Influence of non-local exchange-correlation and spin-orbit interaction on electronic and optical properties of graphene, silicene, germanene, and tinene. 

A. I. Lichtenstein

Generalized Hubbard models for two dimensional hybrid materials — M. Rössner1, E. Saisoclü2, C. Friedrich2, S. Blügel2, A. I. Lichtenstein3, M. I. Katsnelson4, and T. O. Wehling1

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We present effective generalized Hubbard models for the description of novel two dimensional materials. The local and non-local partially screened Coulomb interaction as well as hopping integrals are calculated from first principles for silicene and graphene on a metallic substrate. We consider interactions up to the 6th nearest neighbor in real space and investigate the long range behavior of the dielectric function in k-space. We compare the resulting silicene Hubbard model to the corresponding model for pure graphene. Thereby we find values of $U/t = 10$ eV for the on-site and $V_{t} = 0.5$ eV for the nearest neighbor coupling motivated by the non-local screened Coulomb interaction in silicene, which are slightly bigger than in freestanding graphene. We further show that the ratio of the local to the non-local Coulomb interaction can be controlled by a metallic substrate, which efficiently screens non-local Coulomb terms.

Subgap conductivity in gated bilayer graphene — Maxim Trushin — University of Konstanz, 78457 Konstanz

In the present work [1], the subgap electron transport has been investigated in gated bilayer graphene [2] within the two-band effective model using the finite-size Kubo formula. The conductivity does not vanish even though the temperature is set to zero and the chemical potential gets into the middle of the band gap. In contrast to the universal subgap conductivity observed in the 2D topological insulators [3], the subgap conductivity in bilayer graphene turns out to be sensitive to the band gap size and disorder strength.

The effect can be explained in terms of the quantum mechanical interband coherence which turns out to be important for the chiral carriers. At finite temperature, a competition between the temperature-dependent interband decoherence and thermal activation processes results in the non-monotonic conductivity vs. temperature dependence. The non-monotonicity can be seen as a signature of the interband entanglement responsible for the difference between the transport and spectral gaps. The effect can be observed in gapped bilayer graphene sandwiched in boron nitride where the electron-hole puddles and flexural phonons are strongly suppressed.


Lattice dynamics of few-layer graphene after ultrashort laser excitation — Naira Gregoryan, Eveline S. Zulastra, and Martin C. Garcia

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RKKY interaction in doped graphene monolayer ($K_F \neq 0$) shows Friedel oscillations decaying as $1/r^2$ [1]. In this work we consider the RKKY interaction in AA- and AB-stacked bilayer graphene using exact low energy Green’s functions. Apart from the common site-to-site interaction we discuss impurities located in-between the two carbon layers. Similarly to the monolayer case, we find an oscillatory $1/r^2$ decay for on-site impurities in AA-stacked bilayer graphene. The exchange integral separates into the product of an energy dependent oscillation and an additional modulation resulting from the interlayer coupling. Interestingly, for on-site impurities in AB-stacked bilayer graphene this additional modulation vanishes at low Fermi energies. Moreover, due to the interference of the neighboring site-to-site interactions, at high Fermi energies the RKKY interaction between two plaquette impurities shows a $1/r^3$ behavior.


Coffee break

Ab initio calculations of functionalized graphene nanoribbons — Christian Till, Nina Rosenkranz, Christian Thomsen, and Janna Maultzsch

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Since nearly 30 years the discovery and subsequent research on fullerenes, carbon nanotubes, and graphene fuel expectations on carbon-based nanoelectronics. In this context, thin stripes of the two-dimensional material graphene, so-called graphene nanoribbons (GNRs), draw broad interest as well. In this work, we present a comprehensive ab initio study of the structural, electronic and vibrational characteristics of a 7-armedchair GNR with hydroxyl functionalized edges. Our results show AGNRs with increasing hydroxyl saturation to be particularly stable. In addition, we find a variation of the ribbon geometry under functionalization. An increasing degree of functionalization leads to a compression perpendicular to the ribbon axis. As a consequence we find a linear shift of the band gap with growing edge hydroxylation. With regard to a possible experimental determination of the degree of functionalization, we indicate fingerprint vibrational modes of the hydroxyl groups as well as a substantial shift of Raman active phonons.

N. Rosenkranz, C. Till, C. Thomsen, and J. Maultzsch


Phonon dispersions of AB- and ABC-stacked graphene trilay-
ers and multilayers — Bart Verberck\textsuperscript{1,2}, Karl H. Michel\textsuperscript{1}, and Björn Trauzettel\textsuperscript{2} — \textsuperscript{1}Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — \textsuperscript{2}Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Recently, it was experimentally confirmed that the electronic structure of graphene multilayers crucially depends on how they are stacked. The simplest multilayer for which different stackings can be realised is the trilayer. The ABA variant features both linearly and quadratically dispersed electronic bands near the K-point, while the ABC variant has cubic electronic dispersion. At the same time, the difference between the phonon dispersions for ABA and ABC trilayer graphene is less well established. Detailed knowledge of the phonon spectra is, however, essential for understanding double-resonant Raman scattering experiments, offering a simple means for characterising multilayer graphene samples (number of layers and stacking sequence). Here we present a theoretical study of the phonon dispersions of AB- and ABC-stacked multilayers based on a phenomenological force-constants model. We find that the difference between the phonon spectra for the two variants is much less apparent than the difference between the respective electronic phonon modes around the K-point. We argue that the observed difference in double-resonant Raman scattering signals for ABA and ABC trilayers mainly originates from the different electronic dispersions.

Optical selection rules in graphene quantum dots — Eleftheria Kavousanaki and Keshav Dani — Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology, Graduate University, Okinawa, Japan

We theoretically study the optical absorption of graphene quantum dots for different shapes, sizes and edge types. We calculate the single particle energy spectrum using the tight-binding Hamiltonian and the Dirac-Weyl equation and show that dots with zigzag edges exhibit a degenerate shell of zero energy states, in agreement with previous results. Using standard group theoretical tools, we identify the optical selection rules for triangular and hexagonal quantum dots and discuss the role of light polarization on the absorption spectrum. Finally, we calculate the oscillator strengths and absorption spectra for different quantum dot sizes and identify the contribution of the zero energy states therein.

Electronic reflection for a single layer graphene quantum well — Abir Mhamdi\textsuperscript{1,2}, Emna Ben Salem\textsuperscript{1}, and Sihem Jaziri\textsuperscript{3} — \textsuperscript{1}Laboratoire de Physique de la Matière Condensée, Faculté des Sciences de Tunis, Tunisia — \textsuperscript{2}Institut für Theoretische Physik, Georg-August Universität Göttingen, Germany — \textsuperscript{3}Laboratoire de Physique des Matériaux, Faculté des Sciences de Bizerte, Tunisia

We address the problem of Dirac fermions’ graphene quantum well (GQW) and we focus on the low energy approximation for the Hamiltonian of the system where the former can be described by a Dirac-like Hamiltonian. Interesting relations are obtained and used to discuss the influence of the spin-orbit coupling, which induces an effective mass-like term, on the transport properties of single-layer graphene quantum well. It is found that the reflection probability of incident electrons is sensitive to the effective mass-like term. This can be explained by the dependence of reflection coefficient \( R \) on the incident electrons’ direction and their energies. Notably, we found that the reflection probability for massive fermions with a very small angle, i.e. the wave-vector along the transport direction is zero in the GQW, can be greatly suppressed.