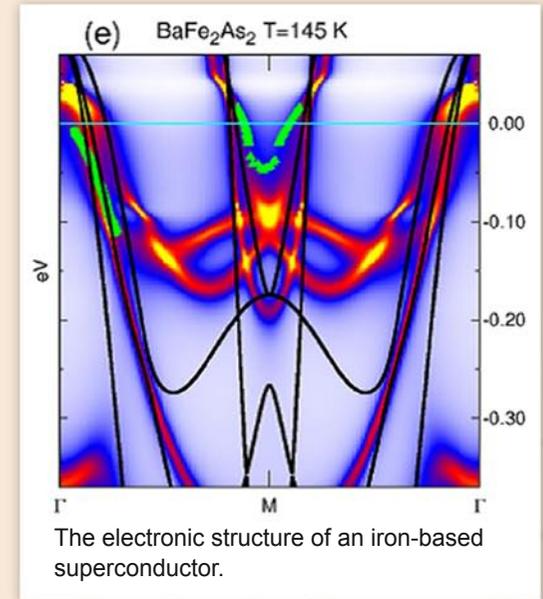
Paul Dirac

In the last few decades many new compounds with intriguing properties have been synthesized and discovered. They are expected to form the foundation of future electronics. A famous example is the unconventional high-temperature superconductors.



Future electronics

The mission of Aryasetiawan group is to develop quantum mechanical methods to study the electronic structure of these complex compounds. In the spirit of Dirac, a strict criterion to be fulfilled is that the method must be theoretically rigorous and at the same time applicable to real materials.

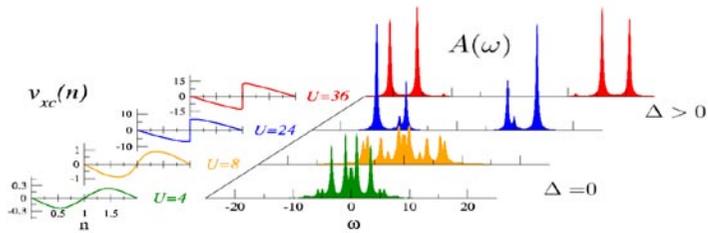


Non-equilibrium phenomena

Many future cutting-edge technologies will likely rely on small ultrafast devices, operating in rapidly changing environments. Furthermore, there is broad consensus among physicists that ground-breaking technological innovations are likely to be based on systems whose properties cannot be described within an independent-particle picture. This is why considerable research effort is currently being devoted in the condensed matter community to the development of theories for systems with strong inter-particle correlations, in- and out-of-equilibrium.

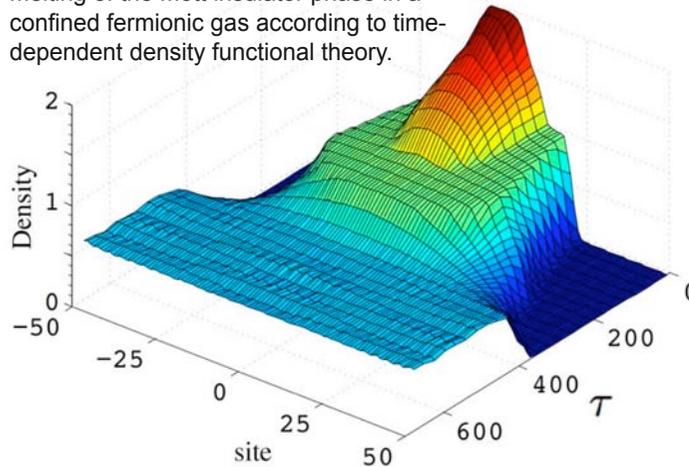


Time-resolved dynamics of non-equilibrium systems



The exchange-correlation potential of DFT in the 3D Hubbard model (left) vs. the metal-insulator transition (right), as a function of electron-electron interactions.

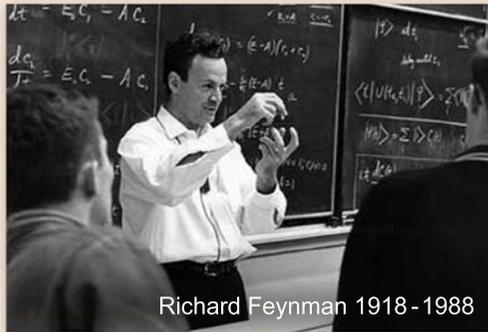
Melting of the Mott insulator phase in a confined fermionic gas according to time-dependent density functional theory.



Since his arrival in Lund, in 2004, Claudio Verdozzi's research has been devoted to developing and applying theoretical and numerical methods to systems with correlations among particles in- and out-of-equilibrium, such as *Green's* function methods, density functional theory and, for finite systems, exact numerical schemes.

The goal is to address open conceptual issues inherent in these approaches and describe situations as diverse as electron transport in nanodevices (together with Carl-Olof Almbladh), ultracold atoms in optical lattices, magnetic clusters, disordered systems and ultra-fast spectroscopy.

The beginning of nanoscience

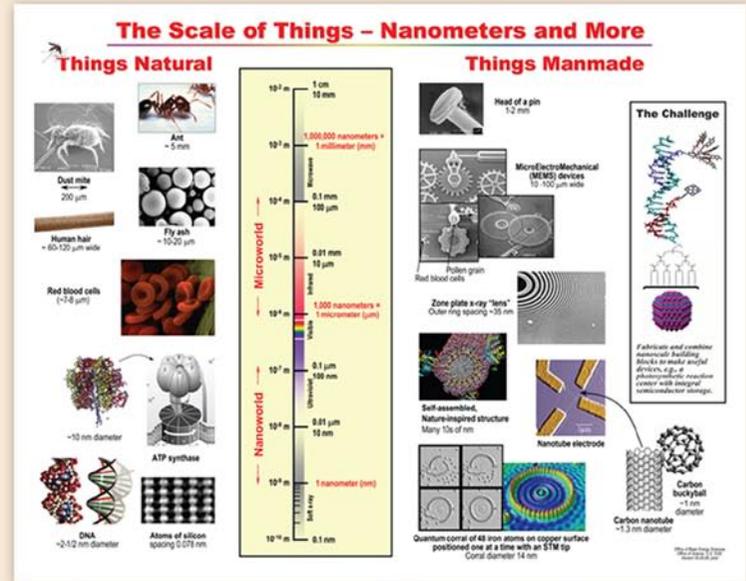


Richard Feynman 1918-1988

In a prescient lecture at Caltech in 1959, the famous American physicist Richard Feynman predicted a new era in materials science where, instead of exploiting materials found in nature, novel artificial systems are created with properties tailored towards targeted applications.

This would be done by manipulating individual atoms on the scale of nanometres, where quantum mechanical effects dominate.

Since then, this vision has spurred vast theoretical and experimental activity, to conceive and realize novel nanomaterials and the theoretical models required to predict and explain their behaviour.



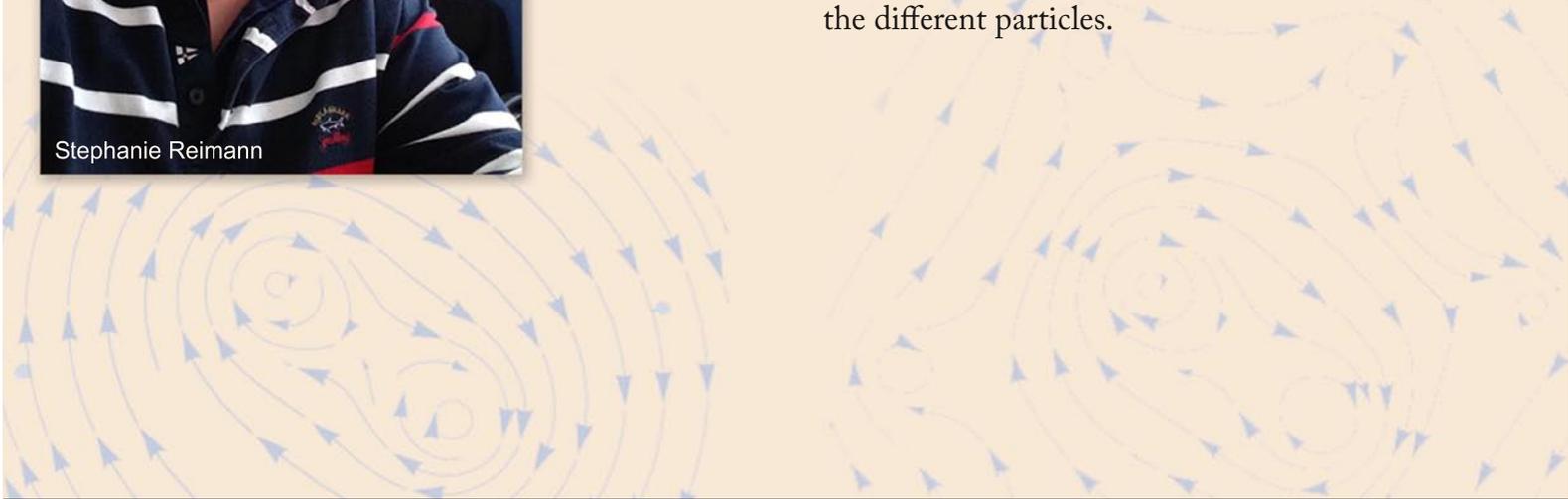
Particle ensembles



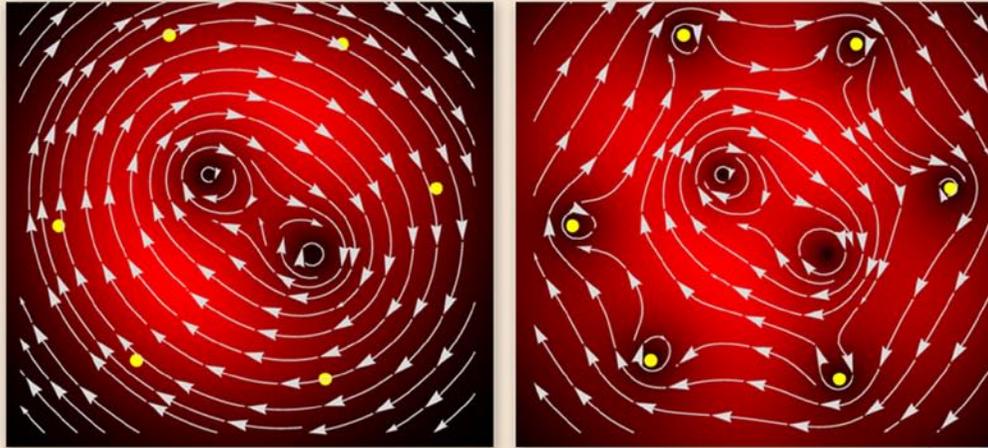
Stephanie Reimann

Stephanie Reimann and her research group are working on theoretical calculations on how small systems, on the nanometre scale, consisting of several interacting particles behave.

One example is small semiconductor systems, e.g. quantum dots and quantum wires, where quantum mechanics determine the laws of physics. Here, the interplay and interactions between the particles are decisive for the physical phenomena being investigated, such as correlations in time and space, vortex formations and the shell structure of the energies of the different particles.



Smart approximations

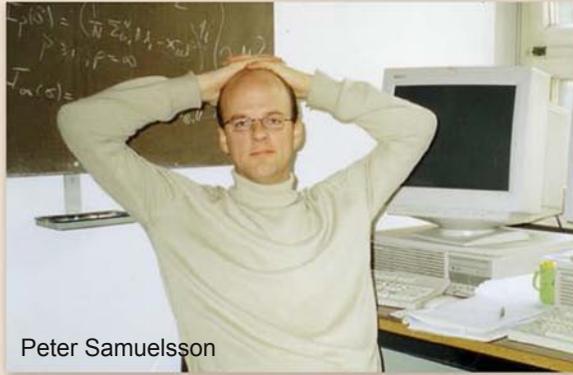


All the particles in the universe can be divided into two types, bosons and fermions. When bosons, such as e.g. different types of atoms, are trapped in small systems, and cooled down to temperatures approaching absolute zero, they can form a *Bose–Einstein* condensate. This very special state can only be explained by quantum mechanics.

Stephanie Reimann and her group have investigated the fundamental properties of Bose–Einstein condensates as well as fermions cooled to very low temperatures. A very interesting example is particles with dipolar properties.

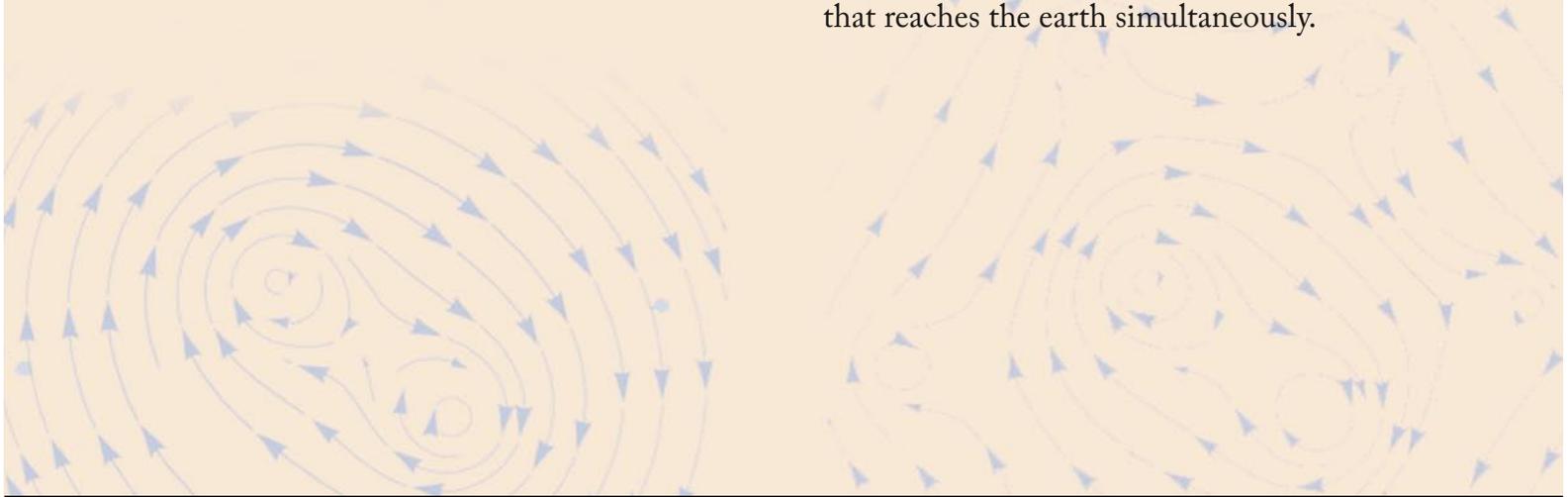


Unexpected relations



Peter Samuelsson and his research group are working on theories for nanoscale systems, especially the transport of electrons through the system. This may lead to better and faster electronic circuits. Quantum mechanical effects that can lead to more reliable transfer of information than is possible today are of special interest.

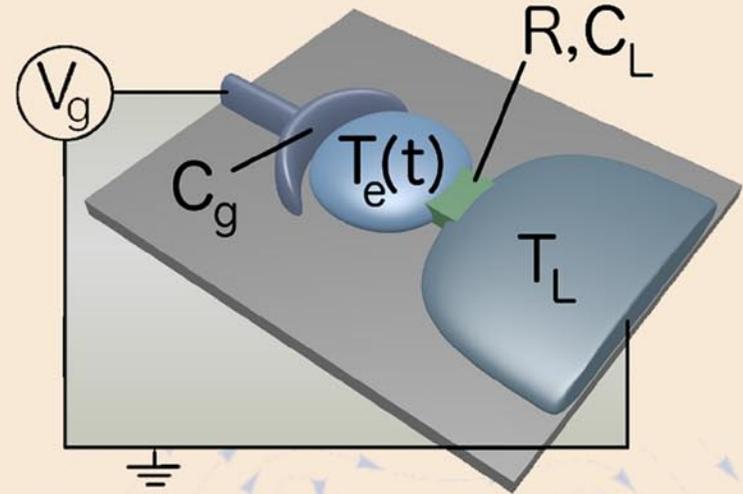
Research carried out by the group has revealed unexpected relations between, on the one hand, quantum information and electrons, and on the other, between light from stars at different distances from the earth that reaches the earth simultaneously.



Useful noise

Another area of research is concerned with noise and the fluctuations in the electric current of nanosystems. Noise is usually regarded as a disturbance to be removed, but the noise itself can contain a lot of information in itself, or, to use the scientist Rolf Landauer's words, *the noise is the signal*. Peter and his group have examined several different aspects of noise in nanoscale systems.

Peter Samuelsson and his group have also investigated the effects on temperature and heat generated in nanostructures when quantum mechanics determine the physical properties of the material. It is hoped that it will be possible to find new, more efficient ways of converting heat into electric energy, by using the unique properties of nanosystems.



Electrons in confined spaces

Andreas Wacker and his research group are working on theories of how electric current, heat and atomic vibrations, is transported through nanoscale systems made of semiconductor materials. Specifically transportation when the nanosystem is not in equilibrium, leading to interesting physical effects.

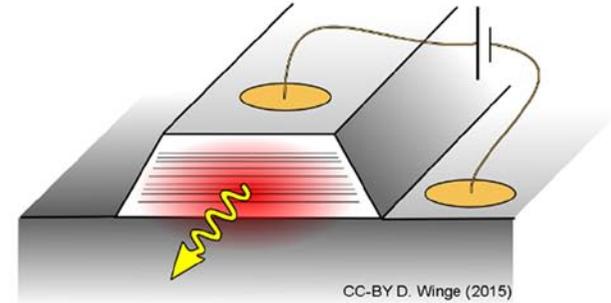
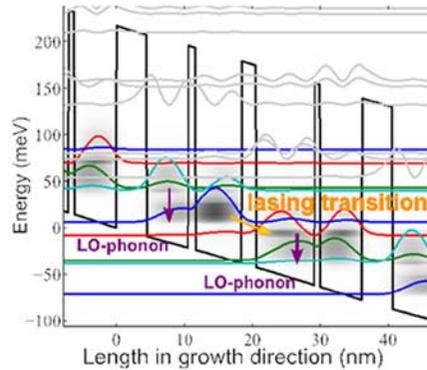
Another important area of interest is how to make better lasers in systems built by different, alternating, semiconductor materials. These so-called quantum cascade lasers have numerous exciting applications in everyday life. Andreas and his group studied the basic quantum mechanical phenomena in these alternating layers of semiconductor systems and how these phenomena can be controlled to increase the performance of the lasers.



Andreas Wacker



The quantum cascade laser



Another area involves transportation through so-called quantum dots, nanoscale specks of semiconductor material. Electrons can jump in and out of the quantum dots and thereby bring both electric charge and heat energy from one side of the dot to the other.

Andreas Wacker has specifically investigated what happens when jumping electrons interact with each other and with the environment in the form of e.g. vibrations of the atoms in the material forming the quantum dot.