Poster Abstracts
SESSION II
(27 August)

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Theoretical study of graphene transport regimes

In recent work [1] we argued that the transport properties of currently available experimental graphene samples are dominated by diffusive carriers scattering off Coulomb impurity centers typically located in or near the substrate. This treatment that included potential screening within the Random Phase Approximation (RPA), impurity scattering using the Ladder Approximation (LA) and employed a self-consistent Fermi-Thomas treatment to determine the low-density minimum conductivity is in excellent agreement with experimental results [2-4].

In the current paper we study graphene monolayers, bilayers [5], nanoribbons [6] and substrate-free graphene [7] and show theoretically that by tuning external parameters, one can access several different transport regimes ranging from the aforementioned diffusive Boltzmann transport to phase-coherent ballistic transport to classical percolation through puddles of electrons and holes. We examine the different crossovers and argue for the experimental conditions necessary to see these different types of transport properties.

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Graphitic structures: network models, C cages properties and solvation of fullerene

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Abstract

We show some results obtained in the recent years about studies performed on graphitic structured systems. These studies have been developed within a semiemprical framework and involved the use of model based on quantum networks, on embedded atoms (the March model), on sum rules and bounds and, finally, on continuum for solvation. We have obtained results on electron density, binding energies, density of states and dispersion relations, dipole polarizabilities and intermolecular forces. We have considered B and C cages, nanotubes and two-dimensional layers. More recently, we have moved the attention to the solvation of fullerene in organic solvents. We have derived an effective fullerene pair potential and we are going to extend this study by means of Monte Carlo computer simulations of liquid solutions including water as solvent for the potential interest in biochemical applications.

High-capacity hydrogen storage by metallized graphene

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Abstract— First-principles plane wave calculations predict that Li can be adsorbed on graphene forming a uniform and stable coverage on both sides. A significant part of the electronic charge of the Li-2s orbital donated to graphene is accommodated by its distorted π^*-bands. As a result, semimetallic graphene and semiconducting graphene ribbons change into good metals. It is even more remarkable that Li covered graphene can serve as a high-capacity hydrogen storage medium with each adsorbed Li absorbing up to four H_2 molecules amounting to a gravimetric density of 12.8 wt %.

Developing safe and efficient hydrogen storage is essential for hydrogen economy.[1] Recently, much effort has been devoted to engineer carbon based nanostructures [2-5] which can absorb H_2 molecules with high storage capacity, but can release them easily in the course of consumption in fuel cells.

In this study [6], we predict that functionalized by Li graphene can be a potential high-capacity hydrogen storage medium. The process is achieved in two steps: Initially, graphene is metallized through charge donation by adsorbed Li atoms to its π^*-bands. Subsequently, each positively charged Li ion can absorb up to four H_2 by polarizing these molecules. At the end, the storage capacity up to the gravimetric density of g_d=12.8 wt % is attained. These results are important not only because graphene is found to be high capacity hydrogen storage medium, but also because of its metallization through Li coverage is predicted.

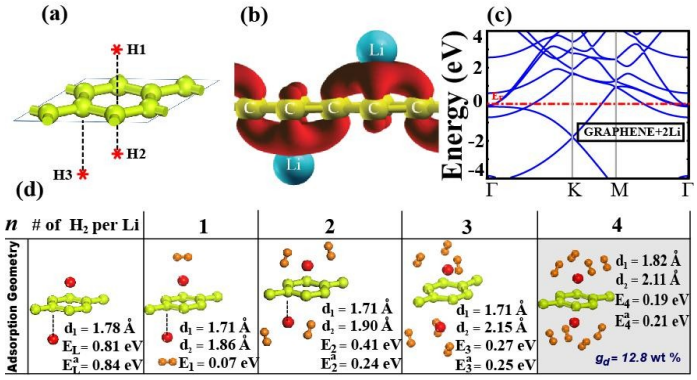

Fig.1: (a) Various adsorption sites H1, H2 and H3 on the (2x2) cell (b) Charge accumulation, $\Delta\rho^+$, calculated for one Li atom adsorbed to H1-site, second Li adsorbed to H3-site of the (2x2) cell of graphene and (c) corresponding band structures. (d) Adsorption sites and energetics of Li adsorbed to the (2x2) cell of graphene and absorption of H_2 molecules by Li atoms. For H1+H2 or H1+H3 configuration corresponding to double sided adsorption, E_L is the binding energy of second Li atom and E^a_L is the average binding energy. Shaded panel indicates the most favorable H_2 absorption configuration. For H1, H1+H2 and H1+H3 configurations, E_1 is the binding energy of the first H_2 absorbed by each Li atom; E_n (n=2-4) is the binding energy of the n^{th} H_2 molecule absorbed by each Li atom; E^a_n is the average binding energy of n H_2 molecules absorbed by each Li.

Adsorption of a single (isolated) Li atom on the hollow site of graphene (i.e. H1-site above the center of hexagon) is modeled by using (4x4) cell of graphene with 1.70 A^0 minimum Li-graphene distance and with a minimum Li-Li distance of 9.77 A^0, resulting in a binding energy of E_L=1.93 eV. The energy barrier to the diffusion of a single Li atom on the graphene sheet through top and bridge sites are calculated to be ΔQ=0.35 eV and 0.14 eV, respectively.

For H1 adsorption site (see Fig. 1 (a)), the binding energy is calculated to be E_L=0.86 eV. The binding energies are relatively smaller at the bridge site (above the carbon-carbon bond of graphene) and top site (on-top of the carbon atoms) to be 0.58 and 0.56 eV, respectively. The binding energy of the second Li for the double sided adsorption with H1+H2 and H1+H3 configurations described in Figure 1 (a), are E_L=0.82 and 0.84 eV, respectively.

The charge accumulation and band structure calculated for H1+H3 adsorption geometry is presented in Figure 1 (b) and (c), respectively. As a result of Li adsorption, the charge donated by Li is accumulated between Li and graphene and is accommodated by 2p π^*-bonds of carbons. The empty π^*-bands become occupied and eventually get distorted. Occupation of distorted graphene π^*-bands gives rise to the metallization of semimetallic graphene sheets. By controlled Li coverage one can monitor the position of Fermi energy in the linear region of bands crossing at the K-point of the Brillouin zone.

The absorption of H_2 molecules by Li+graphene in H1+H2 and H1+H3 geometries are investigated in this paper. The binding energy of the first absorbed H_2, which prefers to be parallel to graphene, is generally small. However, absorption of two or more H_2 molecules concomitantly by each Li occurs with a different binding mechanism but with a higher binding energy: First, a small amount of charge is transferred to H_2 molecule. Secondly the covalent bonding of hydrogen molecule is polarized and one of the H atoms closest to the positively charged Li becomes negatively charged. Charge transfer from Li to H_2, Coulomb attraction between Li and polarized H_2 and the van der Waals interaction are responsible for the formation of mixed weak bonding between H_2 molecules and Li+graphene complex. As the number of absorbed H_2, n, increases, the positive charge on Li as well as the minimum distance between H_2 and Li slightly increases. Maximum number of absorbed H_2 per Li atom is four, and the maximum gravimetric density corresponding to H1+H2 geometry at θ=25 % coverage is g_d=12.8 wt % (in Fig.1 (d)). This is much higher than the limit (g_d=6 wt %) set for the feasible H_2 storage capacity.

In conclusion, two crucial features of Li covered graphene revealed in this abstract may be of technological interest. These are high metallicity and high hydrogen storage capacity of graphene functionalized by Li atoms.

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Electron-electron correlation effects in graphene and graphite

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We studied the effect of electron-electron correlation on the full three dimensional dispersion of the pi-bands, Fermi velocities and effective masses of graphite within GW approximation. The results are then compared with recent experiments obtained by angle resolved photo-emission spectroscopy, fig. 2. The band structure by density-functional theory strongly underestimates the slope of the bands and the trigonal warping effect. Including GW corrections, however, yields remarkable agreement in the vicinity of the Fermi level [1]. This demonstrates the breakdown of the independent electron picture in semi-metallic graphite and points towards a pronounced role of electron correlation. Then we determined the dependence of the electron-phonon coupling (EPC) on various approximations, ranging from standard Density Functional Theory (in LDA or GGA approximation) to the pure Hartree-Fock. The electron-phonon coupling is a fundamental parameter in determining the electronic transport properties in carbon nanotubes [3] and in the interpretation of Raman spectroscopy data, fig. 1 (see for instance reference [2]).

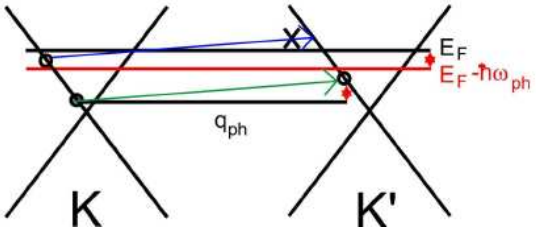

Figure 1: The double resonant Raman.

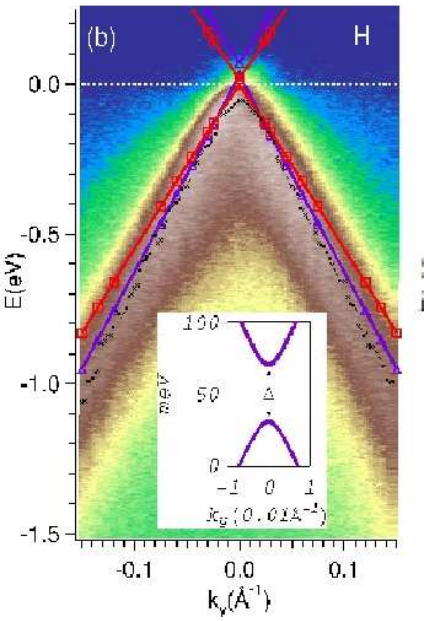

Figure 2: Renormalization of the band structure.

Thanks to these ingredients, renomalized band structure, and electron-phonon coupling beyond the LDA approximation, we were able for the first time to give a quantitative and not only qualitative description of double resonant Raman experiments in graphite and graphene.

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Electric Field Induced Gaps in Graphene Multilayers

Graphene is a rapidly rising star on the horizon of materials science and condensed matter physics. A huge amount of theoretical and experimental papers have been devoted to the investigation of the low-energy electronic properties of ultrathin graphite films, including graphene monolayers and bilayers. This activity followed the successful fabrication of ultrathin graphite films. Besides the high mobility and minimum conductivity, graphene shows very interesting behavior in the presence of a magnetic and electric fields [1, 2].

It is known that the band structure of bilayer graphene can be controlled by an applied electric field so that the electronic gap between the valence and conduction bands can be tuned between zero and midinfrared energies [1, 3].

In this poster we will show that by applying a perpendicular electric field the multi-layer graphene gap can be tuned and that the gap depends on the number of layers. We use a tight-binding approach to calculate the band structure of the multilayer graphene structure in an external electric field, in particular, for three and four graphene layer systems. A self consistent calculation is performed to take into account induced charges on the graphene layers.

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Supercurrent in Graphene Josephson Transistors

We investigate electrical transport in single or bi-layer graphene devices coupled to superconducting electrodes. In these two-dimensional Josephson junctions, we observed gate tunable supercurrent, multiple Andreev reflections and hysteretic current-voltage characteristics. Latest experimental progress on dependence of supercurrent on temperature, number of layers and source-drain separation will be discussed.

Superfluidity of magnetoexcitons and magnetobiexcitons in quantum wells' and graphene layered structures

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The Bose-Einstein condensation and superfluidity of quasi-two-dimensional spatially indirect magnetobiexcitons in a slab of superlattice with alternating electron and hole layers consisting from the semiconducting quantum wells (QWs) and graphene superlattice in high magnetic field are considered. The two different Hamiltonians of a dilute gas of magnetoexcitons with a dipole-dipole repulsion in superlattices consisting of both QWs and graphene layers (GLs) in the limit of high magnetic field have been reduced to one effective Hamiltonian a dilute gas of two-dimensional excitons with the renormalized effective mass of the magnetoexciton, which depends on the magntic field. This Hamiltonian does not include the vector potential. Moreover, for N excitons we have reduced the problem of $2N \times 2$ dimensional space onto the problem of $N \times 2$ dimensional space by integrating over the coordinates of the relative motion of an electron and a hole. The instability of the ground state of the system of interacting two-dimensional indirect magnetoexcitons in a slab of superlattice with alternating electron and hole layers in high magnetic field is found. The stable system of indirect quasi-two-dimensional magnetobiexcitons, consisting of pair of indirect excitons with opposite dipole moments is considered. The density of the superfluid component $n_s(T)$ and the temperature of the Kosterlitz-Thouless phase transition to the superfluid state in the system of two-dimensional indirect magnetobiexcitons, interacting as electrical quadrupoles, are obtained for both the QW and graphene realizations.

It is discussed and proposed an experimental observation of the BEC and superfluidity of 2D spatially indirect magnetoexcitons in two-layer graphene. It is shown that the superfluid density $n_S(T)$ and the temperature of the Kosterlitz-Thouless phase transition T_c increase with the increment of the excitonic density and decrement of the magnetic field and interlayer separation.

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Hydrogen on graphene: from ideal to realistic model.

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Density-functional calculations of electronic structure, total energy, structural distortions, and magnetism for hydrogenated single-layer graphene are performed. It is found that hydrogen-induced magnetism can survive only at very low concentrations of hydrogen single-atom regime whereas hydrogen pairs with optimized structure are usually nonmagnetic. Chemisorption energy as a function of hydrogen concentration is calculated, as well as energy barriers for hydrogen binding and release.

For modeling a realistic hydrogenation process calculation of chemisorption energies for case of edges, Stone-Walls defects, vacancies, impurities and extrinsic ripples are performed. Shown dramatical changes in hydrogenation process in finite graphene sample and in the case of presence of extrinsic defects.

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Band gap and depth profile studies of titania/carbon nanotube nanocomposites

In our previous work, we have shown that the addition of multi-walled carbon nanotubes (MWNTs) combined with a CO_2 laser treatment can significantly increase the wettability and the photocatalytic activity of TiO_2 films [1]. Here, we propose the mechanism of two previously observed phenomena: a) the interstitial charge transfer due to the combination of TiO_2 and MWNTs responsible for the enhanced photocatalytic activity obtained; and b) the selective removal of amorphous carbon and some other impurities from the coated nanocomposite due to the CO_2 laser sintering. The proposed mechanisms were supported by band gap and depth profile studies of the films and are here discussed.

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Cross Andreev Reflection in Ballistic pn Graphene junctions

Beenakker predicted that Andreev reflection may be specular in graphene [1]. I have studied [2] the interplay of superconductivity [3] with the very special dynamics of massless relativistic quasiparticles at a bipolar pn junction [4], and in particular the cross Andreev process that was already observed in nonrelativistic metals [5]. The presence of Dirac conical points in the band structure of graphene enables to observe a pure crossed Andreev reflection in a three-terminal n-doped graphene/superconductor/p-doped graphene (G_1SG_2) bipolar heterojunction. Accordingly the injected Cooper pairs from S are splitted in electrons which further propagate in opposite directions within G_1 and G_2 respectively. Indeed both elastic cotunneling and local Andreev reflection may be totally suppressed owing to the presence of Dirac points in the spectrum of G_1 and G_2. Using Dirac-Bogoliubov de Gennes formalism, the probability for the cross Andreev process is shown to oscillate as a function of the superconductor width. The predicted phenomena could be observed in ultraclean suspended graphene junctions [6,7].

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Electronic properties of chemically modified graphene nanoribbons

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Graphene nanoribbons (GNRs) are the counterpart of nanotubes in graphene nanoelectronics. The confinement of the electronic wavefunctions and the presence of the edges open a bandgap, making them suitable for the realization of devices. When GNRs are cut from a single layer, their edges could in general consist of a combination of regions having an armchair or a zigzag geometry [1]. Chemical impurities, atomic substitutions and functional groups can be an effective way to modify the electronic properties of the ribbons and, in principle, a route to control them. Furthermore, chemical impurities are likely to be a by-product of the production processes. In particular H, O and oxygen containing radicals could be present on the ribbon edges or as adsorbates.
We present a Density Functional Theory study of the electronic properties of zigzag and armchair GNRs with either bulk or edge N, B or O substitutional atoms, edge functionalization [2] or chemisorptions of OH, O and H radicals [3].

In armchair ribbons semiconductor-metal transitions result from the atomic substitution of a bulk carbon atom with N or B atoms [2], while H and OH radicals chemisorbed on the surface increase the bandgap and introduce impurity levels in the gap [3]. These are highly localized in the middle of the gap, with orbitals localized in the vicinity of the adsorbates.

Zigzag ribbons present a lifting of the spin degeneracy upon single edge functionalization, or atomic substitution [2], or OH and H chemisorption [3]. This can lead to a half-semiconductor or even half-metal behaviour. Semiconductor-metal transitions are observed for high concentration of oxygen substitution and shrinkage of the bandgap is observed for double-sided NH_2 edge functionalization [2].

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Asymmetric transport in asymmetric T-shaped graphene nanoribbons

We propose an asymmetric T-shaped graphene nanoribbon (TGNR) which shows peculiar transport properties. In the vicinity of the Fermi level, the electron transmissions from the vertical graphene nanoribbon (GNR) to the two ends of the horizontal GNR are highly asymmetric. The electrons mostly transmit to one horizontal arm while are blocked by the other one. It is originated from the local asymmetric couplings between the intersection of the junction and the two horizontal arms. The asymmetric transport is very robust even the T-shaped junction has large size. Thus the asymmetric TGNR can be served as important components of nanocircuits.

The tube-tube interaction effects on the electronic and optical properties of carbon nanotube bundles.

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The electronic and optical properties of single walled nanotubes and nanotube bundles are systematically investigated using a first-principles method based on density-functional theory in the local-density approximation. At first, we will study the dielectric function of isolated armchair and zigzag nanotubes with diameter range from 4 Å to 20 Å, and the results will be compared with the results calculated by method of graphene of Brillouin zone-foldings. Then we will present the electronic structure and the dielectric function of a number of the armchair〔(3,3), (4,4),(5,5), (6,6)〕, and zigzag〔(5,0), (6,0), (9,0), (10,0)〕nanotube bundles for different rotational angles. The effect of the interactions between the tubes in the bundle on the dielectric functions will be presented and discussed.

Induced superconductivity and multiple Andreev reflections in graphene

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We have investigated electronic transport of few-layer graphene (FLG) and single graphene layer, prepared by mechanical exfoliation of graphite, connected to superconducting electrodes.
For the first device, a FLG flake is connected to two tungsten electrodes, separated by 2.5 μm, grown by focused ion beam. Whereas the tungsten electrodes are superconducting below 4 K, the proximity effect in FLG develops below 1 K, and is characterized by a factor 2 differential resistance drop at low bias. We find multiple Andreev reflection peaks at voltages corresponding to submultiples of $2\Delta/e$ (with Δ the superconducting gap of the electrodes), which persist up to fields of a few tesla.
For the second device, by standard lithography technique we have contacted a monolayer of graphene using Tantalum as superconducting electrodes separated by 450 nm. By applying strong dc currents through this junction we manage to increase the transparency of the junction going progressively from a regime of incoherent multiple andreev reflection with no supercurrent to a regime of high transmission where a supercurrent of 500 nA appears.

Long Spin Coherence Length in Multilayer Graphene

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Spin transport in graphite-based materials such as carbon nanotubes, single-layer graphene [1], and multilayer graphene (MLG) [2] has attracted considerable attention in recent years because coherent spin transport is expected over a long distance due to the weak spin-orbit and hyperfine interactions. Gate control of spin conduction in such materials is also of high interest from the viewpoint of realizing multi-functional spintronic devices and clarifying the underlying physics. In this report, we study the relation between the spin and the charge transport in MLG by changing the gate voltage and clarify its physical meaning.

The device shown in Fig. 1 was fabricated by the standard micromechanical cleavage of bulk graphite followed by the electron beam lithography and metal deposition. The thickness of the MLG film was 2.5 nm. The nonlocal detection signal measured at 4.2 K, shown in the inset of Fig. 2, displayed sharp transitions between a positive value R_P and a negative value R_{AP}, corresponding to the parallel and antiparallel configuration of magnetization in the Co electrodes, respectively. This bipolar behavior confirms the spin injection from the Co electrode and the spin accumulation in the MLG. The main panel of Fig. 2 shows the spin signal, defined as $R_s \equiv R_P - R_{AP}$, as a function of the resistance R of the MLG, obtained by changing the gate voltage. It is clear that R_s is a monotonically decreasing linear function of R. According to the general theory [3], such linear relation is obtained only when the contact resistance between MLG and FM satisfies some special conditions [2,3], which give a lower limit to λ_N: $\lambda_N >> 8.4$ μm for our sample [2]. The obtained spin relaxation length is longer than those of conventional metals and even than that of graphene [1]. This result shows the superiority of MLG for spintronic devices.

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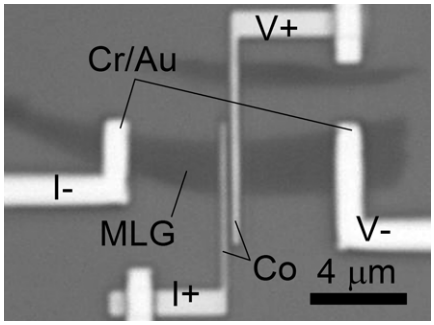

Fig. 1 (left) Optical micrograph of the sample for the nonlocal measurement. Configuration and materials of the electrodes are indicated.

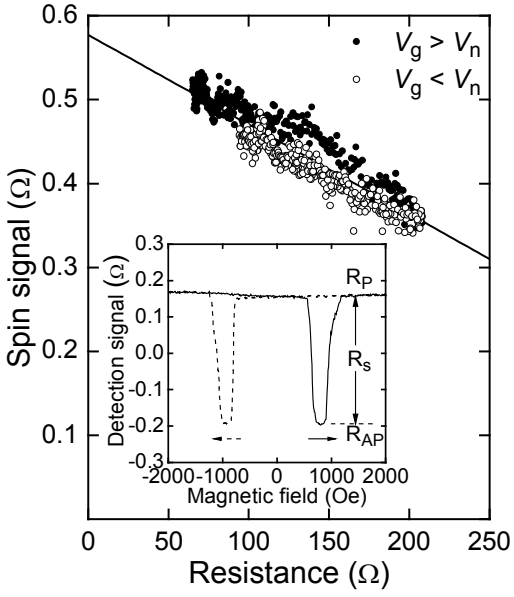

Fig 2. (right) Relation between spin signal and resistance. The solid (open) symbols correspond to the data obtained at $V_g > V_n$ ($V_g < V_n$), where $V_n = 1.5$ V is the charge neutrality point. Inset: Non-local detection signal as a function of the applied magnetic field at $V_g = 0$. Arrows indicate the sweep direction.

Magnetic confinement of massless Dirac fermions in graphene and conductance quantization of snake states

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We exploit inhomogeneous magnetic fields to guide and confine carriers in a monolayer of graphene. As examples we discuss magnetic quantum dots [1,2] and magnetic electron waveguides [3]. Contrary to confinement by electrostatic fields sharp non-decaying quantum dot levels are found, similar as for the familiar electrostatic Schrödinger quantum dot. In graphene waveguides the properties of uni-directional snake states are discussed. For a certain magnetic field profile, two spatially separated counter-propagating snake states are formed, leading to conductance quantization insensitive to backscattering by impurities or irregularities of the magnetic field.

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A. De Martino, L. Dell'Anna, and R. Egger
Phys. Rev. Lett. 98, 066802 (2007)

[2] *Magnetic confinement of massless Dirac fermions in graphene*
A. De Martino, L. Dell'Anna, W.Häusler, R. Egger
Talk presented for the symposium on graphene during the 'Fruehjahrstagung' of the German Physical Society, Regensburg, March, 26-30 th 2007.

[3] *Conductance quantization and snake states in graphene magnetic waveguides*
T.K. Ghosh, A. De Martino, W. Häusler, L. Dell'Anna, R. Egger
Phys. Rev. B 77, 081404(R) (2008)

Graphene for Future Mobile Devices

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Our goal is to build a device for mobile internet, a gateway between the digital and the real world. The device will connect its user to other users, services and local environment. With its sensors it can be used to detect specific chemicals or free frequencies of the radio field for cognitive radio.

The main challenges for enhancing the wireless communications of mobile devices are: size, thermal management, speed, frequency range and energy consumption.

To meet these challenges, we are investigating externally controllable materials, manufacturing, characterizing the properties, tailoring and patterning nanoscale structures and designing systems and devices with desired properties e.g. low energy consumption.

The recently discovered material, graphene, is a promising candidate for such applications in the design of future mobile device electronics. The band structure of the hexagonal lattice gives graphene exceptional electronic properties. For example, the electron conduction in this material is attributed to electrons propagating with a single velocity. By confining the graphene sheet into a ribbon geometry the allowed values of velocities are quantized in one direction – hence the material can become a semiconductor with a tunable band gap. This allows tailoring of the electronic properties of the graphene sheet in a multitude of ways.

We have developed and implemented an extended tight-binding simulation method for calculating the electronic properties of a graphene ribbon, which can be efficiently used for the design of future graphene-based electronic and spintronic devices.

Industrial applications of graphene sheets require efficient large scale manufacturing methods of the material on novel compatible substrates, and its functionalization into different forms and sizes of ribbons. In conjunction with the theoretical calculations, we are studying the challenges of manufacturing graphene, with assessment and verification of the potential of our designs for new mobile device technologies.

Theoretical Calculation of Optical Absorption Spectra with Exciton Effects in Boron-Nitride Nanotubes

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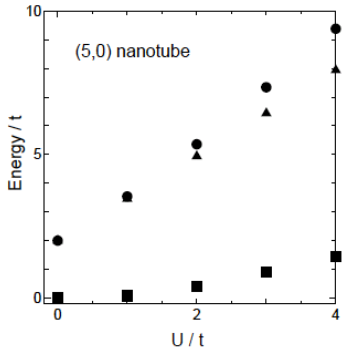
Optical studies in carbon and boron-nitride (BN) nanotubes are being in intensive progress experimentally as well as theoretically. In this talk, we will discuss exciton effects in single-wall BN nanotubes. Linear absorption spectra are calculated with changing the (n,m) geometries of the nanotubes. We use the following model [1]:

$$\begin{aligned} H &= E_{\rm B}\sum_{i\in{\rm B},\sigma} c^{\dagger}_{i,\sigma}c_{i,\sigma} + E_{\rm N}\sum_{i\in{\rm N},\sigma} c^{\dagger}_{i,\sigma}c_{i,\sigma} \\ &- t\sum_{\langle i,j\rangle,\sigma}(c^{\dagger}_{i,\sigma}c_{j,\sigma}+{\rm h.c.}) + U\sum_{i}(c^{\dagger}_{i,\uparrow}c_{i,\uparrow}-\frac{n_{\rm el}}{2})(c^{\dagger}_{i,\downarrow}c_{i,\downarrow}-\frac{n_{\rm el}}{2}) \\ &+ V\sum_{\langle i,j\rangle}(\sum_{\sigma}c^{\dagger}_{i,\sigma}c_{i,\sigma}-n_{\rm el})(\sum_{\tau}c^{\dagger}_{j,\tau}c_{j,\tau}-n_{\rm el}), \end{aligned}$$

where E_B (=+t) and E_N (=-t) are the site energies at the B and N sites, respectively; the sum with i∈B and i∈N are taken over the B and N atoms, respectively; t (>0) is the hopping integral of π electrons between the nearest neighbor i-th and j-th sites; the sum with ‹i,j› is taken for all the pairs of the nearest neighbor sites; n_{el} is the average electron density of the system. Exciton effects are calculated using the CI technique [2]. We use the convention V=U/2. The figure displays the U dependence of the band gap (●), the lowest exciton energy (▲), and the binding energy of the exciton (■) for the (5,0) nanotube.



The energy gap is about 6 eV at U/t=2 with t=1.1 eV. The binding energy of the exciton is 0.46 eV for the same parameters. This energy agrees well with that of other theoretical investigations. We find that the energy gap and the binding energy are almost independent of the (n,m) geometries of the nanotubes. This novel property contrasts with that of the carbon nanotubes which show metallic and semiconducting properties depending on the geometries. Comparison with recent experiments will be discussed in the talk.

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Dispersion of Electronic States in Bilayer Nanographene Ribbons

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Single-layer and multi-layer graphenes are being investigated intensively, after the success of peeling out them from the bulk graphite. Electronic properties under magnetic field are quite unique, and the quantum Hall effects exhibit the non half-integer nature. The Landau levels are quantized at the integer values due to the presence of the Dirac fermions in the single layer graphene. There is a Landau level just at the Fermi energy, and its presence effects on the electronic properties of nano-devices.

On the other hand, the electronic states of the spatially limited systems, for example, nanographenes have surface induced states. The nanographene ribbon with zigzag edges, shown in the Figure, has localized electronic states along the edge carbon atoms. It has been discussed that the magnetism in low temperatures is related with the edge states of the nanographens.

In this paper, the inter-layer interaction effects are studied with the tight-binding model, in view of the recent experiments of multi-layer graphenes. There are two-types of A-B stacking patterns shown in the Figure. The nearest neighbor hopping integral t is considered in each layer. The weak hopping interaction t_1 is assumed at closed circles between layers. We look at wave function patters of electrons, and consider how the localized v.s itinerant properties change. We find that edge state in the type I stacking is affected easier than that of the type II stacking, because the edge atoms are near to the inter-layer interaction points (closed circles).

(a)

(b)

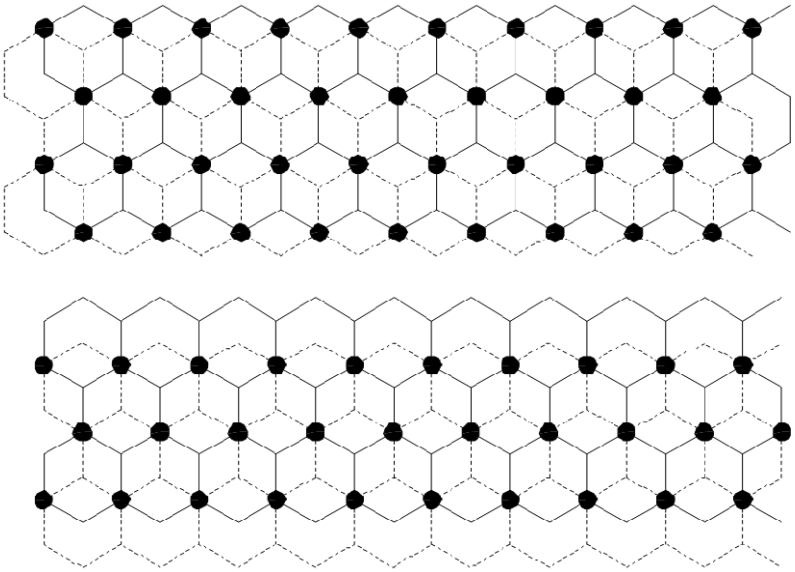

Figure: (a) Type I and (b) type II stacking patterns of bilayer nanographenes. The solid and dotted lines indicate upper and lower layers, respectively. There are weak hopping interactions between layers at the solid circles.

Suppression of spin polarization in graphene nanoribbons by edge defects and impurities

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We investigate the effect of edge defects (vacancies) and impurities (substitutional dopants) on the robustness of spin polarization in graphene nanoribbons (GNRs) with zigzag edges by using density functional theory calculations. The stability of the spin state and its magnetic moments is found to continuously decrease with increasing the concentration of the defects or impurities. The system generally becomes nonmagnetic at the concentration of one edge defect (impurity) per ~10 Å. The spin suppression is shown to be caused by the reduction and removal of edge states at the Fermi energy. Our analysis implies an important criterion on the GNR samples for spintronics applications

First principles characterisation of electronic and vibrational properties of graphenes and carbon nanotubes interacting with surfactant solutions

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Dispersing bundled carbon nanotubes in surfactant solutions has been proven to be an efficient method for isolating them in individual entities. Similar methods may be used for purifiying graphene sheets obtained by cathalitic plasma deposition, allowing the investigation of their electronic and vibrational properties.

Although a lot of experimental work has been performed in order to perfect these individualisation methods, it is not completely understood the way various surfactants imprint a specific signature to the Raman spectrum of graphene and carbon nanotubes, depending on their type: anionic, cationic or neuter.

Using *ab initio* and DFT simulation techniques we characterize the electronic and vibrational properties of graphenes and carbon nanotubes, surrounded by surfactant solution, in order to clarify the nature of the interaction between them.

The experimental implication in the Raman and absorption spectra are discussed.

Unconventional temperature dependence of proximity-induced supercurrent in multilayer graphene

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Superconducting proximity effect in superconductor (S)-normal metal (N) junctions is one of the phenomena which manifest the quantum-mechanical phase coherence of electron transport in the system. For single-layer graphene, the gate-controllable supercurrent was observed [1] and it was recently pointed out that the critical supercurrent and the subgap structures in the I-V curve are quantitatively explained by the diffusive junction model of the conventional SNS junctions [2]. On the other hand, for multilayer graphene, no report has been reported so far. Although some exotic properties coming from the linear dispersion relation of single-layer graphene might be lost in multilayer graphene, effect of finite screening length of the electric field combined with the gate-controllable carrier density provides an interesting system. Here, we report experimental study of the gate-controlled superconducting proximity effect in multilayer graphene.

In our sample, a film of multilayer graphene is connected to two aluminum superconducting electrodes, forming a SNS junction, and gate electric field is applied from a back gate. The critical supercurrent displays an ambipolar behavior, and for a fixed normal-state resistance the electron critical supercurrent with positive gate voltage is always larger than the hole critical supercurrent with negative gate voltage (electron-hole symmetry breaking). Furthermore, the critical supercurrent steeply increases with lowering temperature, approximately proportional to $\exp(-T/T_0)^2$, which has never been observed in other systems. The junction thickness and length dependence of the critical supercurrent will be discussed.

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Doping graphene with metal contacts

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Graphene is often seen as a free-standing two-dimensional sheet. However, graphene studied experimentally always exists in some environment that might include atomic and molecular impurities, an insulating substrate, a gate electrode and metallic leads. In a free-standing graphene sheet the Fermi energy coincides with the conical (Dirac) points but adsorption on metallic (or insulating) substrates can alter its electronic properties significantly. Recently, we have shown that, for example, graphene on the hexagonal boron nitride will have a band gap of at least 53 meV [1].

Since electronic transport measurements through a graphene sheet require contacts to metal electrodes [2] it is also essential to have a full understanding of the physics of metal-graphene interfaces. We study how graphene is doped by adsorption on metal substrates using *ab-initio* density functional theory. We find that weak bonding on Al, Ag, Cu, Au and Pt, while preserving its unique electronic structure, can still shift the Fermi level with respect to the conical point by ~ 0.5 eV. At equilibrium metal-graphene separations, the crossover from p-type to n-type doping takes place for a clean metal surface work function of ~ 5.4 eV that is much larger than the work function of 4.5 eV for free-standing graphene.

We propose a simple analytical model that describes the numerical results for the Fermi level shift in graphene and work function of graphene-covered metal surfaces solely in terms of the clean metal surface work function. The model provides a general description of doping, and can be applied to a variety of other metals, greatly extending the applicability of our numerical results.

We also find a class of metals such as Co, Ni, Pd and Ti that strongly absorb graphene. Graphene p_z-states are hybridized with d-states of the metal surfaces. The chemisorption then leads to a large bandgap opening in graphene and to decrease of the clean metal surface work function much lower than the work function of free-standing graphene. Based on the latter observation, we consider graphene absorbed upon Co, Ni, Pd and Ti as being n-type doped [4].

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Graphite and Graphene as Perfect Spin Filters

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Based upon the observations (i) that their in-plane lattice constants match almost perfectly and (ii) that their electronic structures overlap in reciprocal space for one spin direction only, we predict perfect spin filtering for interfaces between graphite and (111) fcc or (0001) hcp Ni or Co [1]. The spin filtering is quite insensitive to roughness and disorder. The formation of a chemical bond between graphite and the open d-shell transition metals that might complicate or even prevent spin injection into a single graphene sheet can be simply prevented by dusting Ni or Co with one or a few monolayers of Cu while still preserving the ideal spin-injection property.

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The Magnetic effect of Nonmagnetic Defects on Graphene

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We study the effect of nonmagnetic defects on graphene. After its discovery, the graphene have attructed much experimental and theorical attention. Magnetism in carbon-based materials has been a controversial problem. Apart from magnetic defects, the nonmagnetic-defect-induced mechanism is the most probable mechanism in those materials. In this presentation, we focus on vacancy-induced magnetism.

Electrons in graphene can be described with a half-filled Hubbard model on a honeycomb lattice. We then introduce a vacancy as short-range strong scattering potential on a lattice point. Resorting to a mean field approximation and diagonalizing the approximated Hamiltonian, we can determine the electron number and spin densities at each lattice point.

We then find that a vacancy induces short-range ferrimagnetic order around itself. This order is caused by a quasilocalized vacancy state induced by a strong potential. In cases with extended vacancies, the moment formation depends on the geometrical structure and the difference in the numbers of vacancies on two sublattices. The magnetic moment is necessarily induced when the number of vacancies on one sublattice is unequal to that on the other sublattice, in accordance with Lieb's theorem. We further discuss the possible magnetic moment formation on realistic edges in graphene.

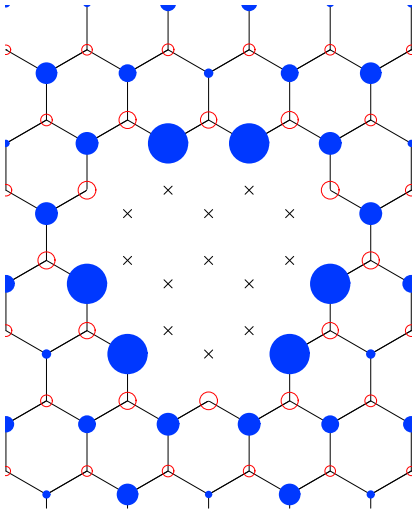

Figure 1: Spin density around defects. Area of each circle is proportial to the magnitude of spin density. Filled circles represent positive moments and open circles represent negatige moment.

The quasilocalized states are formed around defects. Owing their high degeneracy and the small energy gap, these states are spin polarized. This means that its electoron properties depend typically on these states, in particular, when one takes advantage of spin degrees of freedom. Thus, graphene with defects has the possibility of new spintronics devices.

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Title:
Effects of extended and localized states on spin Hall polarization in ballistic Rashba structures

Abstract:
The spin Hall polarization in ballistic Rashba systems is studied by considering both the contributions of extended and localized states simultaneously. In a narrow Rashba strip, the localized states are found to contribute dominantly to the total polarization, while in a wide strip, it is the extended states that determine the behavior of total polarization. Since the contributions from the two kinds of states are of opposite signs, their competition leads to spin flipping of the total polarization with the variation of sample width or Rashba strength. The critical flipping width of the sample is found to be closely related to the characteristic length of the Rashba system. It is expected that the flipping phenomenon would be detectable in the ballistic transport experiments. While in a semi-infinite Rashba system, the spin polarization of extended and localized states are both positive and no spin flipping would occur.

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Graphene Dirac billiards as quantum dots

We report on quantum confinement effects in ballistic graphene Dirac billiards. We investigate the density of states of these quantum dots as a function of varying edge roughness and point defects (i.e. disorder). We thereby change the nearest neighbor spacing distribution continuously from a regular Poissonian to a Wigner-Dyson statistics. This transition can well be described by the Hasegawa distribution functions. Moreover, we find a stable dependence of the second moment of the distribution on the edge roughness. This suggests that the roughness of fabricated graphene billiards can be estimated from the distribution of measured Coulomb blockade peaks.

Charge injection and Electric Force Microscopy investigations in tailored graphene sheets and ribbons.

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The electronic properties of carbon nanotubes have triggered a renewed research interest in the behaviour of graphitic materials and recent discoveries were a major breakthrough in moving towards electronic nanodevice technology. Remarkable mesoscopic electronic properties have been observed in few-layered and monolayered graphene in the past two years so that small domains of thin graphitic structures are now envisaged as an alternative platform for integrated nanoelectronics.

In this context, we will present our recent results in preparing, manipulating and tailoring few layer (FLG) and monolayer graphene in order to realize "all-graphene" devices. Complementary to transport studies in side-gated transistor devices presented elsewhere [1], we show how Electric Force Microscopy (EFM) can be used to contact graphene islands or nanostructured domains, inject charges and subsequently study both qualitatively and quantitatively, the two-dimensional delocalization or/and confinement of charges in the graphene structures [2]. In this regard the EFM studies over other organic systems like pentacene monolayers [3] and DNA [4] or semiconducting nanoparticles such as silicon nanocrystals [5] have already been established as an excellent electrical characterization tool. A quantitative analysis follows a simple model for estimating the carrier charge density with respect to number of layers of graphene islands. These studies are exploited within all-graphene devices, tailored with by Focused Ion Beam into side-gated transistor patterns [1]. As a less damaging and/or contaminating approach, we will show the manipulation and tailoring of graphene sheets by AFM nanolithography to produce islands seperated by trenches of a few tens of nanometers [6].

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Early stages of oxidation of nanostructured carbon: Atomic oxygen on graphene and graphite surfaces.

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We analyze the first steps in the oxidation of clean and defective graphene and graphite materials by combining Density Functional Theory (DFT) calculations, X-Ray photo emission spectroscopy (XPES), and Scanning Tunneling Microscopy (STM). The binding energy of the carbon 1s core level is measured by XPES as a function of exposure to atomic oxygen. With respect to the reference binding energy in graphite, the adsorption of O induces a large C 1s binding-energy shift of 1.75 eV and several new features in the energy range between 0 and -0.5 eV. The origin of these energy shifts are identified by DFT calculations employing the final state approximation for the calculation of the core-level shifts. Besides allowing a precise correspondence between binding-energy shifts and local adsorption geometry of the Oxygen ad-atoms, the calculations reveal that the measured surface binding effects are solely due to the outermost graphene layer, with little contributions from inner layers of graphite, and thus from the inter layer π conjugated bond. Moreover, we investigate the high-coverage regime by providing insights into the clustering of O adatoms, as well as the effect of surface defects and of surface strain. Defect distribution and strain have been further investigated by Scanning Tunneling Microscopy (STM) that complements the XPS data.

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Modelling of carbon nanoscale devices: towards a new generation of extremely integrated electronic circuits.

Carbon nanostructures are considered as key materials for microwave, electronic and optical applications. An accurate modelling of these new emerging materials, from the atomistic- to the micro-scale, is crucial for understanding their behaviour.
In the present contribution we are dealing with the following challenges:
- ballistic transport problem and scattering by lattice discontinuities in graphene nanoribbons (GNR),
- Dirac partial differential equation and transmission-line models for charge propagation in GNR,
- optical transition energy and Coulomb interaction for the characterization of excitonic shifts in carbon nanotubes (CNT), and sensitivity of absorption to photon polarization.

MULTIWALL CARBON NANOTUBE HIGH FREQUENCY RESONATOR

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We report on the measurement of a doubly clamped multiwall carbon nanotubes (MWNT) resonator electrostatically actuated. A resonant frequency of f=206MHz and quality factor of Q~16 has been detected in air at atmospheric pressure with an AFM room pressure technique similar to the one reported by D. Garcia-Sanchez, et.al. (PRL 99, 085501). Using the elastic beam theory and the geometrical parameters of the device the Young's modulus E=0.43TPa can be estimated. This value is in agreement with DC deflection measurements on the same carbon nanotube source. This implies that the built-in mechanical stress in the case of MWNTs is negligible.

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Hall effect in multilayer graphenes

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We discuss Hall effects of multilayer graphenes in weak- and strong-magnetic field regimes. We consider three stacking structures: Bernal, rhombohedral, and simple hexagonal types, and discuss how the physical behavior reflects the difference of the structures. For weak-magnetic field regime, we found plateaux in Hall conductivity as a function of the gate voltage, but the plateaux appear in different values depending on the structures.[1] For bilayer system in strong-magnetic field, we observed crossover of integer quantum Hall effect from two independent monolayer type system to strongly coupled bilayer systems by changing the ratio of interlayer hopping energy and the gate voltage.[2]

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How to detect the pseudospin-$\frac{1}{2}$ Berry phase in a photonic crystal with a Dirac spectrum

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We propose a method to detect the geometric phase produced by the Dirac-type band structure of a triangular-lattice photonic crystal. The spectrum is known to have a conical singularity (= Dirac point) with a pair of nearly degenerate modes near that singularity described by a spin-$\frac{1}{2}$ degree of freedom (= pseudospin). The geometric Berry phase acquired upon rotation of the pseudospin is in general obscured by a large and unspecified dynamical phase. We use the analogy with graphene to show how complementary media can eliminate the dynamical phase. A transmission minimum results as a direct consequence of the geometric phase shift of π acquired by rotation of the pseudospin over 360° around a perpendicular axis. We support our analytical theory based on the Dirac equation by a numerical solution of the full Maxwell equations.

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Structural properties and energetics of doped graphene nanoribbons

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Abstract

Structural properties and energetics of Li, Al, and BN doped armchair and zigzag graphene nanoribbons have been studied. The graphene nanoribbons have been formed from the lines of carbon atoms. Li and Al atoms have been attached to the carbon atoms and BN have been substituted into carbon atoms. The geometry optimization of the systems have been performed using semi-empirical self-consistent-field molecular-orbital methods at PM3 level. The single point energy calculations on optimized geometries have been performed by density functional theory within B3LYP exchange-correlation functional using 6-31G basis set. The structural, thermodynamical, vibrational properties, as well as some selected molecular orbital eigenvalues, and dipole moments have been reported.

Andreev reflection in graphene nanoribbons

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(Dated: June 5, 2008)

We study Andreev reflection in graphene nanoribbon/superconductor hybrid junctions. By using a tight-binding approach and the scattering formalism we show that finite-size effects lead to notable differences with respect to the bulk two-dimensional case. Conservation of pseudoparity, a quantum number characterizing the ribbon states, yields a suppression of Andreev reflection in a wide range of energies, inducing an insulating behavior even when the junction is biased. Electron conduction can be restored by applying a gate voltage, indicating potential applications of graphene nanoribbon/superconductor junctions as electron transistors.

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Magnetic confinement of electrons and direction-dependent transmission in graphene nanostructures

A two-dimensional (2D) honeycomb lattice of carbon atoms that can be viewed either as a single layer of graphite or an unrolled nanotube known as graphene, as well as that of multi-layer graphene has led to an intensive investigation of graphene's electronic properties. They possess unusual properties, such as very high electron mobility, an unconventional quantum Hall effect, and a strong electric field effect due to gapless and linear in 2D momentum energy spectrum [1]. The electrons in these structures are described as chiral, massless charged fermions and their behavior is governed by the 2D Dirac equation. The study of their properties points to new basic phenomena and the development of graphene-based, nanoelectronic devices.

We theoretically investigate transmission through the magnetic barriers in graphene-based nano-structures. Several particular cases are considered: a magnetic step, single and double barriers, δ -function barriers as well as barrier structures with inhomogeneous magnetic field profiles but with average magnetic field equal to zero. Bound states are obtained for a magnetic step and various barrier structures. The transmission exhibits a strong dependence on the direction of the incident wave vector and an angular confinement with a proper choice of the parameters involved. In general the resonant structure of the trans-mission is significantly more pronounced for i) Dirac electrons with *linear* spectrum compared to those with a *parabolic* spectrum, and ii) Dirac electrons in complex multi-barrier structures relative to the same electrons in single or double magnetic barriers. The results extend significantly the limited ones of Ref. [2] and contrast substantially with those of Ref. [3] pertaining to electrons with a *parabolic* spectrum.

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Dirac Antifermion-fermion condensates in the presence of magnetic fields

Abstract: We solve the Dirac equation in the presence of a constant magnetic field in (3+1) and (2+1) dimensions. Quantizing the fermion field, we calculate the $\bar{\psi}\psi$ condensate from first principles for parity conserving and violating Lagrangians for arbitrary field strength. We extend the analysis in the background of a thermal bath. We make a comparison with the results already known in the literature for some particular cases and point out the relevance of our work for possible physical applications.

Correspondence between Andreev reflection and Klein tunneling in bipolar graphene

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Andreev reflection at a superconductor and Klein tunneling through an n-p junction in graphene are two processes that couple electrons to holes — the former through the superconducting pair potential Δ and the latter through the electrostatic potential U. We derive that the energy spectra in the two systems are identical, at low energies $\varepsilon \ll \Delta$ and for an antisymmetric potential profile $U(-x,y) = -U(x,y)$. This correspondence implies that bipolar junctions in graphene may have zero density of states at the Fermi level and carry a current in equilibrium, analogously to superconducting Josephson junctions. It also implies that nonelectronic systems with the same band structure as graphene, such as honeycomb-lattice photonic crystals, can exhibit pseudo-superconducting behavior.

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Magnetoexcitons and magnetoplasmons in graphene.

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The dynamical polarizability of two dimensional graphene in a strong perpendicular magnetic field is calculated at arbitrary wave vector and frequency, in the Random Phase Approximation. We only consider completely filled Landau levels. From the obtained polarizability, we study the screening effects, the renormalized two dimensional Coulomb interaction and the collective excitations (magnetoexcitons, magnetoplasmons). We stress the differences with the usual two-dimensional electron gas. Special attention is paid to the intrinsic interband contribution to the screening.

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Effect of electron-electron interaction on the Fermi surface topology of doped graphene.

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The electron-electron interactions effects on the shape of the Fermi surface of doped graphene are investigated. The actual discrete nature of the lattice is fully taken into account. A π-band tight-binding model, with nearest-neighbor hopping integrals, is considered. We calculate the self-energy corrections at zero temperature. Long and short range Coulomb interactions are included. The exchange self-energy corrections for graphene preserve the trigonal warping of the Fermi surface topology, although rounding the triangular shape. The band velocity is renormalized to higher value. Corrections induced by a local Coulomb interaction, calculated by second order perturbation theory, do deform anisotropically the Fermi surface shape. Results are compared to experimental observations and to other theoretical results[1].

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Ground-state carrier density in graphene

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We calculate the carrier density dependent ground state properties of graphene in the presence of random charged impurities in the substrate taking into account disorder and interaction effects non-perturbatively on an equal footing in a self-consistent theoretical formalism. We provide detailed quantitative results on the dependence of the disorder-induced spatially inhomogeneous two-dimensional carrier density distribution on the external gate bias, (i.e. the average density), the impurity density, and the impurity location. We find that the interplay between disorder and interaction is strong, particularly at lower impurity densities. We show that for the currently available typical graphene samples, inhomogeneity dominates graphene physics at low ($<< 10^{12}$ cm^{-2}) carrier density with the density fluctuations becoming larger than the average density.

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Graphene nanoconstriction as a single-level quantum dot

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Quantum dot having a single relevant electronic level, that shows only spin degeneracy, is widely considered as a key ingredient for solid-state quantum information processing. Recently, such a single-level quantum dot (SQD) was proposed to be realized in graphene constrictions with predominantly *armchair* edges [1, 2] in order to exploit the superior spin coherence expected in carbon nanostructures. This is the theoretical proposal to build SQD by using graphene nanoconstriction with *zigzag* edges only. The work was motivated by recent experiment by Li *et al.* [3] reporting fabrication of a 120-degree graphene kink with zigzag edges. On the other hand, in the existing proposals to build SQD in graphene [1, 2] the sections of an insulating-armchair nanoribbon are used to trap an electron in the device [4].

Earlier, we have shown [5] using tight-binding calculations, that the *asymmetric* kink consists of two nanoribbons with zigzag edges rotated to form a 120-degree kink, blocks the lowest propagating mode. Here, we first briefly discuss the evolutions of the kink conductance with its geometrical parameters W_1 and W_2 to show the blocking mechanism works effectively except from the *symmetric* case $W_1 \approx W_2$, when the resonant tunneling may appear. The analysis is extended to the case of nonzero edge magnetization, which may appear in nanoribbons with zigzag edges [6].

Here, the two kinks are joined together to form a *double kink*, which shows narrow conductance peaks associated with a charge density localized in a central section. The decay rates of such localized states comparable as of their counterparts in the system of Ref. [2]. This indicates each kink traps an electron as effectively as an insulating-armchair nanoribbon of the similar size and, subsequently, the double kink operates as SQD in graphene. We also consider a *double quantum dot* (DQD), formed in nanostructure containing *four* kinks, to illustrate the scalability of the proposed device.

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Spin transport in graphene nano-ribbons

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Abstract

Graphene is emerging as a very versatile material with properties that could be tuned for many device applications. Recently a demonstration of spin injection into graphene which has a low-spin orbit coupling and hence long spin relaxation times and lengths has aroused an interest in using graphene for possible spintronic applications. Zigzag graphene nano-ribbons have been shown to have an inherently magnetic structure, and in our work here, we investigate how efficiently they can transport spin from one spin polarized electrode to another. The role of vacancy on its spin valve characteristics will also be discussed.

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Field theoretic description of graphene in an electromagnetic background, at finite temperature and density

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Abstract.

We present the evaluation of the effective action, at finite temperature and density, for Dirac fields in the presence of an electromagnetic background, in three Euclidean dimensions. Apart from explaining (in the low temperature limit) the behavior of the Hall conductivity for graphene, our results show the existence of a direct relationship between the selection of a phase for the Dirac determinant and the generation (or lack thereof) of Berry's phases and Chern-Simons terms.

Extremal transmission at the Dirac point of a photonic band structure

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We calculate the effect of a Dirac point (a conical singularity in the band structure) on the transmission of monochromatic radiation through a photonic crystal. The transmission as a function of frequency has an extremum near the Dirac point, depending on the transparencies of the interfaces with free space. The extremal transmission $T_0 = \Gamma_0 W/L$ is inversely proportional to the longitudinal dimension L of the crystal (for L larger than the lattice constant and smaller than the transverse dimension W). The interface transparencies affect the proportionality constant Γ_0, and they determine whether the extremum is a minimum or a maximum, but they do not affect the "pseudo-diffusive" $1/L$ dependence of T_0.

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Side-gated transport in FIB-fabricated multilayered graphene nanoribbons

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We present the fabrication and investigation of the low-temperature transport properties of a multi-layer graphene-based transistor device with side gate voltage. We fabricate micron long sub-100nm graphitic ribbon using a combination of a resist free method and focus ion beam (FIB) lithography technique [1,2].
Temperature dependence ($40\ K < T < 300\ K$) of the (I-V) characteristics in these nanoribbons reveals an increasing non-linearity and the opening of a gap in the zero-bias region with decreasing temperature. Gate modulated transport with double side-gate ($-30\ V < V_G < 30\ V$) shows that the amplitude of this gap decreases with increasing applied gate voltage. Symmetry is also observed for both positive and negative applied gate voltage.
We believe that the electronic transport can be simply interpreted in terms of Coulomb Blockade (CB) along a linear array of N tunnel junctions between graphene islands. Further, we propose a simple and intuitive model to describe such transport properties that closely match our experimental findings. In this framework, the role played by natural and/or ion-induced defects dominates and supersedes any "edge effects" from the ribbon sides, as suggested in other reports [3].
We believe that our preliminary study on graphitic layer represent the first step towards a more comprehensive and thorough understanding of the electron transport in mono-layer graphene sheet-based device.

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Interacting particles in two dimensions: numerical solution of the four-dimensional Schrödinger equation in a hypercube

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We study numerically the Coulomb interacting two-particle stationary states of the Schrödinger equation, where the particles are confined in a two-dimensional infinite square well. Inside the domain the particles are subjected to a steeply increasing isotropic harmonic potential, resembling that in a nucleus. For these circumstances we have developed a fully discretized finite difference method of the Numerov-type that approximates the four-dimensional Laplace operator, and thus the whole Schrödinger equation, with a local truncation error of $\mathcal{O}(h^6)$, with h being the uniform step size. The method is built on a 89-point central difference scheme in the four-dimensional grid. As expected from the general theorem by Keller [Num. Math. **7**, 412 (1965)], the error of eigenvalues so obtained are found to be the same order of magnitude which we have proved analytically as well. Based on this difference scheme we have obtained a generalized matrix Schrödinger equation by vectorization. In the course of its numerical solution group theoretical methods were applied extensively to classify energy eigenvalues and associated two-particle wave functions. This classification scheme inherently accounts for the symmetry property of the two-particle state under permutation, thereby making it very easy to fully explore the completely symmetric and antisymmetric subspaces of the full Hilbert space. We have obtained the invariance group of the interacting Hamiltonian and determined its irreducible representations. With the help of these and Wigner-Eckart theorem, we derived an equivalent block diagonal form of the eigenvalue equation. In the low-energy subspace of the full Hilbert space we numerically computed the ground state and many (≈ 200) excited states for the noninteracting as well as the interacting cases. Comparison with the noninteracting exact results, which we have found analytically too, reveals indeed that already at a modest resolution of $h \approx 1/15$ our numerical data for the eigenvalues are accurate globally up to three or more digits of precision. Having obtained the energy eigenvalues and eigenstates we calculated some relevant physical quantities with and without interaction. These are the static two-particle densities labeled by irreducible representations, one- and two-particle density of states and some different measures of entanglement, including the reduced density matrix and the von Neumann entropy. All these quantities signal concordantly that the symmetric states (with respect to permutation of particles) as well as their energies are affected by the interaction more dramatically then their antisymmetric counterparts.

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Title: *Electron-electron interactions and Dirac liquid behavior in graphene bilayers*

Abstract:

We study the e ect of electron-electron interactions in the quasiparticle dispersion of a graphene bilayer within the Hartree-Fock-Thomas-Fermi theory. We nd that the electronic uid can be described in terms of an e ective Lorentz invariant theory with renormalized mass and velocity, the Dirac liquid. We show that the Dirac liquid can quantitatively describe recent cyclotron resonance experiments in this system.

Non-adiabatic geometric phase induced by relative vibrations of two sublattices in graphene

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We investigate the geometric phase of electron states under relative vibrations of two sublattices in graphene by solving the time-dependent Schrödinger equation using the Floquet scheme. In a period of vibration the fermions acquire different geometric phases depending on their momenta. Two regions are obtained in the momentum space: the adiabatic region where the geometric phase can be approximated by the Berry phase and the chaotic region where the geometric phase drastically fluctuates in changing parameters. The energy of fermions due to vibrations shows spikes in the chaotic region. The results suggest a possible dephasing mechanism which may cause classical-like transport properties in graphene.

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Title:	The effect of domain wall in graphene
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Abstract：

We use the tight-binding approximation based on the π-states of carbon, and consider about the discrete model with just the nearest sites hopping. By means of an improved transfer matrix approach (ITMA) recently developed by us, we study the following properties for single-layer graphene.

1、 The energy band of graphene strip and the transport properties of a graphene bar with zigzag and armchair open boundary are studied. The relationship of the scaling behaviour of the graphene bar and the transmission coefficient, and the oscillation are analyzed.

2、 A spin domain wall is introduced in graphene strip. Its effect on the Dirac point is studied, and its comparison with the effect from electric p-n junction of graphene is presented.

3、 We obtain the analytic expressions of eigen-energies and wave functions for a graphene strip with open zigzag or armchair boundary. The comparison of the results with our numerical calculation is presented. The consistent results are received.