HL 57 Theory of electronic structure

Time: Friday 11:00–12:45 Room: BEY 118

HL 57.1 Fri 11:00 BEY 118

Magnetic band structure of GaAs and InSb in ultrahigh magnetic fields — •Christian Ammann, Christian Strahberger, and Peter Vogl — Walter Schottky Institut, Technische Universität München, D-85748 Garching, Germany

The availability of ultrahigh magnetic fields for solid state investigations calls for reliable theoretical predictions of the electronic band structure in ultrahigh fields. We have calculated the magnetic band structure and optical absorption spectra of bulk GaAs and bulk InSb by means of an empirical $sp^3d^5s^*$ tight binding model where the magnetic field is incorporated non-perturbatively to capture effects that can only arise by taking the entire Brillioun zone into account. In fields up to 1000 T, the band structure can be interpreted in terms of Landau ladders arising from all valleys throughout the BZ whereas the spectrum shows a fractal behavior for higher fields. There is a strong dependence of the magnetic band structure on the B-field direction because of zone folding effects. We find the lowest $L\downarrow$-band state to cross the lowest $\Gamma\uparrow$-band state in GaAs at 600 T. The effective Lande g factor in InSb shows a strongly sublinear behavior due to strong hybridization of Γ and L band states beyond 100 T. For GaAs as well as InSb, we find efficient optical absorption in the far infrared range for intra-valence band transitions for B-fields between 100 T and 500 T.

HL 57.2 Fri 11:15 BEY 118

Excitons in stackes of ZnSe/CdSe quantum dots — •Tchelidze Tamar — Tbilisi State University, Department of Exact and Natural Sciences, Chavchavadze Ave.3 0218 Tbilisi Georgia

We investigated electron hole interaction in the flat 2D-quantum dot heterostructures with arbitrary number of stacked quantum dot layers. The calculation were carried out on the basic of obtained recurrent formula, which derives single particle energies and wave functions of electrons and holes in quantum dot heterostructures with n stacked layers from the single particle energies and wave functions for heterostructure with n-1 stacked layers. Interaction of electrons and holes were considered by means of direct diagonalizing of Hamiltonian matrix. We studied the dependence of exciton binding energy, probabilities of optical transitions in dependence on quantum dot and barrier layer size, as well as on the number of stacked layers. We have investigated the influence of impurities on the electron-hole Coulomb interaction in single and double stacks of quantum dots. We studied how the presence of one-charged donor and acceptor impurities affects on the exciton binding energy and probability of radiation decay in the flat 2D-quantum dots and quantum dot molecules.

HL 57.3 Fri 11:30 BEY 118

Orbital Functionals in Current Spin Density Functional Theory — •Stefano Pittalis, Stefan Kurth, Nicole Helbig, and E.K.U. Gross — Freie Universität Berlin, Theoretische Physik, Arnimallee 14 D-14195 Berlin

The proper description of non-relativistic many-electron systems in the presence of magnetic fields within a density-functional framework requires the paramagnetic current density and the spin magnetization to be used as basic variable besides the electron density. However electron-gas-based (LDA-type) functionals of Current-Spin-Density Functional Theory (CSDFT) exhibit derivative discontinuities as a function of the magnetic field whenever a new Landau level is occupied, which makes them difficult to use in practice. Since the appearance of Landau levels intrinsically is an orbital effect, it is appealing to use orbital-dependent functionals. Therefore, here CSDFT is presented in the framework of exchange-correlation energy functionals which are explicit functionals of two-component Kohn-Sham spinors. The integral equations for the exchange-correlation components of the scalar and vector potential and the magnetic field are derived in the formalism of the optimized effective potential method and a simplifying approximation to these equations is suggested. The formalism is then applied within the exchange-only limit to study two-dimensional quantum dots and atomic ground states.

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All-electron *GW* approximation in the augmented-plane-wave basis-set limit — •Christoph Friedrich[1], Arno Schindlmayr[1], Stefan Blügel[1], and Takao Kotani[2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of Chemical and Materials Engineering, Arizona State University, Tempe, AZ 85287-6006, USA

The GW approximation for the electronic self-energy yields quasiparticle band structures in very good agreement with experiment, but almost all calculations so far are based on the pseudopotential approach. We have developed an implementation within the all-electron linearised augmented plane-wave (LAPW) method, which treats the core electrons explicitly. As errors resulting from the linearisation of the basis set are frequently overlooked, we here aim to investigate its influence on the GW self-energy correction. A systematic improvement is achieved by including additional local orbitals defined as second and higher energy derivatives of solutions to the radial scalar-relativistic Dirac equation, which constitute a natural extension of the LAPW basis set. Within this approach the linearisation error can be systematically reduced, and the exact augmented-plane-wave basis-set limit can be reached. While the electronic self-energy and the quasiparticle energies benefit from the better description of the unoccupied states, the resulting band gaps remain relatively unaffected.

HL 57.5 Fri 12:00 BEY 118

Calculation of non-resonant x-ray Raman spectra by real-space multiple-scattering — •Henning Sternemann[1], Christian Sternemann[1], Juha Aleksi Soininen[2], and Metin Tolan[1] — [1]Exp. Physik I / DELTA, Universität Dortmund, 44221 Dortmund — [2]Div. X-ray Physics, Dept. Physical Sciences, University of Helsinki, Finland

Non-resonant x-ray Raman scattering is a valuable tool to reveal detailed information on the structural and electronic properties of matter. Low energy absorption edges can be studied with a high incident x-ray energy. In order to extract information out of the measurements it is often necessary to use computer simulations. Whereas most bandstructure methods require periodic boundary conditions and small unit cells, an extension of the ab initio real-space multiple-scattering approach [1] to non-resonant x-ray Raman scattering [2] is not confined by this limitation. We present calculations of K- and L-edges for simple elements such as Na and Si as well as for more complex materials like doped silicon clathrates.

[1] A. L. Ankudinov *et al.* Phys. Rev. B**65**, 104107, (2002), http://leonardo.phys.washington.edu/feff/
[2] J. A. Soininen *et al.* Phys. Rev. B**72**, 045136, (2005)

HL 57.6 Fri 12:15 BEY 118

GW Calculations Starting from Generalized Kohn-Sham Schemes: Application to InN — •Frank Fuchs[1], Jürgen Furthmüller[1], Friedhelm Bechstedt[1], and Georg Kresse[2] — [1]Institut für Festkörpertheorie und -optik, FSU-Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Materialphysik and Center for Computational Materials Science, Universität Wien, Austria

The GW approximation of Hedin is arguably the most successful approach for the calculation of quasi-particle (QP) energies. Its accuracy has been proven for a variety of systems. Usually, GW corrections are calculated in a 'one shot' fashion, calculating G_0 and W_0 from solutions of the Kohn-Sham equations with an exchange-correlation potential in local density or generalized gradient approximation (LDA/GGA). However, this standard approach fails for a number of systems such as InN which share shallow 'semi-core' electrons and a 'negative gap' in LDA/GGA. Here we present GW calculations which start from solutions of generalized Kohn-Sham (gKS) equations [1]. Such a procedure yields a positive gap for all the investigated gKS functionals. However, a crucial dependence on the wave-function details is found for the semi-core states. The calculations were performed using a model dielectric function for the GW self-energy. The electron-ion interaction was modeled via the PAW method which provides direct access to the all-electron wave functions.

[1] A. Seidl et al., PRB **53**, 3764 (1996)

HL 57.7 Fri 12:30 BEY 118

Path-integral treatment of a translation invariant many-polaron system — •F. Brosens[1], S. N. Klimin[1,2], and J. T. Devreese[1,3] — [1]TFVS, Department of Physics, Universiteit Antwerpen, B-2610 Antwerpen, Belgium — [2]State University of Moldova, Kishinev, Moldova — [3]Department of Semiconductor Physics, TU Eindhoven, NL-5600 MB Eindhoven, The Netherlands

Using an extension of the Jensen-Feynman inequality for systems of identical particles, we derived an upper bound for the ground state energy of a translation invariant system of N interacting polarons, taking into account the Fermi-Dirac statistics of the electrons. The developed approach is valid for arbitrary coupling strength.

For sufficiently large values of the electron-phonon coupling constant and of the Coulomb coupling strength, a stable multipolaron ground state can be formed. The total spin of the system then takes its minimal value. The stability region of the multipolaron state becomes narrower if the number of electrons increases. For a stable multipolaron state, the addition energy exhibits peaks corresponding to closed shells. These features of the addition energy, as well as the total spin as a function of the number of electrons, might be observable experimentally, e.g., by capacitance and magnetization measurements in high-Tc superconductors.

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