Workshop on Graphene

August 29 - September 2, 2011, San Sebastián, Spain

Abstract Booklet

Organizing Committee

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General information

Dear Workshop Participant,

On behalf of the Donostia International Physics Center, the Air Force Office of Scientific Research and Hunter College, we extend a warm welcome to our Workshop on Graphene. We hope you will find the workshop program most stimulating and your attendance most worthwhile. The aim of the workshop is to gather researchers working in graphene physics to stimulate the interaction between them and to develop a greater awareness of recent progress that has been made in the field.

The Organizing Committee

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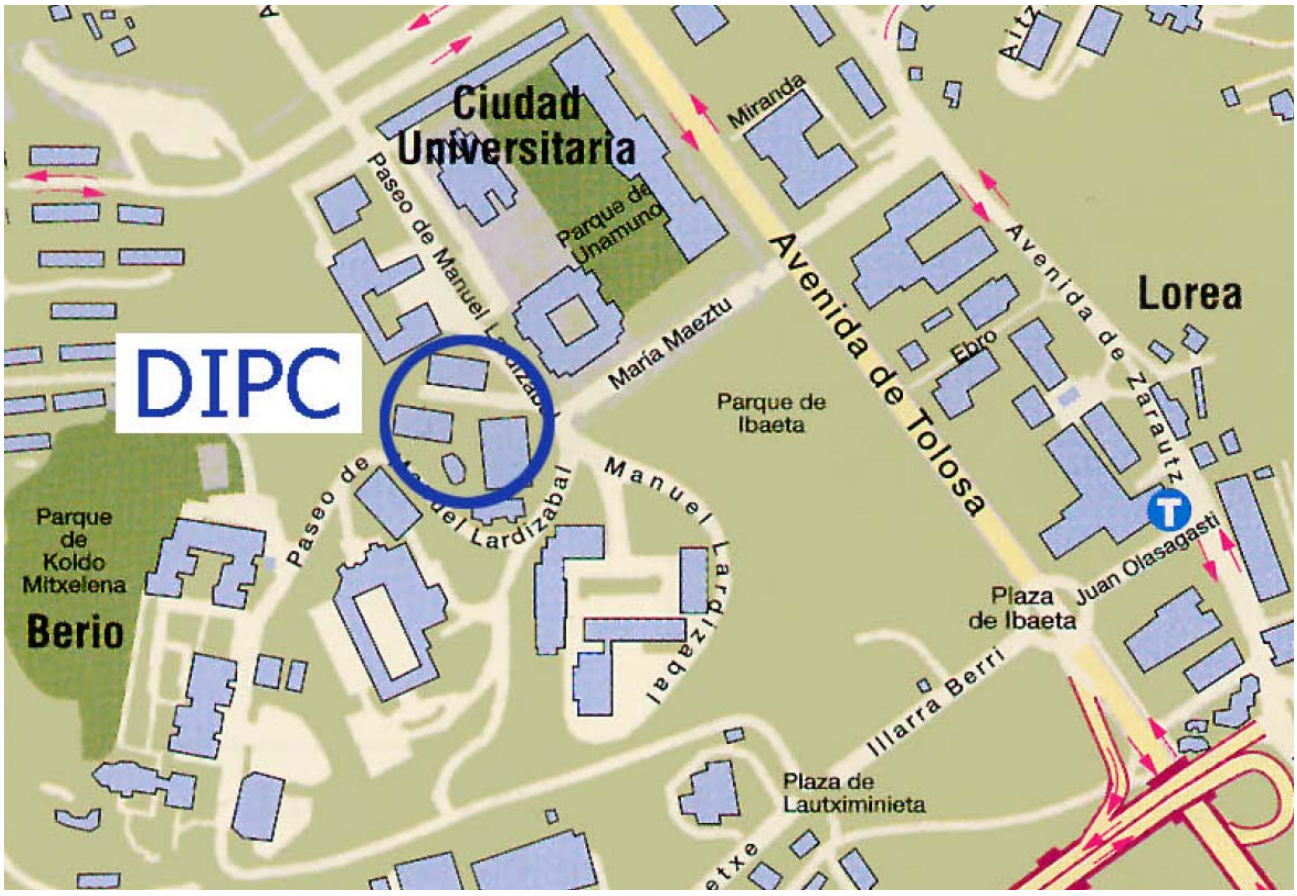
A map of DiPC's immediate environs



Workshop lunch venue

List of abstracts

The following are the abstracts for all presentations given at the Workshop on Graphene held at the Donostia International Physics Center between August 29 and September 2, 2011. The abstracts are arranged in alphabetical order by the last name of the (first named) author. Following the *List of abstracts* is the workshop *Program* that gives the timetable for the talks. At the end of the *List of Abstracts* you will find a map indicating Workshop Dinner venue location.

Effects of a potential barrier on spin currents along a nanotube

Y. Abranyos[1], P. Fekete[2], and G. Gumbs[1]
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Using a continuum model, we obtain analytical expressions for the spin-split energy bands of electrons on the surface of nanotubes in the presence of a Rashba-like spin-orbit interaction (SOI) arising from the asymmetry in the electron's confining potential onto the surface of the nanotube. We find that the energy separation between spin-split levels within a subband increases as the Rashba parameter increases and as the radius of the nanotube decreases. Electrons occupying the spin-split energy levels can be excited to yield intra-SO and inter-SO transitions leading to some plasmon excitation with frequencies in the terahertz regime. The presence of the SOI interaction leads to several interesting effects on the resulting plasmon excitations, including the fact that not all single-particle transitions between subbands contribute to the collective excitations.

Dirac electrons in superlattice potentials

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At low energies, electric carriers in graphene obey the two-dimensional Dirac equation. Therefore, quantum mechanics effects when graphene carriers are confined or subject to potentials varying in the nanoscale, may be quite different than what occurs in conventional semiconductor based electronic systems. In this presentation, we discuss the effect of one-dimensional potentials on the electronic properties of graphene using the continuum Dirac equation appropriate at low energies.

In the case of a periodic potential of the form $V(x) = V_0 \cos(G_0 x)$, new zero energy Dirac points emerge whenever the condition $J_0(2V_0/\hbar v_F G_0)$ is satisfied [1]. In the case of piecewise constant potentials new Dirac points are present throughout the band structure, and in the special case of a particle-hole symmetric potential they occur, as in the cosine potential case, at zero energy [2]. In the case of piecewise constant potentials new Dirac points are present throughout the band structure, and in the special case of a particle-hole symmetric potential they occur, as in the cosine potential case, at zero energy [2].

We also study transport in undoped graphene in the presence of a superlattice potential both within a simple continuum model and using numerical tight-binding calculations [3]. The continuum model demonstrates that the conductivity of the system is primarily impacted by the velocity anisotropy that the Dirac points of graphene develop due to the potential. When the superlattice generates new Dirac points the conductivities can be approximately described by the anisotropic conductivities associated with each Dirac point. Tight-binding calculations demonstrate that this simple model is quantitatively correct for a single Dirac point, and that it works qualitatively when there are multiple Dirac points. Remarkably, for a two-dimensional potential which may be very strong but introduces no anisotropy in the Dirac point, the conductivity of the system remains essentially the same as when no external potential is present.

Finally, we demonstrate that the electronic spectrum of graphene in a one-dimensional periodic potential will develop a Landau level spectrum when the potential magnitude varies slowly in space [4]. The effect is related to extra Dirac points generated by the potential whose positions are sensitive to its magnitude. We develop an effective theory that exploits a chiral symmetry in the Dirac Hamiltonian description with a superlattice potential, to show that the low energy theory contains an effective magnetic field.

Work done in collaboration with H. A. Fertig, P. Burset, A. Levy Yeyati, J. Sun, D. P. Arovas, E.-A. Kim, and K. Ziegler.

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Spectral properties of phonon peaks in optical conductivity of graphenes

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The detection and analysis of the spectral properties of optical phonons in single-layer and multilayer graphene provides a powerful tool not only for investigating the role of the underlying electron-phonon interaction, but also for a careful characterization of the systems. The large majority of the studies in this field have been performed so far by using Raman spectroscopy, focusing on the gate voltage dependence of the frequency and of the linewidth of the phonon peak. Recent experiments in gated bilayer graphene revealed however a clear phonon resonance at $\omega_0 \approx 0.2$ eV also in the IR spectra with several interesting features, the most spectacular of which is a giant enhancement of the phonon E_u intensity as a function of the gate voltage [1]. In addition, the phonon peak presents a pronounced Fano asymmetric shape, also strongly modulated by the gate voltage, pointing out a coupling of the phonon mode to a continuum of electron-hole excitations [1, 2].

In this contribution we show how these features can be analyzed and predicted on a microscopic quantitative level using the charge-phonon theory applied to the specific case of graphene systems [3]. We show in particular how the phonon intensity and the Fano asymmetry are strictly related, stemming out from the quantum interference between the electronic and phononic degrees of freedom. Within this context we are also able to elucidate the relative role of the E_u and E_g phonon modes in regards to the infrared activity and the Fano asymmetry of the observed phonon peaks. We present thus a complete phase diagram for the strength of the phonon modes and their Fano properties as functions of the chemical potential μ and of the gated-induced electronic Δ gap, showing that a switching mechanism between the dominance of the E_u or E_g mode can be controlled by the external gate voltage. We discuss how the present analysis can be generalized as well to multilayer systems with different stacking order. Such controlled quantitative theory can provide thus a useful roadmap for the characterization of graphenic systems by optical infrared means.

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Magneto-optical excitations of graphene under periodic magnetic fields

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Low-frequency optical excitations of graphene in a periodic magnetic field are calculated by the tight-binding model and gradient approximation. Quasi-Landau levels and two partial flat bands exist in the low-energy region. Each quasi-Landau level possesses an original and four extra band-edge states, which lead to the principal peaks and subpeaks in the optical absorption spectra, respectively. These two kinds of peaks obey two different selection rules because their wave functions present different features. The intensity, frequency, and number of the absorption peaks are related to the period, strength, direction of a modulated magnetic field, and the electric polarization direction. The anisotropic absorption spectra, induced by the different modulated directions and electric polarization directions, are obtained and explained by the characteristics of the wave functions.

Metal-insulator transitions in graphene

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In this work we show the metal-insulator (MI) quantum phase transitions that appear in the quantum Hall effect in graphene, namely the plateau-insulator (PI) and plateau-plateau (PP) transitions. For this purpose we have performed magneto-transport experiments with the magnetic field (up to 28 T) as the driving parameter in the temperature range from 4 K up to 230 K. The Hall (ρ_{xy}) and longitudinal (ρ_{xx}) resistivities were measured by the standard 4-probe low frequency *AC* lock-in technique while the graphene sample was obtained by mechanical exfoliation over a Si/SiO_2 wafer with subsequent e-Beam lithography and the evaporation of *Au/Ti* contacts.

We have also studied a trilayer graphene sample processed in Hall bar geometry. We have studied the temperature dependence of the Hall and longitudinal resistance in the temperature range 2-190 K and using as a driving parameter the magnetic field up to 22 T. We have observed the presence of the $\nu = 6$ quantum Hall (QH) plateau in our sample. To our knowledge this is the first report of a QH plateau in non-suspended trilayer graphene. This result is in agreement with the expected series for the QH plateaus in trilayer graphene: $\nu = \pm 6, \pm 10, \ldots$ see Refs. [1] and [2] and references therein.

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Transmission and conductance across a square barrier potential in monolayer graphene

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The transport properties and the tunneling resonance in graphene have attracted very much attention [1,2]. We have studied the transmission coefficient (*T*) and the conductance

across a square barrier in monolayer graphene. We obtained an analytical expression for the transmission coefficient of a square barrier in graphene which depends on the one hand, on the energy (E) and the angle of carrier incidence (φ), and on the other hand on the barrier potential (V_0) and of the barrier length (D).

We also calculate the conductance using the Landauer-Büttiker formalism [3]. We define the effective conductance as the conductance per unit width (W) in a sheet of graphene using fundamental units e^2/h. By using the previous expression for T, we obtain the effective conductance across a square barrier in monolayer graphene.

Finally, we consider that in an experiment of electronic transport across a barrier in a graphene sheet the carriers will arrive at different angles. We therefore calculate a weighted conductance in accordance with a certain probability distribution dependent on the angle of incidence to the barrier.

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Aharonov-Bohm interferences from local deformations in graphene

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One of the most interesting aspects of graphene is the tied relation between structural and electronic properties. The observation of ripples in the graphene samples both free standing and on a substrate has given rise to a very active investigation around the membrane-like properties of graphene and the origin of the ripples remains as one of the most interesting open problems in the system. The interplay of structural and electronic properties is successfully described by the modeling of curvature and elastic deformations by fictitious gauge fields that have become an experimental reality after the suggestion that Landau levels can form associated to strain in graphene and the subsequent experimental conformation. Here we propose a device to detect microstresses in graphene based on a scanning-tunneling-microscopy setup able to measure Aharonov-Bohm interferences at the nanometer scale. The interferences to be observed in the local density of states are created by the fictitious magnetic field associated with elastic deformations of the sample.

Electron-electron interactions in graphene

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The effects of the electron-electron interactions in clean single layer graphene, and in graphene with defects is discussed. In high mobility suspended graphene recent experiments show a significant enhancement of the Fermi velocity, in agreement with Renormalization Group arguments. Resonances associated to vacancies and strongly coupled adatoms lead to an unusual Kondo effect, defined by a ferromagnetic coupling, the absence of a Kondo temperature, and the involvement of many electron channels.

Electronic and optical properties of graphene layers in response to magnetic fields

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A complete tight-binding model is developed to study the electronic and optical properties of graphene layers in response to magnetic fields. Since the magnetic field and all atomic hoppings are simultaneously taken into account without introducing any approximation, the calculated results are accurate over a wide energy range. The wave functions and their spatial distributions appropriately characterize the Landau levels. Moreover, the concept of sublattices provides a straightforward way to clearly identify the optical spectra, including the selection rules and relative absorption rates. Those spectral structures are substantially impacted by the interlayer interactions and the stacking sequence. Our numerical results can provide guideline and new spectral features for future experiments.

Edge states and flat bands in graphene nanoribbons with arbitrary geometries

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Graphene nanoribbons (GNR), stripes of nanometric widths cut from graphene, are the subject of a growing interest. They exhibit edge-localized states, which may play an important role in transport and magnetic properties. For instance, the magnetic properties of nanoribbons are directly related to the existence of localized edge states [1]. All these edge terminations have been experimentally identified by different techniques, such as scanning tunneling microscopy [2,3], high-resolution transmission electron microscopy [4], or atom-by-atom spectroscopy [5]. It is thus important to identify general edges and nanoribbons that present localized edge states, as well as their degeneracy and characteristics.

We prescribe general rules to predict the existence of edge states and zero-energy flat bands in graphene nanoribbons and graphene edges of arbitrary shape [6]. No calculations are needed. For the so-called minimal edges, the projection of the edge translation vector into the zigzag direction of graphene uniquely determines the edge bands. By adding nodes to minimal edges, arbitrarily modified edges can be obtained; their corresponding edge bands can be found by applying hybridization rules of the extra states with those belonging to the original edge. Our prescription correctly predicts the localization and degeneracy of the zero-energy bands at one of the graphene sublattices, confirmed by tight-binding and first-principles calculations. It also allows us to qualitatively predict the existence of $E = 0$ bands appearing in the energy gap of certain edges and nanoribbons.

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Manifest of electron interactions in quantum Hall effect in graphene

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The quantum Hall ferromagnetism (QHFM) and fractional quantum Hall effect (FQHE) in 2-dimensional electron gas with multiple internal degrees of freedom provides a model system to study the interplay between spontaneous symmetry breaking and emergent topological order. In graphene, the structure of the honeycomb lattice endows the electron wavefunctions with an additional quantum number, termed valley isospin, which, combined with the usual electron spin, yields four-fold degenerate Landau levels (LLs). This additional symmetry modifies the QHFM and FQHE with intriguing interplay between two different spin flavors. As a consequence, it is conjectured to produce new incompressible ground states in graphene, reflecting strong electron interactions. In this presentation we report multiterminal measurements of the FQHE in high mobility graphene devices fabricated on hexagonal boron nitride substrates. The measured energy gaps of observed FQHE are large, particularly in the second Landau level where they measure up to ten times larger than those reported in the cleanest conventional systems. In the lowest Landau level, the hierarchy of FQH states reflects the additional valley degeneracy. We will also discuss the implication of QHFM with spin and valley spin degree of freedoms.

RKKY interaction in graphene

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We consider Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between two magnetic impurities in graphene. The consideration is based on the perturbation theory for the thermodynamic potential in the imaginary time representation. We present a new proof of the theorem, which states that the RKKY interaction on the bipartite lattice at half filling is ferromagnetic between magnetic impurities on the same sublattice and is antiferromagnetic between impurities on opposite sublattices. We also propose a method of analytical calculation of the integrals, defining the interaction, which is simpler than the methods, used previously, and allows to evade some problems which plagued those methods.

The effect of pressure on the magnetic moments of multilayer graphene

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The magnetic behavior of graphene and its multilayer compounds is one of the most interesting aspects of these systems. Magnetic order has been observed, by different experimental techniques, in pure carbon-based materials and has been associated with the presence of disorder [1]. By now, it seems clear that magnetic features in carbon structures are related to the existence of unpaired spins at defects induced by under-coordinated carbon atoms existing in vacancies, voids, edges or alike defects. A key issue for the presence of these spins is the bipartite character of the lattice.

We study the magnetic properties of vacancy-induced states in bilayer and multilayer graphene, in the presence of topological defects, pentagonal or heptagonal rings, which break the bipartite nature of the lattice [2]. With an unrestricted Hartree-Fock calculation of the Hubbard model we show that a slight frustration of the bipartite property of the honeycomb lattice alters the magnetic properties predicted by the Lieb's theorem. Furthermore, we analyze

the effect of external pressure on the behavior of the localized magnetic moments [3] with particular emphasis on the two inequivalent types of vacancies that appear in the Bernal stacking of multilayer graphene [4,5].

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Collective and coherent properties of graphene structures

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Electron-hole pairing caused by Coulomb interaction in the system of independently gated graphene layers separated by dielectric barrier is discussed. The theory of Cooper pairing of massless, spatially separated Dirac electrons and holes at strong coupling in graphene bilayer is presented. Various factors leading to enlargement of the critical temperature at strong coupling beyond Bardeen-Cooper-Schrieffer model predictions are considered. These factors are multi-band character of the pairing, dynamical and correlation effects. Importance of correlation effects is demonstrated.

We consider disorder effect on electron-hole pairing in the system. The influence of charged impurities on temperature of phase transition is studied. The quantum hydrodynamics of the system is considered and phase stiffness of electron-hole condensate and temperature of Berezinskii-Kosterlitz-Thouless transition to the superfluid state are calculated.

Dependence of critical temperature on mismatch of Fermi lines of *e* and *h* and value of trigonal warping of their spectrum is obtained. We predict appearance of the state with finite value of Cooper pair momentum Larkin-Ovchinnikov-Fulde-Ferrell-like (LOFF) state at mismatch of the Fermi lines above the critical value. We show that spatial structure of the order parameter in LOFF-like state can be reconstructed from the dependence of tunnel current between the layers on value and direction of parallel magnetic field.

Collective properties of graphene structures in high magnetic fields are discussed. Drag effects in graphene structures are considered.

States with spontaneously broken time reversal symmetry in graphene

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This talk will describe recent prediction of chiral superconductivity from repulsive interactions in doped graphene [1]. Chiral superconductors feature pairing gaps that wind in phase around the Fermi surface (FS) by multiples of 2π, breaking time-reversal symmetry (TRS) and exhibiting a wealth of fascinating properties. The search for experimental realizations of chiral superconductivity, a holy grail of correlated electron physics, greatly intensified in the last few years with the advent of topological superconductivity. Here we show that chiral superconductivity with a *d+id* gap structure can be realized in graphene monolayer, a system of choice of modern nanoscience. We demonstrate that when graphene is doped to the vicinity of a Van Hove singularity in the density of states (DOS), repulsive electron-electron interactions induce *d*-wave superconductivity. Our renormalization group analysis indicates that

superconductivity dominates over competing density wave orders, and also indicates that interactions select the chiral *d+id* state over TRS-preserving *d*-wave states. The *d+id* state exhibits exceptionally rich phenomenology, including a charge Hall effect at zero magnetic field, a quantized spin and thermal Hall conductance, and a quantized boundary current in magnetic field. This, as well as Majorana modes localized at the boundaries and vortex cores, makes it a highly desirable state in diverse areas of nanoscience.

Reference

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Spin-orbit coupling and spin relaxation mechanisms in graphene

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Graphene is considered as a potential material for spintronics devices due to the weakness of the spin-orbit (SO) coupling and practically absence of nuclear magnetic moments. The intrinsic SO coupling between at graphene π electrons is a second order process since it involves virtual transitions into σ states [1]. However, the measured spin diffusion lengths [2] are much shorter than the theoretically expected ones [3]. We analyze different mechanisms which lead to an enhancement of the SO coupling based on the mixing of π and σ electronic states. We consider the case of a sp^3-like distortion of the lattice coordination, as the one induced by adatoms which hybridize directly with carbon atoms [4]. Also we consider the effect of flexural phonon modes. Importantly, the mechanism induced by phonons is not associated with a spatial inversion asymmetry, so the enhanced SO coupling is the intrinsic term discussed by Kane and Mele [5]. We report an enhancement of almost two orders of magnitude.

Also spin relaxation is investigated. We study the Elliot-Yafet mechanism, that is, spin relaxation during a momentum scattering event, which is considered to play the major role in single layer graphene. We show that in the doped regime the amount of spin relaxation in a scattering event behaves as $S \propto \Delta/\epsilon_F$ independently of the nature of the scatterer, where Δ is the effective SO coupling strength and ϵ_F is the Fermi energy. This result implies the relation $\tau_s/\tau_p \propto \epsilon_F^2/\Delta^2$, where τ_s is the spin relaxation time and τ_p is the momentum relaxation time. This result is not compatible with the experimental data. Importantly, this relation does not hold when the SO coupling is locally enhanced due to the presence of heavy adatoms or resonant impurities. Other extrinsic mechanisms are based on this local enhancement of the SO coupling.

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Bernstein modes in graphene

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In this talk, I will present a theoretical description of Bernstein modes that arise as a

result of the coupling between plasmon like collective excitations (upper-hybrid mode) and inter-Landau-level excitations, in graphene in a perpendicular magnetic field. These modes, which are apparent as avoided level crossings in the spectral function obtained in the random-phase approximation, are described to great accuracy in a phenomenological model. Bernstein modes, which may be measured in inelastic light-scattering experiments or in photo-conductivity spectroscopy, are a manifestation of the Coulomb interaction between the electrons and may be used for a high-precision measurement of the upper-hybrid mode at small nonzero wave vectors.

Charged particle energy loss in epitaxial, irradiated and free-standing multi-layer graphene

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We present a formalism and numerical results for the energy loss of a charged particle scattered at an arbitrary angle from epitaxially grown multilayer graphene (MLG) for single, double and bi-layer configurations. It is compared with that of free-standing graphene layers as well as those irradiated by a circularly polarized laser field. Specifically, we investigated the effect of the substrate/radiation induced energy gap on one of the layers. The gap yields collective plasma oscillations whose characteristics are qualitatively and quantitatively different from those produced by Dirac fermions in gapless graphene. The range of wave numbers for undamped self-sustaining plasmons is increased as the gap is increased, thereby increasing and red-shifting the MLG stopping power for some range of charged particle velocity. We exploit our formalism to interpret several distinct features of experimentally obtained electron energy loss spectroscopy (EELS) data.

Magnetism of graphene with defects: vacancies, substitutional metals and covalent functionalization

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Magnetic properties of graphenic nanostructures, relevant for future spintronics applications, depend crucially on doping and on the presence of defects. Here we present a theoretical study using density functional calculations of the structural, electronic and magnetic properties of defects such as: substitutional doping with transition metals [1, 2, 3], vacancies [6], chemical functionalization with organic and inorganic molecules [4, 5], light atoms [4], and polymers [4]. We have found that such defects can be used to create and control magnetism in graphene-based materials. Our main results can be summarized as follows:

(i) Substitutional metallic impurities can be fully understood using a model based on the hybridization between the states of the metal atom, particularly the d electrons, and the defect levels associated with an unreconstructed D_{3h} carbon vacancy. We identify three different regimes associated with the occupation of the different electronic levels between hybridized graphene-metals which determine all the magnetic properties obtained by the doping;

(ii) In chemical functionalization, independently of the particular adsorbate, a spin moment of 1.0 Bohr is induced when a molecule chemisorbs on a graphene layer via a single *C-C* covalent bond. This effect is similar to *H* adsorption, which saturates one p_z orbital creating an effect on the electronic structure that resembles a single vacancy in a π-tight-binding,

however with universal character. The magnetic coupling between adsorbates was also studied and showed a key dependence on the sublattice adsorption site;

(iii) Monovacancies under isotropic strain display a rich phase diagram of spin solutions with the geometry configuration. Stretching increases the moment in different spin phases and compression reduces or even kills the magnetic moment. The transition to the non-magnetic solutions can be traced to changes in the local structure of graphene that are associated with the global rippling of the layer.

All these results provide key information about formation and control of defect-induced magnetism in graphene.

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Unoccupied electronic states in layered graphene

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Recently, it was shown that polarization of a two-dimensional graphene sheet by an external charge produces an attractive image potential that supports, in addition to the well-known π^* bands, a double series of Rydberg-like image potential states converging onto the vacuum level. Being quantified in the direction perpendicular to the graphene sheet, in the parallel plane these states have nearly free electron character, like similar states on metal surfaces. A large extension of wave function of image-potential states into the vacuum implies that they are very sensitive to any change of shape and environment of the graphene sheet. Thus, the properties of these states can be modified by an external electric field and a shape/geometry variation. The lowest-energy members of such states have been experimentally observed in graphene sheets grown on some substrates.

Some examples of such unoccupied electronic states in other carbon-based materials, like graphite, multilayer graphene, fullerenes, and nanotubes as having common origin with the graphene image-potential states will be presented.

Photon switching mechanism in graphene and quantum dot hybrid systems

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Recently graphene-quantum dot hybrid systems have been synthesized to study their application in light harvesting and energy conversion [1]. In the present work we have developed a theory for one-photon switching in graphene-quantum dot hydride waveguides and nanofibers. This hybrid nanomaterial is a new and emerging research area which has applications in sensing and advanced information nanotechnology. The electronic properties of graphene have been studied extensively in the literature. However, not much work is done on waveguides and fibers fabricated from graphene sheets and graphene nanotubes. In this paper we have considered that graphene waveguides are fabricated by sandwiching the graphene-quantum dot (GQD) hybrid system between two silica-glass plates. We have also studied photonic switching in graphene waveguides fabricated by sandwiching the GQD hydride within a photonic crystal. In the latter case the plasmon frequency of the graphene lies with the band

gap of the photonic crystal. Probe and control laser fields are applied to monitor the one-photon switching effect in the waveguide, where the excitons in the quantum dots are interacting with plasmons of the graphene. The applied laser fields induce polarizations in the quantum dot and graphene. Therefore, the quantum dot and graphene interact with each other via the dipole-dipole interaction. The quantum dot is also interacting with the photonic modes present in the waveguide due to confinement of the electromagnetic field. The quantum density matrix method [2] has been used to study the power loss in the quantum dot. Numerical simulations were performed to calculate the time-dependent density matrix elements which in turn provide information about the power loss in the quantum dot. It has been found that the power loss in the quantum dot can be switched on and off by the control laser field. This reveals interesting results and can be applied to develop new types of graphene based nanophotonic devices such as nano-switches, nano-transistors, nano-limiters and nano-gates.

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Ballistic transport through quantum wires with scatterers

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Phase-coherent electron transport through quasi-one-dimensional systems has developed into a very active and fascinating subfield of mesoscopic physics. We present a review of this development focusing on ballistic conduction through quantum wires (or constrictions). In quantum wires the electron conductance versus Fermi energy is quantized as a consequence of the reduced dimensionality and the subsequent quantization of transverse momentum. The presence of scatterers in otherwise “clean” wires can strongly suppress the quantum conductance. In the case of attractive scattering potential, sharp resonances in the conductance are generated which are due to quasibound states. These resonances can be of the Fano or Breit-Wigner type, depending on the size or/and strength of the scattering potential. Three types of scattering potential will be discussed: i) a 2D delta-function potential, ii) a rectangular barrier or well, and iii) a 2D Gaussian barrier or well. Thermal effects will also be discussed. Scattering in ballistic quantum wires is formulated in terms of the Lippmann-Schwinger equation, while the Feshbach coupled-channel theory is employed in order to treat Fano resonances.

Infrared optoelectronic properties of graphene and its application in *HgCdTe* infrared detectors

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Graphene has excellent electronic, transport and optical properties, such as high carrier density, high carrier mobility at room-temperature and high light transmittance from UV to infrared. Therefore, graphene is an excellent optoelectronic material which can be used as transparent conductor. At present, graphene has been applied in making better visible optoelectronic devices such as LCD, LED, solar cells, etc.

In this work, we study infrared optoelectronic properties of graphene. It was found

experimentally [1] that there is an infrared optical absorption window and the width of this window can be controlled by applying the gate voltage. This implies that graphene can have even better light transmission in infrared bandwidth. The results obtained from our theoretical work show that the infrared absorption window in graphene is induced by the requirement of different transition energies during inter- and intra-band absorption scattering events. The depth and width of the optical absorption window depend strongly on temperature and carrier density (or gate voltage). In particular, the high-frequency absorption edge depends more sensitively on temperature and carrier density and stronger cut-off of infrared absorption can be observed at lower temperature and larger density.

For application of graphene in infrared optoelectronic devices, we explore the possibility to utilize graphene as infrared transparent electrodes to make better and cheaper *HgCdTe* (MCT) infrared detectors. We grow large size (cm scale) and high quality multi-layer (5-10 layers) graphene films using CVD technique. The graphene films can be transferred onto the MCT wafers at room-temperature without any mechanical and chemical damage. We are able to make μm-scale graphene-electrodes on MCT wafer. It is found that the light transmittance for 5-10 layer graphene on MCT wafer is about 80% in mid-infrared bandwidth at room-temperature and 77 K. The electrical resistance for graphene films on MCT wafer is about 25 times less than that for the wafer itself. These findings indicate that, at least from a physics point of view, graphene can be applied as infrared transparent electrodes for various applications.

Reference

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Modeling electronic properties of single-layer and multilayer graphene

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We present a detailed numerical study of the electronic properties of single-layer and multilayer graphene in the tight-binding model. The algorithms are based on the numerical solution of the time-dependent Schrödinger equation, and applied to calculate various quantities [1-5], such as the density of states, quasieigenstates, dynamic polarization, dielectric function, response function, energy loss function, static and optical conductivities. The presence of the perpendicular magnetic and/or electric field is also discussed. Different realistic disorders are considered, such as resonant impurities (vacancies or hydrogen adatoms), fluctuated on-site potentials, and random hoppings. The advantage of our numerical method is that the computer memory and CPU time is linearly dependent on the size of the system, and therefore it could be applied to large samples consisting by hundreds of millions of carbon atoms.

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Phonon instabilities in graphene

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Recent progress in doping of graphene with various types of non-carbon atoms has opened a new field to study two-dimensional materials with adjustable physical parameters. We study the thermal distribution of out-of-plane and intervalley phonons in these materials. Due to the two electronic bands there are two out-of-plane phonon modes with respect to the two sublattices. One of these modes undergoes an Ising transition by spontaneously breaking the sublattice symmetry. We calculate the critical point, the renormalization of the phonon frequency and the average lattice distortion. This transition might be observable in doped graphene by Raman scattering and transport experiments. For the intervalley phonons there are also two modes due to the two spatial directions. The two modes are degenerate and this degeneracy is preserved by weak electron-phonon coupling. A sufficiently strong electron-phonon coupling, however, can result in a splitting into an optical and an acoustic phonon branch, which creates a fluctuating gap in the electronic spectrum. We describe these effects by treating the phonon distribution within a saddle-point approximation. Fluctuations around the saddle point indicate a Berezinskii-Kosterlitz-Thouless transition of the acoustic branch. This transition might be observable in the polarization of Raman scattered light.

Graphene films synthesized via CVD

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Researchers envision many different applications for graphene. Depending on the application the required graphene format can vary from powder/flake to homogeneous film form. The powder form can be obtained starting from graphite while the large area graphene films can be obtained using silicon carbide sublimation and chemical vapor deposition (CVD) methods. In the CVD method, graphene is synthesized via the deposition of a carbon source on a metallic catalyst substrate at high temperatures. Copper and nickel metals have been widely used as graphene catalysts during CVD growth. Copper has been reported to control better the monolayer graphene growth [1]. However, the growth is not the only process that needs to be optimized in order to have high quality graphene on insulating substrates. The graphene transfer process is as important as the growth since the synthesized graphene can easily be damaged during the transfer. After a careful characterization of our monolayer graphene by means of Raman and optical microscopy, the limiting factors for a successful graphene transfer were determined. Moreover, we have also obtained suspended graphene samples which were characterized via High Resolution TEM.

Reference

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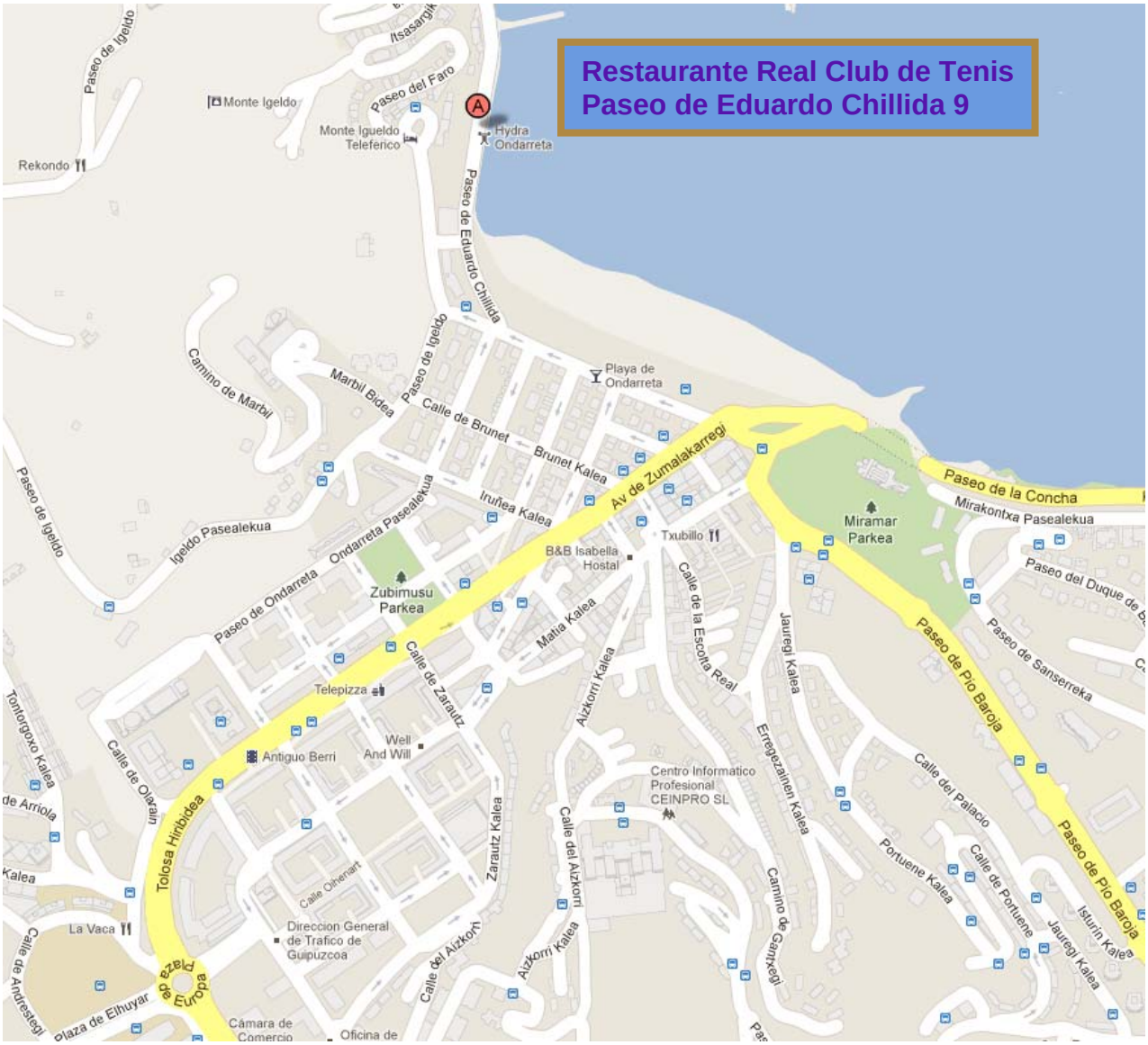
Workshop dinner venue



Workshop on Graphene at Donostia International Physics Center (DiPC)

San Sebastián, Basque Country, Spain

August 29, 2011 – September 2, 2011

Program

Monday, August 29, 2011	
8:30-9:45	Registration
9:45 - 10:00	Welcome remarks Ricardo Díez-Muiño - Director of Centro de Física de Materiales, Spain
Session 1-1	Chair - Danhong Huang - AFRL, US
10:00 - 11:00	Manifest of electron interactions in quantum Hall effect in graphene Philip Kim - Columbia University, USA
11:00 - 11:30	Coffee
11:30 - 12:30	Charged particle energy loss in epitaxial, irradiated and free-standing multi-layer graphene Oleksiy Roslyak - CUNY, USA
12:30 - 13:00	Modeling electronic properties of single-layer and multilayer graphene Shengjun Yuan, IMM, The Netherlands
13:00 - 15:00	Workshop lunch at the Artikutza restaurant - hosted by DiPC see map on page 3
Session 1-2	Chair - Godfrey Gumbs - CUNY, US
15:00 - 16:00	RKKY interaction in graphene Eugene Kogan - Bar-Ilan, Israel
16:00 - 16:30	Magnetism of graphene with defect vacancies, substitutional metals and covalent functionalization Elton J. G. Santos - DiPC, Spain
Tuesday, August 30, 2011	
Session 2-1	Chair - Yonatan Abranyos - CUNY, US
9:00 - 10:00	Electron-electron interaction in graphene Francesco Guinea - ICMM, Spain
10:00 - 11:00	Using low temperature scanning probe techniques to study graphene quantum dots Charles Smith - Cambridge, UK
11:00 - 11:30	Coffee

Session 2-1 Program continues on the next page

11:30 - 12:00	**The electronic and optical properties of graphene layers in response to magnetic field** Yen-Hung Ho - NCKU, Taiwan
12:00 - 12:30	**Collective and coherent properties of graphene** Yurii Lozovik - MIPT, Russia
12:30 - 13:00	**Bernstein modes in graphene** Rafael Roldán - IMM, the Netherlands
13:00 - 15:00	**Workshop lunch at the Artikutza restaurant - hosted by DiPC** see map on page 3
Session 2-2	Chair - Danhong Huang - US AFRL
15:00 - 16:00	**Dirac electrons in superlattice potentials** Luis Brey - ICMM, Spain
16:00 - 16:30	**Spectral properties of phonon peaks in optical conductivity of graphene** Emmanuele Cappelluti - ICMM, Spain
Wednesday, August 31, 2011	
Session 3-1	Chair - Eugene Kogan - Bar-Ilan, Israel
9:00 - 10:00	**Collective modes of graphene** Klaus Ziegler - Universität Augsburg, Germany
10:00 - 11:00	**Unoccupied electronic states in layered graphene** W. Silkin - DiPC, Spain
11:00 - 11:30	**Coffee**
11:30 - 12:30	**States with spontaneously broken time reversal symmetry in graphene** Leonid Levitov - MIT, US
13:00 - 15:00	**Workshop lunch at the Artikutza restaurant - hosted by DiPC** see map on page 3
15:30	**Trip to the Chillida Leku Museum** board bus for trip from DiPC
Thursday, September 1, 2011	
Session 4-1	Chair - Paula Fekete, USMA, US
9:00 - 10:00	**Infrared optoelectronic properties of graphene and its application in *HgCdTe* infrared detectors** Wen Xu - ISSP, China
10:00 - 11:00	**Photon switching mechanism in graphene and quantum dot hybrid systems** Mahi Singh - UWO, Canada
Session 4-1 Program continues on the next page	

11:00 - 11:30	**Coffee**
11:30 - 12:00	**Magneto-optical excitation of graphene under periodic magnetic field** Y. H. Chiu - NCKU, Taiwan
12:00 - 12:30	**The effect of pressure on the magnetic moments of multilayer graphene** María P. López-Sancho - ICMM, Spain
12:30 - 13:00	**Ballistic transport through quantum wires with scatterers** Vassilios Vargiamidis - AUTH, Greece
13:00 - 15:00	**Workshop lunch at the Artikutza restaurant - hosted by DiPC** see map on page 3
Session 4-2	**Chair - Danhong Huang - AFRL, US**
15:00 - 16:00	**Aharonov-Bohm interferences from local deformations in graphene** Fernando de Juan - IU, USA
16:00 - 16:30	**Transmission and conductance across a square barrier potential in monolayer graphene** Cristina Hernández Fuentevilla - USAL, Spain
21:00	**Workshop dinner at the Tennis restaurant - hosted by DiPC** see map on page 17
Friday, September 2, 2011	
Session 5-1	**Chair - Mahi Singh - UWO, Canada**
9:00 - 10:00	**Edge states and flat bands in graphene nanoribbons with arbitrary geometries** Andres Ayuela Fernandez - DiPC, Spain
10:00 - 10:30	**Metal-insulator transitions in graphene** Enrique Diez - USAL, Spain
10:30 - 11:00	**Spin-orbit coupling and spin relaxation mechanisms in graphene** Hector Ochoa - ICMM, Spain
11:00 - 11:30	**Coffee**
11:30 - 12:00	**Effects of a potential barrier on spin currents along a nanotube** Paula Fekete, USMA, US
12:00 - 12:30	**Graphene films synthesized via CVD** Amaia Zurutuza, Graphenea, Spain
12:30 - 13:00	**Closing Remarks**
13:00 - 15:00	**Workshop lunch at the Artikutza restaurant - hosted by DiPC** see map on page 3
15:30 - 16:30	**Tour of nanoGUNE - Graphenea and other experiments**