Bogoliubov Laboratory of Theoretical Physics Joint Institute for Nuclear Research

DUBNA NANO 2012 conference

International Conference

DUBNA-NANO2012

July 9-14,2012 • Dubna, Russia

Section

GRAPHENE AND OTHER CARBON NANOSTRUCTURES

NEUTRON STUDIES OF CARBON NANOSTRUCTURES

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The possibilities of neutron scattering in the research of carbon nanomaterials are outlined. The examples of the structure analysis of crystalline solids, films and layered structures and dispersed systems are given. Among the covered questions are quasi-1D fullerene structures, chirality and hydrogen storage capacity of single-wall carbon nanotubes, water in pores and at interfaces in liquid dispersions of nanodiamonds and fullerene solutions, as well as in the clusters of shungites. The application of nanodiamond powders in fundamental neutron physics is discussed.

The experiments on small-angle neutron scattering from cluster solutions of carbon nanoparticles are considered with respect to the application of the kinetic equations based on the nucleation theory approach. The models of dissolution processes and cluster growth are presented.

NONLINEAR OPTICAL RESPONSE OF GRAPHENE AT MULTIPHOTON RESONANT EXCITATION IN STRONG LASER FIELDS

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Many fundamental nonlinear QED processes,specifically, electron-positron pair production in superstrong laser fieldsof ultrarelativistic intensities, have theircounterparts in graphene where incomparably weaker electromagnetic fieldsare required for its experimental realization [1].

In the present work the microscopic theory of the creation of particle-holecoupled states in graphene via multiphoton resonant excitation by laser fields of moderate intensities is developed. We considerthe multiphoton interaction regime and nonlinear optical response of a graphene, considering particle-hole quantum dynamics in the vicinity of the K point. The evolutionary equation for single-particledensity matrix is formulated arising from the second quantized formalism.The time-dependent single-particle density matrix in the given field of alaser radiation is calculated in the multiphoton resonant approximation. TheRabi oscillations of Fermi-Dirac sea in a graphene at multiphoton excitation depended onthe time, momentum, and photons number are considered and analyzedalso on the base of numerical simulations. The obtained results demonstrateRabi oscillations of Fermi-Dirac sea in the graphene that correspond tomultiphoton excitation by moderately strong laser radiation. The latter can already be observed for such laser fields where the work of electric field on a wave period is comparable to photon energy. For the mid-infrared lasers multiphoton interactionregime can be achieved at the intensities $10^7 W/cm^2$, for the picosecond time scales. Hence, the described Rabi oscillations of the particle distribution function may be experimentally probed by pump-probe, picosecond time-resolved photoemission spectroscopy. The considered process, apart from fundamental interest, also has practical applications. In particular, particle-holeannihilation from the coherent superposition states will cause intensecoherent radiation of harmonics of the applied wave-field, which is also discussed in the present work.

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HEAT CAPACITY OF SINGLE – WALLED CARBON NANOTUBE BUNDLES SATURATED WITH NITROGEN

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The heat capacity $C_{SWNTs+N2}$ of bundles of single – walled carbon nanotubes (SWNTs) closed at their ends and saturated with N_2 has been investigated in the interval 2-40 K. The ratio n_{N2}/n_C=0.6%, n_{N2}, n_C – are the numbers of N_2 molecules and C atoms, respectively, in the sample. According to the estimates, this concentration of nitrogen could well suffice for the formation of one chain per groove when the N_2 molecules occupy the grooves on the outer surface of SWNT bundles.

The heat capacity $C_{SWNT+N2}$ was measured using an adiabatic calorimeter [1]. The curve $C_{SWNT+N2}(T)$ increases monotonically with a rising temperature. The temperature dependence $C_{SWNTs+N2}$ has a feature at 33 K. For pure SWNTs we observed a similar feature in the curve $C_{SWNT}(T)$ near 36 K [2], which is due to the radial breathing modes (RBM). It is likely that the filling of the grooves by N_2 molecules leads to the depression of the RBM frequencies in the SWNTs and hence shifts the feature towards lower temperatures. $C_{SWNT}(T)$ and $C_{SWNT+N2}(T)$ were measured on the same SWNT sample before and after saturation with N_2 gas.

It is found that filling SWNT bundles with nitrogen gas to the concentration 0.6% enhances considerably the heat capacity in the whole interval of the temperatures investigated. The ratio $C_{SWNT+N2}/C_{SWNT}$ is equal to about 2.5 at 2 K<T<15 K and decreases linearly with a growing temperature down to ~ 2 and 1.6 at 25 K and 40 K, respectively. This large effect in the heat capacity is mainly due to the contributions of the translational and rotational degrees of freedom of the N_2 molecules.

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PLASMON NANOOPTICS WITH PRISTINE AND HYBRI CARBON NANOTUBE SYSTEMS

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In general, plasmons cannot be excited by light in optical absorption since they are longitudinal excitations while photons are transverse. In small-diameter ($\sim$1 nm) semiconducting carbon nanotubes (CNs), light polarized along the CN axis excites excitons which, in turn, can couple to the nearest (same-band) interband plasmons by applying an electrostatic field perpendicular to the CN axis[1,2]. Both of these collective excitations originate from the same electronic transitions and, therefore, occur at the same (low) energies $\sim$1 eV, as opposed to bulk semiconductors where they are separated by tens of eVs. Their coexistence at the same energies in CNs is a unique feature of confined quasi-1D systems where the transverse electronic motion is quantized to form 1D bands and the longitudinal motion is continuous. We discuss how low-energy interband plasmon excitations can efficiently mediate enhanced electromagnetic absorption (Fig.1) by pristine semiconducting CNs[3] and bipartite entanglement in hybrid metallic CN systems[1]. We develop a theory for (non-linear) optical monitoring and control of the phenomena above.

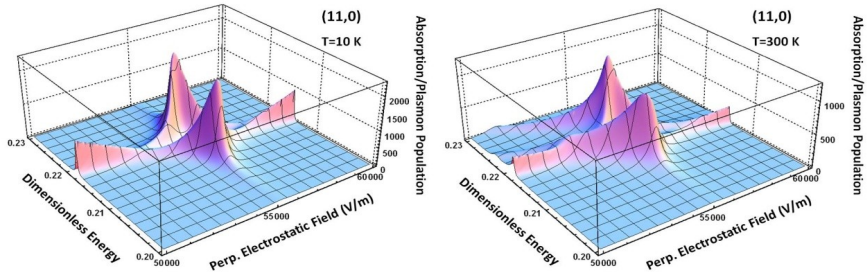

Fig. 1. Low- and high-temperature (left and right, respectively) plasmon population (also representting increased electromagnetic absorption by excitons) for the first bright exciton coupled to the nearest interband plasmon resonance in the (11,0) nanotube in a perpendicular electrostatic field. Dimensionless energy is defined as [Energy]/$2\gamma_0$ where γ_0 = 2.7 eV is the C-C overlap integral.

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NOVEL METHOD OF LARGE AREA GRAPHENE FABRICATION

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For studying of physical properties of graphene and fabrication of graphene devices large area graphene samples are necessary. Our fabrication method does not demand special expensive equipment and can be easily implemented. Single-layer graphene flakes with the size up to 200 mkm and few-layer graphene flakes with the size up to 2000 mkm were obtained by this technique. These flakes were can be produced on various substrates including transparent ones. Atomically thin films of other laminated materials can be also obtained using this method.

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THEORETICAL INVESTIGATION OF PROPERTIES OF THE CURVED GRAPHENE NANOSTRUCTURES

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Results of the theoretical investigation of mechanical and electronic properties of the curved graphene nanostructures are presented in this work. We considered axial compression of graphene structures in a regime of real time. The simulation of the compression process was carried out by means of the tight-binding molecular modeling method (MDTB)[1]. Monolayer and bilayer graphene nanoribbons are subjects of this investigation. As a result of investigation it was found that the monolayer and bilayer graphene became a wave-like at the increase of compression (see fig.1,2). The number of half-waves generated by compression depends on the size of graphene structures.

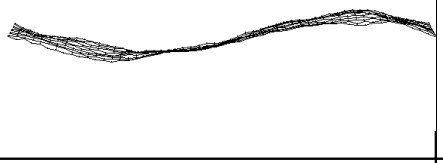

Fig.1. Atomic structure of the curved monolayer graphene nanoribbon

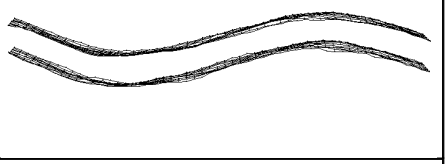

Fig.2. Atomic structure of the curved bilayer graphene nanoribbon

The distribution of the local stress by coordinates of atoms for monolayer and bilayer curved graphene was calculated by means of the original developed method. It was established that the stress ~1.8 GPa is critical stress for the deformed graphene structures.

We calculated electronic spectrum of the curved graphene nanoribbons by means of the quantum chemical tight-binding method and parallel algorithms. As a result of calculations it was established that the ionization potential of the curved graphene is less in comparison to the planar graphene.

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NONLINEAR SPIN WAVES IN GRAPHENE STRUCTURES

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It is known a number of experimental and theoretical works which investigated the magnetic properties of graphene structures. This is due, among other things, with the prospects of using graphene as a material for the needs of the future nanoelectronics and spintronics. In particular, the well-known paper [1] reported the presence of ferromagnetic properties at temperatures up to 200° C and above in a single-layer graphene films that are free from impurities, and in [2] the issues of propagation and relaxation of the spin-polarized current pulse in the graphene film are studied. In papers [3-4] there was proposed a quantum field theoretical model describing the possible mechanism of ferromagnetism in graphene as a result of spontaneous breaking of spin symmetry of the surface density of valence electrons. The possible spatial configurations of the localized spin density were described.

In this paper we investigate such spatially localized nonlinear spin configurations of the valence electron density on the graphene surface as kinks, and their interactions, as well as quasibound metastable states of the interacting kinks and antikinks, that are breathers. The spectrum of such breathers is investigated. It is shown that under certain conditions, this spectrum has a discrete sector, which, in turn, allows us to speak about the possibility of coherent quantum generation of spin waves in graphene structures, which is important in terms of practical applications in nanoelectronics and spintronics.

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CHEMICAL AND PHYSICAL METHODS FOR THE PRODUCTION OF GRAPHENES

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Graphite is a layered mineral composed of weakly bonded graphene sheets with a large aspect ratio. A peculiarity of graphite is its layered structure formed by parallel two-dimensional graphene sheets weakly coupled by van der Waals interaction. Each graphene sheet looks like a hexagonal network of carbon atoms connected by strong covalent "in-plane" σ–σ bonds [1].

Nanographite has attracted more scientific attentions for the past decade years owing to their unique properties, such as excellent electrical conductivity, high thermal resistance, low thermal expansion coefficient and our ability to influence these properties through chemical functionalization.. Nanographite with a large surface area and high electrical conductivity has been widely used in various fields such as electrodes of supercapacitors, advanced catalyst supports, chromatographic packing, energy storage, gas sensors and self-assembled films [2-4].

There are a number of methods for generating graphene and chemically modified graphene from graphite and derivatives of graphite, each with different advantages and disadvantages. Here we review the use of different methods to produce new materials composed of graphene and chemically modified graphene. These techniques can in general be classified into three different routes: namely (i) mechanical peeling, (ii) epitaxial graphene growth and (iii) solution-based reduction of graphene oxide.

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MECHANICAL AND EMISSION PROPERTIES OF THINNEST STABLE BAMBOO-LIKE NANOTUBES

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The use of carbon bamboo-like nanotube became possible as nanoindentor and nanoemiterov. Consequentlythe study of electronic structure and topology of the framework is necessary.

Single- wall CBNTs with the inner bridges with the diameter 2.024 nm (the length 3.6 nm) and the diameter 1.6 nm (the length 3.728 m) were investigated by develop tight-binding model for calculating carbon nanoclasters[1].

Following results were obtained:

1) The method of calculation of map of local stresses developed was developed[2].

The calculation of map local stresses was carried out for CBNT with diameter 1.36 nm and 2.024nm. Analyses stability of CBNT was carried out by the calculation of the map of the local stresses. The critical stresses at which UBNT begins destruction is approximately 11 GPa. It is established that carbon bamboo-like nanotube with diameter 2.024nm is thinnest stable bamboo-like nanotube and the maximum stress achieved in this tube is ~ 8 GPa.

2) CBNT with the diameter 2.024nm destructed under compression, which carried out with speed 10m/sec, after 8.44 ps in the area of bridge (destruction equal ~ 3%).

3) CBNT with diameter 2.024nm destructed under stretching , which carried out with speed 10m/sec, after 19 ps in the area of bridge (destruction equal ~ 5%)

4) CBNT with smaller diameter do not differ from the hollow nanotubes On the emission properties. Therefore, the nanotubes can be used in electronics as a strong and elastic needle nanoemitterov diameter ~ 2 nm. *References*

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THE SYNTHESIS OF HELICAL CARBON NANOTUBES IN THE PECVD PROCESS

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Carbon nanotubes has been discovered more than 20 years ago, but interest of them growing steadily. At the moment a lot of new technologies and research methodologies of carbon nanotubes are developed. However, no device or technology using carbon nanotubes as main element were not produced. Recently, a lot of experiments are conducted according to a geometric modification of carbon nanotubes based on the physical electric and magnetic properties. The results of modifications are helical carbon nanotubes and tori that can be used in micro-electromechanical systems.

The main purpose of this work is the develop laboratory system for coiled carbon nanotubes into rings and spirals production. Developed nanomaterial can be used for production conductive percolated surface for electro stimulated growth culture in cells. For this purpose has been studied the world experience of creation a helical carbon nanotubes, and developed the laboratory system for coiled carbon nanotubes into rings and spirals production. Systems consists of the discharge chamber with the electrodes in which the metal catalyst in coal-rods, and the interelectrode gap are fed carbon containing gases such as methane with argon daring, a vapor of ethanol and carbon dioxide. The process based on the decomposition of carbon-containing gas in the discharge plasma, and deposition on the catalyst by structuring the carbon nanotubes of different geometry.

The obtained samples of nanomaterial were analysed on the device which combines scanning probe microscope and Raman spectrometer. The topography of the carbon material was investigated using a semi-contact method of atomic force microscopy. The chemical structure of the material constitution was studied by analyzing Raman spectrum. At the result we were shown that structure of nanomaterial obtained in our system depends on gas which we used in system. The materials obtained from methane gas were helical carbon nanotubes which has following parameters: diameter of the carbon nanotubes about 15 nm, diameter of the helix of nanotubes about 1 micron.

FIELD EMISSION FROM CARBON NANOTUBES

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So far the question of field emission mechanism from carbon nanotubes remains open. Traditionally, field emission current-voltage characteristics of carbon nanotubes are interpreted by Fauler-Nordgeim model, developed for metals with dimension 3D and Fermi electronic gas [1]. But it is known, that thin carbon nanotubes should be considered as quantum wire (quasi-1D structures) and therefore, Fauler-Nordgeim model shouldn`t be used for them. It means, that it's impossible to use this model to understand the nature of anomalously low threshold values of intensity of electric field Eb, at which emission of electrons begins and anomalously high density of emission current j [2]. Also the influence of ambipolarity of carbon nanotubes (CNT) on field emission wasn`t considered.

The object of this work was to study the influence of quantum-well effects and ambipolarity of CNT on field emission of them.

It was theoretically shown that canals with anomalously high density appear by field emission from thin CNT on current-voltage characteristics as the result of dimensional quantization charge carrier.

The experimental measuring current-voltage characteristics at field emission conducted with single nanotubes cathodes in system of scanning electron microscopy Carl Zeiss NEON 40 showed the presence of emission beginning threshold and strong oscillation of current on current-voltage characteristics, which we connect with presence canals of conductivity.

Possible mechanism of field emission with CNT and more detailed results of researches will be discussed.

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THE UNIQUE BEHAVIOR OF THE ELECTROMAGNETIC WAVES IN GRAPHENE AT THE INTERFACE BETWEEN TWO DIELECTRIC MEDIA

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The influence of the optical contrast between the two media, located on the opposite sides of graphene on the behavior of electromagnetic waves with TE and TM polarization was studied. It was found that TE-polarized waves, predicted to exist only in graphene [1], becomes leaky due to the increase of the optical contrast. In considered case TE-mode frequency lies only in the window determined by the contrast. Analytical expressions describing the frequency range and extent of leakage depending on the contrast were deduced. The different characteristics of leaky modes: the wave vector, phase and group velocities, the characteristic length of leakage were studied in detail. The sensitivity of TE-modes to changes in contrast was estimated. Near the frequency where the imaginary part of the conductivity of graphene vanishes, the very high sensitivity and very low detection limit were observed. The considered effect can be used for design of highly sensitive optical sensors based on graphene. We expect that they can outperform modern plasmon resonance sensors [2] by several orders.

The work was supported by Russian Foundation for Basic Research and the Grant of President of Russian Federation MK-5288.2011.2.

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MECHANISM OF ENDOHEDRAL VOID CONFINEMENT OF CARBON AND GOLDEN FULLERENES

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A large series of different fullerenes including the ordinary, classical ones, such as C20, C28, C36, C42, C60, C80 and the golden fullerenes were studied quantum chemically, invoking the density functional theory, in order to elucidate the mechanism of their endohedral void confinement @. It is demonstrated, choosing atoms He and Li, and molecules Li2, H2O, and CH4 as dopants, that the void confinement is not a simple one of a 'particle-in-box" type [1], rather is that causes a change of the oxidation state of dopants, thus revealing a hole existence within a void. Character of a hole is probed via corresponding protonation of void and compared with the exohedral one. A change of the charge state of dopant under void confinement reveals rather specific spectroscopic features of dopants that result in blue shifts of their stretching vibrational modes and quite unusual mechanism of bonding between dopant species within a void, similar to that for dicationic complexes of benzene [2]. The model of endo-void confinement is proposed and developed for modeling a confinement of the complexes of methane within classical fullerenes.

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TO THE PROBLEM OF THE INTRINSIC MAGNETISM IN CARBON-BASED SYSTEMS

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The development of experimental techniques over the recent years opened the possibility for synthesis and investigations of a wide class of new substances with unusual combination of properties. As a rule, magnetic materials can be metals, semiconductors or insulators which contain the ions of transition metals or RE-metals with unfilled shells. During the last decade the search for macroscopic magnetic ordering in exotic materials has attracted big attention. In particular, the carbon-based materials were pushed into the first row of researches. Carbon materials are unique in many ways. They are characterized by the various allotropic forms that carbon materials can assume, including the graphene - a monolayer of carbon atoms densely packed in a honeycomb lattice. It was conjectured that in addition to its transport properties a rich variety of magnetic behavior may be expected in graphene, including even a kind of intrinsic ferromagnetism. Some hypothesis were claimed that connected possible spin-ordering effects with the low-dimensionality and Dirac-like electron spectrum of graphene, thus inspiring a new kind of magnetism without magnetic ions [1]. In the present study, these questions were analyzed and critically reconsidered to elucidate the possible relevant mechanism (if any) which may be responsible for observed peculiarities of the ”magnetic” behaviour in these systems, in the approach of quantum theory of magnetism [2, 3]. On the basis of this analysis the conclusion was made that the thorough and detailed experimental studies of this problem only may lead us to a better understanding of the very complicated problem of magnetism of carbon-based materials. References

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QUANTUM COHERENT EFFECTS IN NANOSTRUCTURES BASED ON LAYERED MATERIALS

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We studied quantum coherence in layered superconductors, charge density wave (CDW)materials and graphite using various nanostructures fabricated by focused ion beams. Using mesa type structures we studied synchronization of intrinsic Josephson junctions in layered high temperature superconductor $Bi_2Sr_2CaCu_2O_{8+x}$ by magnetic field oriented across the layers[1].Those structures have also been used for interlayer tunneling spectroscopy of CDW gap and intragap states [2].We found effect of induction of CDW state by high magnetic field in $NbSe_3$ [3] and in graphite[4].

We will discuss a new type of threshold nonlinearity in $NbSe_3$ in the in-plane direction across the conducting chains in high magnetic fields which is accompanied by generation of electromagnetic radiation. Finally we consider quantum interference effects on thin graphite crystals containing nanoholes. On graphite and graphene samples with nanoholes we found oscillations of magnetoresistance with a period corresponding to the flux quantum per nanohole area [5]. The existence of Aharonov-Bohm type effect on samples of non-ring geometry is attributed to the existence of the edge states around a hole. The work has been supported by RFBR grants No 11-02-01379-a, No 11-02-90515-Ukr_f_a, 11-02-12167-ofi-m, state contracts No 16.740.11.0146 and No 16.513.11.3066.

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INVESTIGATION OF COOLING ON GROWTH NANOSIZED GRAPHITE LAYERS

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Graphene is a new material with an outstanding thermal and electrical conductivity, high mechanical and thermal stability [1]. This facts makes grapheme a promising properties, it is necessary to develop reliable and technologically advanced methods that will obtain large quantities of graphene with the given parameters.

In our experiments, the formation of graphene is the result of thermal decomposition of gaseous carbon compounds on the surface of a metal catalyst. The experiments investigated the decomposition of C2H5OH at temperatures of 650-750oC.

The results of atomic force microscope investigation showed that the parameters of graphene films strongly depend on the combination of several factors. The first parameter is a grain size of a Ni catalyst, i.e., roughness of the substrate should be minimal. The second parameter is a concentration of carbon-containing mixture in the reaction zone. Also the number of layers increases an important factor is the rate of cooling of the sample after CVD growth.

To control the last factor we made a new growth device where the substrate is heated by an induction method. This method eliminates the use of inert gas to cool the substrate. The cooling rate of the substrate in such a way was 20oC/sec., This allows to obtain films with thickness up to 3 nm. With decreasing cooling rate.

Investigation of Raman-spectra of the resulting structures allows us to speak about the dependence of the number of layers of material on the shooting range. The comparative height of the characteristic peaks of 1350 cm-1 and 2700 cm-1 clearly describes the thickness of the material.

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LOCALIZED STATES FOR ZIG-ZAG – ARMCHAIR JUNCTION OF CARBON NANOTUBES

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Carbon nanotubes are the most promising structure for modern nanoelectronics. The quantum graph model of junction of ”zig-zag” and ”armchair” single-wall carbon nanotubes is considered. The structures of such type (particularly, connection of single-wall nanotubes of zig-zag type (2N, 0) and armchair type (N, N)) were synthesized few years ago [1]. The nanotubes coupling causes the disturbance of the crystal structure. As a result, one obtains additional electron refraction at the interface.

Hence, the conductivity changes and localized states concentrated near the interface appears. It can be the background for creation of new nanoelectronic devices (diode, transistor, etc.). There are few mathematical models for description of transport and spectral properties of such structures. We use the quantum graph model of the system. This model is explicitly solvable and allows us to find the transfer matrix explicitly and to describe the spectrum completely. The model is analogous to that suggested in [2]. A condition on appearance of states localized near the interface is provided. All localized states are explicitly calculated.

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THE ELECTRONIC PROPERTIES OF SINGLE AND DOUBLE WALL CARBON NANOTUBES

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The electronic spectra of single wall (SWN) and also double wall (DWN) nanotubes using tight binding approximation are investigated. We focus on the double wall zig-zag and armchair nanotubes. The influence of nanotube curvature on the electronic spectra is also treated. The impact of the external magnetic field on the spectral characteristic of double wall nanotubes is computed. The strong changes of the electronic spectra caused by the different geometry of the nanotube are found. The field change the gap between valence and conductive band in the double wall nanotubes. We found the strong change of the electronic spectra for the double walled carbon nanotubes due to external magnetic field. The difference in the fermi energy between outer and inner nanotube for DWN was found which originate from the different hybridization of pi orbital. We will study the electronic states of finite size nanotubes. We would like examine the influence of nanotube curvature on the flat bands and how nanotube size and curvature influences the edge states in different types of nanotubes. We will also investigate within the effective mass approximation the influence of the topological defects in the nanotubes on their electronic spectra. We will analyze different boundary conditions at the end of the nanotubes and how the conditions effected finally their electronic properties. We will present also a theory of the long-wavelength low-energy electronic structure of graphite nanotubes. The transfer of electrons are described by wrapping a massless two dimensional Dirac Hamiltonian onto a curved surface of nanotubes. The effect of inhomogeneous nanotube shape deformations as some small hyperboloidal bending are analyzed analytically within a perturbation scheme. We find very different semimetal characteristic for the double wall zig-zag and armchair nanotubes. The results of our calculations will be presented analytically as well as numerically.

ELECTRONIC DENSITY OF STATES OF CARBON NANOTUBES

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Extraordinary electrical properties of carbon nanotubes (CNTs) together with their excellent mechanical stability make these systems very attractive for nanoelectronic applications. That is why the theoretical and experimental study of electronic structure and density of states (DOS) $\nu(\varepsilon)$ of CNTs is necessary. The following phenomena in CNTs have been reported in literature:

- depth of the minimum in the DOS at the Fermi level ε_F decreases when temperature increases;
- curve of $\nu(\varepsilon)$ near ε_F becomes more narrow when chirality indices of metallic nanotubes increase;
- doping of CNTs with the different chemical elements and impurities complexes results in appearance or disappearance of energy gap near ε_F for metallic or semiconducting CNTs, respectively;
- DOS increases when concentration of impurities rises;

In the present work we have observed that all these peculiarities of DOS may be explained by the multiple elastic electron scattering on impurities and structural inhomogeneous of short-range order type. Using the temperature Green function method we have obtained the contribution to DOS:

$$\Delta\nu(\varepsilon)=\frac{2.45(\pi)^{3/2}}{(C_h a\gamma_0)^{3/2}\tau}\frac{\left(\left(\frac{\sqrt{3}\pi a\gamma_0}{6C_h}-\varepsilon\right)^2+\frac{1}{4\tau^2}\right)^{1/2}}{\left(\frac{\sqrt{3}\pi a\gamma_0}{6C_h}-\varepsilon\right)^{3/2}},$$

where a is lattice constant, C_h is chirality of nanotubes, γ_0 is the transfer integral between first neighbor p_z orbitals and, finally, τ is electron relaxation time calculated in [1] taking into account the multiple elastic electron scattering on impurities and structural inhomogeneous of short-range order type. We have shown that τ depends on temperature, concentration of impurities and defects and short-range order coefficient. Thus the contribution to DOS from the electron scattering on impurities and structural inhomogeneous may lead to a strong dependence of DOS on temperature, concentration of impurities and defects of structure, chirality and the type of short-range order. This is in a good agreement with the corresponding experimental data and the results of calculations performed by the different methods.

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WHY THE CHEMICAL ACTIVITY OF GRAPHENE CHANGES UNDER DEFORMATION: INSIGHT FROM QUANTUM CHEMISTRY

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Deformation of graphene is tightly connected with odd electron correlation since it concerns changing interatomic distances. Obviously, strengthening the electron correlation results in the growths of the number of effectively unpaired electrons N_D and, thus, increasing chemical reactivity. Stretching the bond from its equilibrium value of 1.326Å up to R_{crit}=1.395Å does not cause the appearance of the unpaired electrons. Above R_{crit} the number N_D gradually increases up to a clearly vivid knee that is characterized by $N_D \cong 2$ at R=1.76Å, that evidences a complete radicalization of two odd electrons. Further stretching concerns mainly two σ electrons that gradually become unpaired as well resulting in $N_D \cong 4$ at 2.5Å.

A similar stretching of C-C bonds can be highlighted when comparing the carbon skeletons of the pristine (5, 5) nanographene and those canopy-like and basket-like ones subjected to one-side hydrogen adsorption on either fixed or free standing membrane, respectively [1]. As a whole, changes in the C-C bond lengths result in increasing N_D from 31e to 46e and 54e, respectively. Both findings evidence an undoubted strengthening of the odd electron correlation caused by the chemically-stimulated deformation of the carbon skeleton.

Besides the static deformation discussed above, graphene can be dynamically deformed by the application of external stress. For this case, quantum molecular theory suggests the mechanochemical-reaction approach [2-4]. The relevant forces of response are calculated as the energy gradients along specifically introduced mechanochemical internal coordinates. When applied to the description of the deformation of both (5, 5) nanographene [2, 3] and (5, 5) nanographane [4] under uniaxial tension, the calculations highlighted a pronounced changing in the number of effectively unpaired electrons N_D of the sample in due course of its deformation thus revealing strengthening of its chemical reactivity.

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CHIRAL MODEL OF GRAPHENE

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The chiral model of graphene based on the SU(2) order parameter is suggested in the long-wave approximation, the ideal graphene plane being determined by the kink-like solution. Corrugation of the graphene surface is described in the form of ripple and rings. The approximate solution corresponding to an infinite carbon nanotube is found.

EFFECT OF CORRELATION AND RASHBA INTERACTION ON THE ENERGY LEVELS OF PARABOLICALLY CONFINED QUANTUM DOT

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We present a theoretical study of the ground state energy of a parabolically confined quantum dot in the presence of the Rashba spin-orbit interaction (SOI) and electron-electron interaction in an external magnetic field. With a simple and physically reasonable model potential for electron - electron interaction term, we have solved the problem exactly. Our results indicate that the presence of SOI reduces the total energy of the system quadratically. With increasing number of electrons in the system, the reduction in energy due to SOI becomes stronger. The effect of SOI becomes more significant at larger magnetic fields. Electron – electron interaction increases the total energy of the system. It increases quadratically with the number of electrons in the statem. Also electron – electron interaction energy increases linearly with an incease in external magnetic field. Our results are found to be in excellent agreement with exact numerical solutions reported in the literature.

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COMPUTATIONAL STRATEGY FOR GRAPHENE: INSIGHT FROM ODD ELECTRONS CORRELATION

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The correlation of odd electrons in graphene turns out to be significant so that the species should be attributed to correlated one. This finding profoundly influences the computational strategy addressing it to configurational-interaction computational schemes. Owing to serious problems related to the schemes realization in practice, a compromise can be suggested by using single-determinant approaches based on either Hartree-Fock or Density-Functional Theory in the form of unrestricted open-shell approximation. Both computational schemes enable to fix the electron correlation, while only the Hartree-Fock theory suggests a set of quantities to be calculated.

Four characteristic quantities that involve the energy misalignment, the number of effectively unpaired electrons, the squared spin value, and interatomic distance between the electrons have been suggested to classify the extent of the odd electron correlation. Basing on these criteria, graphene is significantly correlated. Within the Hartree-Fock approach, the finding provides a quantitative description of magnetic, chemical, and mechanical properties of the species [1, 2]. The magnetic constant J is directly connected with the correlation extent. Chemical properties are governed by the correlated-electron algorithm that allows for performing stepwise computational addition of any addend to the graphene body. The electron correlation is highly sensitive to the graphene deformation since the interatomic spacing is the main regulator of the former. Both static and dynamic deformation is considered in the paper. In view of these findings, a correlated-electron explanation of peculiarities related the density images of the graphene bubbles found on different substrates has been suggested that looks more natural than that one proposed from the position of an artificial 'gigantic pseudo-magnetic field'.

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EFFECTIVE MODULI OF MWCNT AND CARBON NANOFIBERS BASED ON GRAPHENES: CONTINUUM APPROACH

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Carbon nanofibers based on graphenes (CNFG) and MWCNT have cylindrical high-anisotropy structure. The structure results in similar anisotropy of their mechanical and thermal properties [1, 2]. The stress distributions in the CNFG and MWCNT are inhomogeneous under longitudinal compression and extension. So one have to evaluate effective elastic moduli of a single MWCNT or a single CNFG from experimental results. These moduli do not coincide generally with elastic moduli of folded graphene sheets from which nanotubes and nanofibers are made.

The effective elastic modulus E_f and the effective Poisson ratio ν_f are derived in terms of continuum mechanics and elasticity for cylindrically anisotropic bodies [3]:

$$E_f = E_z\left(1 + h\frac{k-1}{k+1}\left(\nu_{z\theta} - \nu_{zr}\right)\right)$$

$$\nu_f = \nu_{zr} + \frac{h(k-1)}{k}\left(\frac{E_z}{E_r} - \nu_{zr}^{\,2}\right).$$

The effective modulus and Poisson ratio are used in estimating the G peak strain sensitivity for MWCNT and CNFG, and to study splitting of the peak [4]. The values of the sensitivity are in good agreement with those obtained elsewhere [1,4].

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MOMENTUM AND SPIN DYNAMICS OF DIRAC PARTICLES AT EFFECTIVE DIMENSIONAL REDUCTION

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We consider an example of an effective dimensional reduction for a Dirac particle in a curved spacetime and use it for investigation of general properties of Dirac particles in effective two-dimensional spaces. The reduction is just effective because the particle remains in the three-dimensional space while one of its dimensions is compactified. This is assumed to be a model for the generic low-dimensional structures. We perform the Foldy-Wouthuysen transformation of the covariant Dirac equation for three spatial dimensions and determine general properties of momentum and spin dynamics at the above reduction. We use the specific metric admitting such a reduction [1]:

$$ds^2 = dt^2 - [\rho_1(z)]^2 d\Phi_1^2 - [\rho_2(z)]^2 d\Phi_2^2 - [\rho_3(z)]^2 dz^2 \qquad (1)$$

where $\rho_3(z)^2 = 1 + [\rho_1'(z)]^2 + [\rho_2'(z)]^2$, the primes define derivatives with respect to z, and all the functions on z are arbitrary. We derive the corresponding relativistic Foldy-Wouthuysen Hamiltonian and equations of motion. We formulate general conditions and find general properties of the effective dimensional reduction. When the above conditions are satisfied, the semiclassical equation of spin motion is given by

$$\frac{ds}{dt} = \Omega \times s\,, \quad \Omega = \frac{\rho_2' p_2}{\rho_2^2 \rho_3 E} e_1\,. \qquad (2)$$

Here $p_2(z)$ is the component of the generalized momentum and E is the total particle energy. For a particle in a curved spacetime, the axis of spin quantization coincides with the axis corresponding to the compactified dimension. However, the direction of this axis can be changed by an additional electromagnetic interaction. The semi-classical and classical limits are studied. The work is supported by the Belarusian Republican Foundation for Fundamental Research(Grant No.Ф10D-001).

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MODELING DEFECTS IN GRAPHENE AND NANOGRAFENE

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The ideal structure of graphene is a two-dimensional hexagonal lattice. The presence of defects in graphene leads to a disruption of this structure and to changes in physico-chemical properties of graphene.

Using Metropolis Monte Carlo method, the formation of point defects and stable configurations of graphene and nanographene (which has a small finite size with free boundary atoms) have been studied. The interatomic interactions have been described by the Brenner's reactive empirical bond order potential which was parametrized specifically for carbon and hydrocarbon systems. [1].

Nanographene has been modeled by 112 carbon atoms arranged in a flat plane and in the appropriate configuration for graphene with a lattice constant of 2.46 Å. To simulate a graphene the periodic conditions were superimposed on the boundary atoms of nanographene along its plane. The presence of defects has been modeled as point vacancies and their different combinations in the lattice. We studied their effects on changes in the lattice structure and binding (cohesive) energy of atoms. In particular, it was found that point defects results in decreasing the cohesive energy of studied systems. A number of possible defect patterns and stable configurations of graphene and nanographene are presented and discussed.

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