HL 42: Optical Properties of Quantum dots: Theory and Simulation

Time: Thursday 9:30–13:00 Location: EW 201

HL 42.1 Thu 9:30 EW 201

Gauge invariant k.p envelope function theory and g-factors in quantum dots — •Till Andlauer, Richard Morschl, and Peter Vogl — Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, D-85748 Garching

We present a gauge invariant real space discretization scheme that includes magnetic fields nonperturbatively in the framework of the multiband k.p envelope function theory. Our procedure is based on Wilson's formulation of gauge theories [1]. The magnetic field couples to the envelope functions via phase factors that result from spatial discretization of the gauge covariant derivative. These phase factors contain a discretized curve integral over the vector potential. In addition, the carrier's spin couples to the magnetic field via a Zeeman-term. In the case of infinitesimal grid spacings, our method becomes equivalent to the minimal substitution method. Applying our procedure, we calculate effective electron and hole g-factors of InAs/InP nanowire dots as a function of dot size and magnetic field direction. We obtain excellent agreement with experimental data [2] and show that the changes in g-factors correlate well with the spatial extent of the wave functions. Furthermore, we investigate the influence of strain and high magnetic fields on the g-factors. In the latter case, we find nonlinear Zeeman splittings and strongly deformed eigenstates. [1] K. G. Wilson, Phys. Rev. D 10, 2445 (1974). [2] M. T. Björk et al., Phys. Rev. B 72, 201307(R) (2005).

HL 42.2 Thu 9:45 EW 201

Gain reduction in semiconductor Quantum Dot systems — •Michael Lorke[1], Jan Seebeck[1], Paul Gartner[1], Frank Jahnke[1], and Weng Chow[2] — [1]Institute for Theoretical Physics, University of Bremen — [2]Sandia National Laboratories, Albuquerque, New Mexico

For practical application of quantum dots (QDs) in light emitters as well as for fundamental studies of their emission properties, dephasing processes due to carrier-carrier and carrier-phonon interaction play a critical role. They determine the homogeneous linewidth of the QD resonances, limit the coherence properties of QD lasers and their ultrafast emission dynamics, and have a strong influence on coherent optical nonlinearities. A microscopic theory is used to study the optical properties of semiconductor quantum dots. The dephasing of a coherent excitation and line-shifts of the interband transitions due to carrier-carrier Coulomb interaction and carrier-phonon interaction are determined from a quantum kinetic treatment of correlation processes which includes non-Markovian effects.

Our quantum kinetic theory predicts a new effect, not found in other gain materials. For large carrier densities, the maximum gain can decrease with increasing carrier density. This behavior arises from a interplay of state filling and dephasing, so that a appropriate treatment of the carrier density dependence of dephasing is necessary. Results for the α-factor for QD systems and a comparison of the peak gain between QDs and quantum wells are will be shown. The presented theory will also be used to determine gain spectra in nitride material systems.

HL 42.3 Thu 10:00 EW 201

Theoretical investigation of optical properties of semiconductor nanostructures — •Gudny Gudmundsdottir and Frank Grosse — Institut für Physik der Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Near band edge optical properties of compound semiconductors are determined by excitons. The two particle problem is numerically challenging in semiconductor nanostructures due to their inhomogeneous nature. The one-particle potentials for electron and hole contain the spatially varying band edge potentials given by the local chemical composition and are additionally modified by intrinsic static strain fields and acoustic phonons through deformation potential coupling.

We present calculations of optical properties by solving the time dependent Schrödinger equation for the full three dimensional exciton problem (6 coordinates) in embedded semiconductor quantum dots varying in shape and composition including disorder (alloys). The parallel implementation (MPI) of the computer code allows to treat these complex nanostructures efficiently. Input strain fields are generated from molecular dynamics simulations enabling us to study the influence of phonon wave packets on the optical response of quantum dots.

HL 42.4 Thu 10:15 EW 201

Atomistic Theory of Excitonic Effects in Nanostructures — •Gabriel Bester — Max Planck Institute for Solid State Research, Stuttgart, Germany

The confinement in all three space dimensions given in nanostructures leads to several new phenomena of fundamental interest that can be handled by different levels of theory. For nanostructures of small size, the atomistic nature and ensuing symmetry is most relevant and the system should be viewed as a large assembly of atoms. The adequate description is then atomistic in nature, such as in tight binding or pseudopotential approaches. For larger structures, the atomistic nature tends to become less important while particle-particle correlations become more relevant. In this size regime descriptions such as effective mass in the single band or in the multiband approach (k.p) followed by configuration interaction have established themselves. I will present a theoretical framework, based on empirical pseudoptentials and configuration interaction calculations that enables us to address the intermediate length scale where both, the atomistic nature and correlations are retained. I will illustrate the method by showing recent applications in the realm of quantum dot physics where properties such as quantum entanglement [1], piezoelectricity [2] or Coulomb blockade [3] have been investigated.

[1] Bester et al., Phys. Rev. Lett. 93 047401 (2004). [2] Bester et al. Phys. Rev. Lett. 96, 187602 (2006). [3] Ediger, Bester, et al., Nature Physics 3, 774 - 779 (2007).

15 min. break

HL 42.5 Thu 10:45 EW 201

The phonon bottleneck revisited at low temperatures — •Jan Seebeck[1], Paul Gartner[1,2], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen, Germany — [2]National Institute for Materials Physics, Bucharest-Magurele, Romania

The application of semiconductor quantum dots in optoelectronic devices requires efficient carrier-scattering processes. For low carrier densities the interaction with LO phonons provides fast scattering channels, which can be understood by describing carriers as polarons.

Within a quantum kinetic many-body theory we revisit the phonon bottleneck problem. For low temperatures, an asymptotic phonon bottleneck is observed, where after an initial redistribution of carriers the carrier kinetics freezes, not reaching a thermal distribution in terms of the Kubo-Martin-Schwinger condition. Also non-Markovian effects in the dephasing properties as well as intermediate polar coupling nitride materials are discussed.

HL 42.6 Thu 11:00 EW 201

Plane-Wave-implementation of the $\mathbf{k}\cdot\mathbf{p}$-formalism including strain and piezoelectricity to study the optoelectronic properties of semiconductor nanostructures — •Oliver Marquardt, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung

Optical properties of semiconductor nanostructures such as quantum dots and wires are a direct consequence of their shape, size and material composition. The $\mathbf{k}\cdot\mathbf{p}$ formalism provides a real space approach to compute relevant parameters of nanostructures as e.g. needed to simulate optoelectronic devices such as light and laser emitting diodes. Contributions like strain and piezoelectric potentials entering the $\mathbf{k}\cdot\mathbf{p}$ formalism are typically calculated using continuum elasticity theory.
We have reformulated this approach into a mixed real / reciprocal space formalism and implemented it into our plane-wave DFT-package S/Phi/nX. This allowed us to make efficient use of the existing highly optimized minimization routines as well as the efficient preconditioner techniques in a plane-wave basis set.
We investigate different nanostructures with a focus on the III-nitride materials in the zincblende and wurtzite phase. A detailed comparison to approaches resolving fully the atomistic structure will be shown in order to verify the validity of our approach. Further the influence of the spin-orbital coupling which has been commonly neglected is shown to lift the artificial degeneracy of the hole ground state.

HL 42.7 Thu 11:15 EW 201

Input/Output Characteristics of Semiconductor Quantum Dot Lasers — •Christopher Gies, Jan Wiersig, and Frank Jahnke — Institute for Theoretical Physics, University Bremen, 28334 Bremen, Germany

The field of quantum dot- (QD) microcavity lasers is vividly developing. Initial uncertainties in the definition of a laser threshold and discrepancies in the physics of QDs and two-level atoms have lead us to the development of a microscopic semiconductor laser theory. Effects like Pauli blocking, modifications to the source term of spontaneous emission, and the absence of complete inversion in the carrier system can strongly influence the emission characteristics in QD-based systems. Consequently, we find deviations from predictions of atomic laser models and extracted parameters. With respect to the jump in the input/output curve that is dependent on the spontaneous emission factor β, we discuss various effects that lead to differences between the atomic and the semiconductor model. Our applications focus on the influence of pulsed and continuous wave excitation, which is of great relevance for current experiments.

HL 42.8 Thu 11:30 EW 201

Optical Spin Switching in a Quantum Dot with a Single Mn Atom — •Doris E. Reiter[1], Vollrath Martin Axt[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str.10,48149 Münster — [2]Institut für Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth

Spins in semiconductor quantum dots are promising candidates as basic ingredients for new quantum hardware, e.g. magnetic bits. In a single quantum dot with a single Mn atom as has been fabricated recently the spin of the Mn instead of the exciton spin can be used as new basis for spintronics. The Mn spin has six possible orientations. In contrast to the carrier spins however it is not directly accessible by laser light. Instead, it can be controlled via the exciton, which can be driven by the optical excitation with ultra short laser pulses. Exciton and Mn spin couple to each other via direct exchange interaction. Though stronger coupled, the heavy holes can hardly induce spin flips, but electrons and light holes have great impact on the dynamics of the Mn spin. Starting from an initial state, we show that the Mn spin states can be selectively accessed via flips on ultrashort times scales induced by a sequence of laser pulses.

15 min. break

HL 42.9 Thu 12:00 EW 201

Study of combined decoherence channels of optically controlled spin rotations in quantum dot systems — •Anna Grodecka[1,2], Paweł Machnikowski[2], Carsten Weber[3], Andreas Knorr[3], and Jens Förstner[1] — [1]Computational Nanophotonics Group, University Paderborn, Germany — [2]Institute of Physics, Wrocław University of Technology, Poland — [3]Nonlinear Optics and Quantum Electronics, Technical University Berlin, Germany

It has been recently proposed [1] that coupling to a trion state may lead to a Raman transition between the two Zeeman-split spin states in a quantum dot, which allows for optical coherent control of a spin. However, the question arises whether the intrinsic features of the system may lead to decoherence which counteracts the ideal coherent control.

In this work, we study the combined decoherence channels resulting from the influence of phonon and photon reservoirs, as well as from the imperfections of the evolution of an optical spin control based on an off-resonant coupling of the spin states to a trion state in a doped semiconductor quantum dot. Using a perturbative theory describing the open system evolution we calculate the total error of the spin-based quantum gate. The optimal conditions for coherent operations are indicated and possible ways of reducing the decoherence are discussed [2].

1. P. Chen, C. Piermarocchi, L. J. Sham, D. Gammon, and D. G. Steel, Phys. Rev. B 69, 075320 (2004).
2. A. Grodecka, C. Weber, P. Machnikowski, and A. Knorr, Phys. Rev. B 76, 205305 (2007).

HL 42.10 Thu 12:15 EW 201

The impact of travelling phonon wave packets on quantum dot spectra — •Jan Huneke[1], Vollrath Martin Axt[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie , WWU Münster, Wilhelm-Klemm-Str.10,48149 Münster — [2]Institut für Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth

The influence of phonon wave packets travelling across a semiconductor quantum dot on the optical spectra of the lowest quantum dot transition is analysed. Two situations are compared: (i) a phonon wave packet is generated by the optical excitation of a single quantum dot near a surface, which after reflection at the surface reenters the quantum dot; (ii) a phonon wave packet is generated by the excitation of a nearby second dot and then travels across the quantum dot. The analysis accounts for pure dephasing interactions between electronic and phononic degrees of freedom in quantum dot systems driven by ultrafast laser pulses. For this situation a generating function formalism provides exact analytical results. We find that although the displacement fields crossing the dot are almost identical in these two situations, the real time responses as well as the corresponding spectra exhibit qualitative differences and thus allow for a discrimination of phonon wave packets from different origins. By looking at the analytical results it is possible to trace back the physical origin of the differences in the above considered spectra to the fact that the phonons that cross the dot travel in different quantum mechanical subspaces namely: reflected phonon wave packets propagate in the single pair subspace while wave packets generated by a second dot travel in the two-pair manifold.

HL 42.11 Thu 12:30 EW 201

Coherence properties, photon statistics, and mode properties of quantum-dot based microcavity lasers — •Jan Wiersig[1], Christopher Gies[1], Michael Lorke[1], Frank Jahnke[1], and Martina Hentschel[2] — [1]Institut für Theoretische Physik, Universität Bremen, 28334 Bremen — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden

Semiconductor quantum dots as active material offer several advantages for laser applications. In combination with optical microcavities these systems promise ultra-low thresholds and genuine single-mode lasing [1,2]. This talk reviews our recent progress in developing a microscopic theory for the photon correlation functions $g^{(1)}(\tau)$ and $g^{(2)}(\tau)$ describing the first-order coherence and the photon statistics of quantum-dot-based microcavity lasers. In the transition region from spontaneous to dominantly stimulated emission our theory predicts a qualitative change of $g^{(1)}(\tau)$ from a Gaussian-like to an exponential behaviour in agreement with recent experiments. Moreover, we demonstrate two different approaches to achieve unidirectional laser light emission from deformed microdisk cavities. One scheme is based on avoided resonance crossings [3], the other one on chaotic ray dynamics.

[1] S.M. Ulrich, C. Gies *et al.*, Phys. Rev. Lett. **98**, 043906 (2007).
[2] C. Gies, J. Wiersig, M. Lorke, and F. Jahnke, Phys. Rev. A **75**, 013803 (2007).
[3] J. Wiersig and M. Hentschel, Phys. Rev. A **73**, 031802(R) (2006).

HL 42.12 Thu 12:45 EW 201

Annealing of overgrown InAs/GaAs Quantum Dots: A Tight-Binding Study — •Alexander Kleinsorge[1], Thomas Hammerschmidt[1], and Peter Kratzer[2,1] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany

The electronic and optical properties of quantum dots (QDs) are determined by their atomic structure. A better understanding of this relationship requires input from electronic structure theory. We employ the empirical sp^3s^* tight-binding approach, including 2nd-nearest-neighbor interactions and spin-orbit coupling, preceded by structural relaxation using a potential of the Abell-Tersoff type. Large systems with up to 10^6 atoms can be treated using the folded-spectrum method.

To simulate the intermixing during annealing of InAs QDs in GaAs, we implemented a strain-driven kinetic Monte-Carlo (kMC) method, where the hopping rate of the cation vacancies depends on the differences of the relaxation energy (calculated with the Tersoff potential). Using strain-dependent rates in the kMC-Simulation leads to faster dissolving of the wetting layer. Because of the different shape of the electron and hole wavefunctions, the exciton is associated with a dipole moment which causes the experimentally observed Stark shift. We investigate how the dipole moment of the ground state exciton in a QD depends on the concentration profiles after annealing.