LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN | ARNOLD SOMMERFELD CENTER FOR THEORETICAL PHYSICS

Sommerfeld Theory Colloquium

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Out-of-equilibrium phenomena from a new perspective: an Ab-Initio approach

Ultra-fast optical spectroscopy is a powerful tool for the observation of dynamical processes in several kind of materials. The basic time-resolved optical experiment is the so-called "pump-probe": a first light pulse, the "pump", resonantly triggers a photo-induced process. The subsequent system evolution can be monitored, for example, by the time–dependent transmission changes of a delayed "probe" pulse. The pump pulse photon energy, spectral width and peak intensity creates a certain density of electron-hole pairs in a more or less localized region of space. After the creation of the initial carrier density the time evolution of the single-particle and many-particle excitations is now governed by a non-trivial interplay between electron-electron and electron-phonon scatterings. In this talk I will present a novel approach based on the merging of Non-Equilibrium Green's function theory and Density Functional Theory to investigate the carrier dynamics following a pump excitation. The case of bulk Silicon, a paradigmatic indirect gap semiconductor, is studied by using the Baym-Kadanoff equations. Both the electron-electron (e-e) and electronphonon (e-p) self-energies are calculated fully Ab-Initio by using a semi-static GW approximation in the e-e case and a Fan self-energy in the e-p case. By using the generalized Baym-Kadanoff ansatz the two-time evolution is replaced by the only dynamics on the macroscopic time axis. The enormous numerical difficulties connected with a real-time simulation of realistic systems is overcomed by using a completed collision approximation that further simplifies the memory effects connected to the time evolution. The carrier dynamics is shown to reduce in such a way to have stringent connections to the well-known equilibrium electron-electron and electron-phonon self-energies. This link allows to use general arguments to motivate the

relative balance between the e-e and e-p scattering channels on the basis of the carrier energies.

Wednesday, 6 February 2013, 16:15h, Room A348/349, Theresienstr. 37/III

Prof. A. Scrinzi