Electron properties of chiral carbon nanotubes

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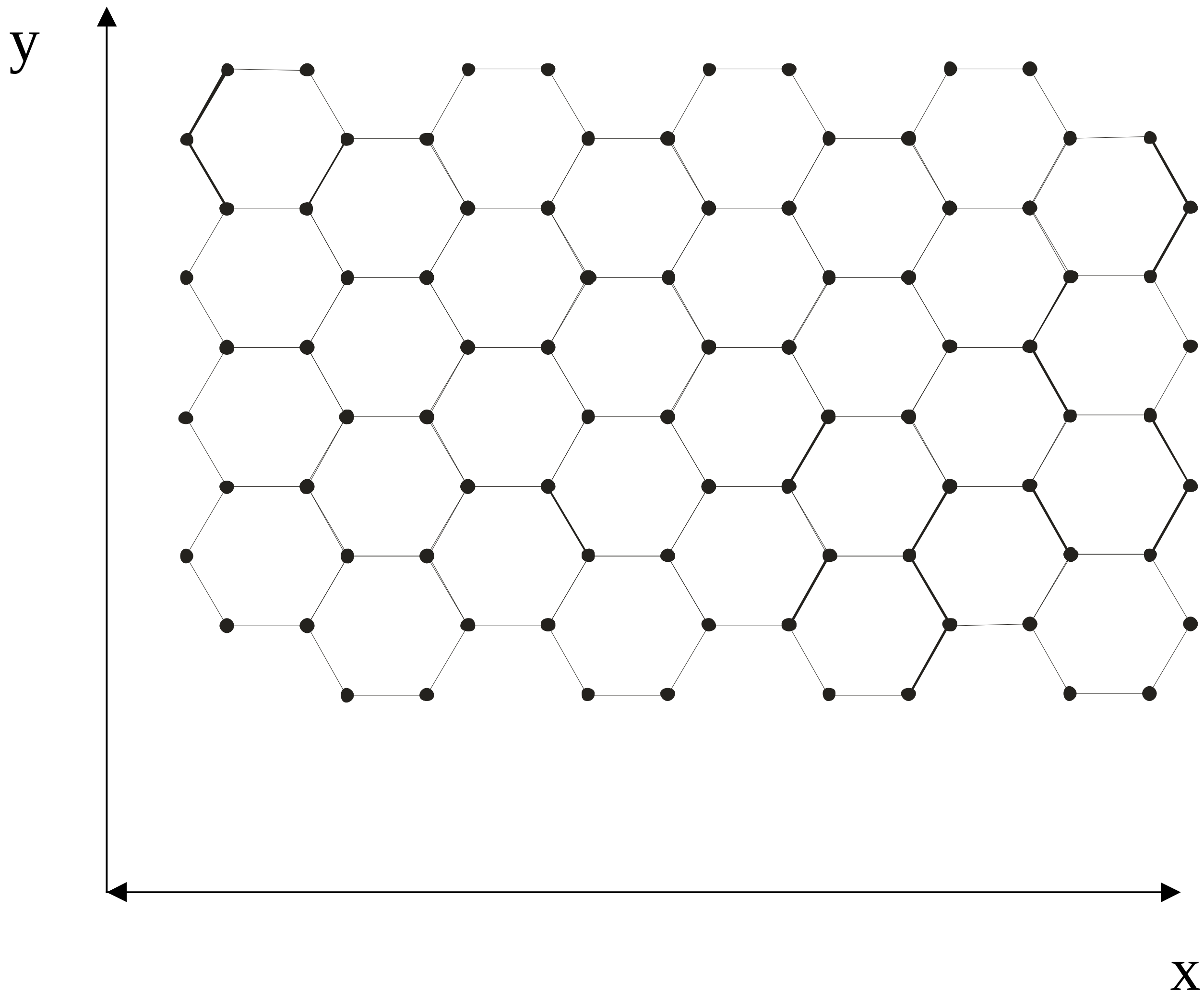
Carbon nanotubes were discovered experimentally by S. Iijima in 1991

[S. Iijima, Nature (London) **354**, 56 (1991)]

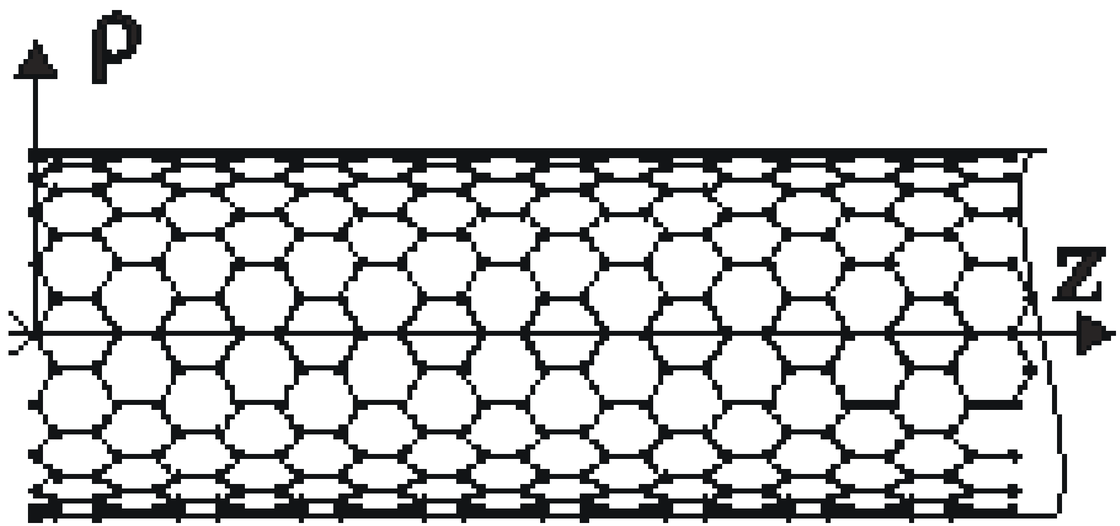
The most important and general results concerning studies of carbon nanotubes are collected in the book

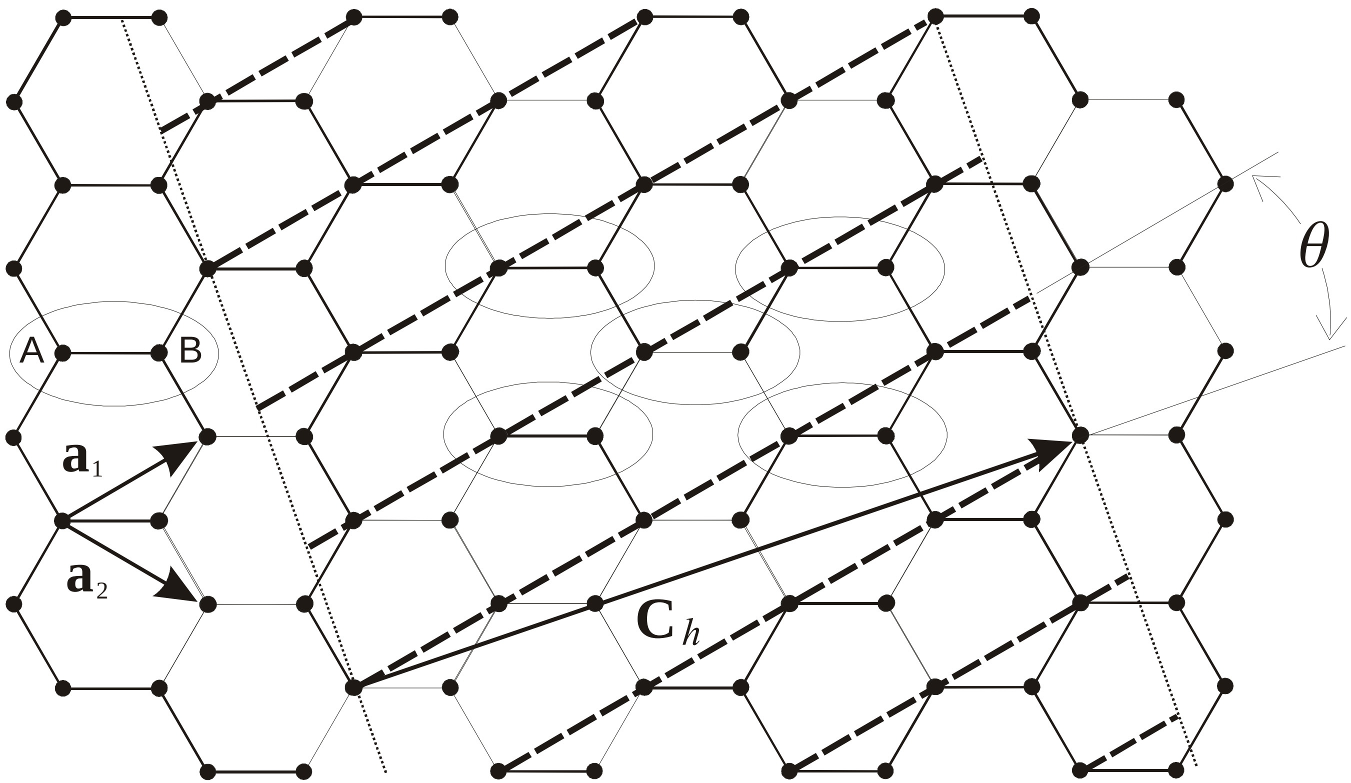
R. Saito, G. Dresselhaus, M. Dresselhaus
"Physical Properties of Carbon Nanotubes"
Imperial College Press, London
(first published 1998; reprinted 1999, 2001, 2002, 2003)

A single graphite sheet



A carbon nanotube





The unrolled graphite sheet. By connecting the head and tail of the chiral vector $\mathbf{C}_h = n\mathbf{a}_1 + m\mathbf{a}_2$ we can construct the nanotube having any crystal structure and commonly describing by two integers *(n,m)*. On the picture, for example, a rolling of (4,1) carbon nanotube is shown. The dashed lines will then form a helix line on the nanotube wall. The θ is a chiral angle describing the value of chirality.

Outline

1. Electron properties of chiral nanotubes in a magnetic field

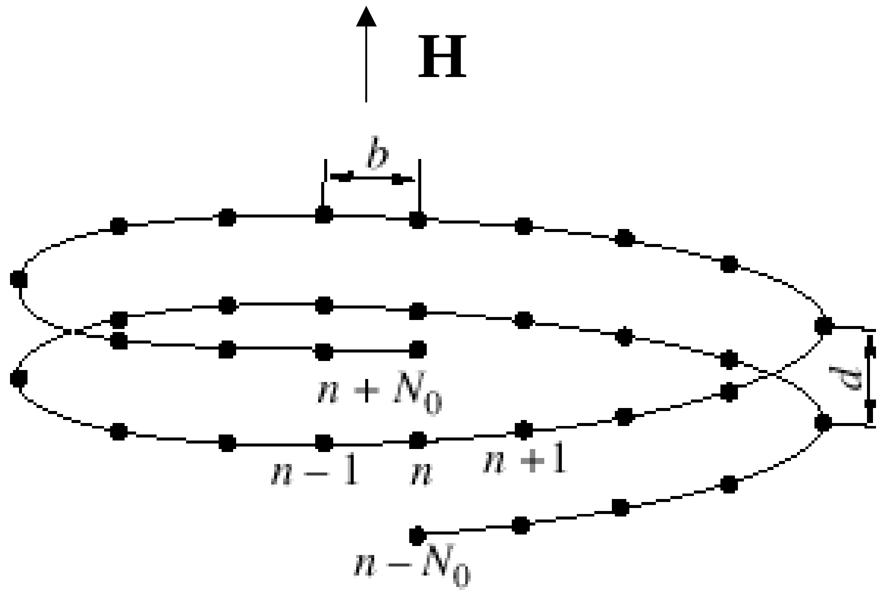
2. Electron properties of chiral nanotubes in an electric field

3. Features of electron-photon interaction in chiral nanotubes

4. Features of electron-electron interaction in chiral one-dimensional structures

5. Conclusion

1. Electron properties of chiral nanotubes in a magnetic field



Fragment of the nanotube composed of atoms arranged along a helical line (schematic).

The Hamiltonian in the tight-binding approximation

$$\hat{\mathscr{H}} = \sum_n (|n\rangle\langle n|\mathscr{H}|n\rangle\langle n| + |n\rangle\langle n|\mathscr{H}|n+1\rangle\langle n+1|$$
$$+ |n\rangle\langle n|\mathscr{H}|n-1\rangle\langle n-1| + |n\rangle\langle n|\mathscr{H}|n+N_0\rangle$$
$$\times \langle n+N_0| + |n\rangle\langle n|\mathscr{H}|n-N_0\rangle\langle n-N_0|)$$

$$\hat{\mathcal{H}} = \sum_n (|n\rangle\langle n|\mathcal{H}|n\rangle\langle n| + |n\rangle\langle n|\mathcal{H}|n+1\rangle\langle n+1|$$
$$+ |n\rangle\langle n|\mathcal{H}|n-1\rangle\langle n-1| + |n\rangle\langle n|\mathcal{H}|n+N_0\rangle$$
$$\times \langle n+N_0| + |n\rangle\langle n|\mathcal{H}|n-N_0\rangle\langle n-N_0|),$$

$$\langle n|\mathcal{H}|n\pm 1\rangle = -A(\quad b \quad)\exp(i\varphi_{n\pm 1}),$$
$$\langle n|\mathcal{H}|n\pm N_0\rangle = -A(\quad d \quad)\exp(i\varphi_{n\pm N_0}).$$

$$\varphi_{n\pm N_0} = 0,$$
$$\varphi_{n\pm 1} = \pm 2\pi\frac{\nu(H)}{N_0},$$

where

$$\nu(H) = \frac{\pi D^2 eH}{4ch}$$

is the number of quanta hc/e in the magnetic flux through the nanotube cross section.

The electron energy spectrum

$$\varepsilon(k) = \varepsilon_0 - 2A(b)\cos\left(kb + 2\pi\frac{\nu(H)}{N_0}\right)$$

$$-2A(d)\cos(N_0 kb).$$

oscillates for change of the magnetic field *H* with period $\Delta\nu(H) = N_0$

[D. A. Romanov and O. V. Kibis, Phys. Lett. A **178**, 335 (1993)]

Oscillations of conductivity with an unusual period were observed in

A. Bachtold, C. Strunk, J.-P. Salvetat, J.-M. Bonard, L. Forro, T. Nussbaumer, C. Schönenberger, Nature 397 (1999) 673.

This period is differ from period of AAS conductivity oscillations $\Delta\nu(H) = 1/2$ caused by weak localization processes

The electron energy spectrum

$$\varepsilon(k) = \varepsilon_0 - 2A(b)\cos\left(kb + 2\pi\frac{\nu(H)}{N_0}\right)$$

$$- 2A(d)\cos(N_0 kb).$$

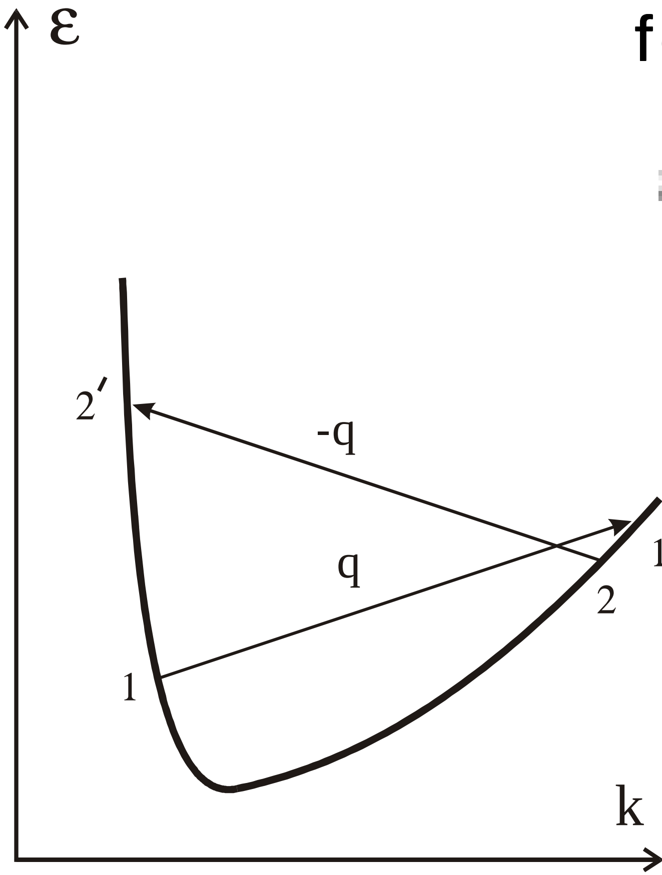
has the asymmetry

$$\varepsilon(\mathbf{k}) \neq \varepsilon(-\mathbf{k})$$

for

$$\frac{\nu(H)}{N_0} \neq z \quad (z = 0, 1, 2, 3, \ldots)$$

Effect of asymmetrical electron-phonon interaction for dispersion



$$\varepsilon(\mathbf{k}) \neq \varepsilon(-\mathbf{k})$$

Matrix elements of electron-phonon interaction potential *V*

$$\left|\left\langle \Psi_{1'} \left| \hat{V}_q \right| \Psi_1 \right\rangle\right| \neq \left|\left\langle \Psi_{2'} \left| \hat{V}_{-q} \right| \Psi_2 \right\rangle\right|$$

[O. V. Kibis, Phys. Lett. A **237**, 292 (1998)]

The asymmetrical electron-phonon interaction leads to the electromotive force of phonon drag

$$\mathcal{E} = \frac{\hbar L}{n_L e} \sum_{q_l} q_l [w_e(q_l) - w_a(q_l)]$$

L is the length of the helix, *n* is the electron density per unit length,
q is the phonon wave vector, w_e and w_a are probabilities of phonon emission and phonon absorption, respectively

The emf of phonon drag appears for a homogeneous heating of electron system

$$\mathcal{E} \propto T_e - T$$

T_e is the electron temperature, T is the phonon temperature

[O. V. Kibis, Phys. Lett. A **244**, 432 (1998)]

The electron system is heated by electric current J :

$$T_e - T \propto J^2 \quad \text{and} \quad \mathcal{E} = \alpha(H)J^2$$

Current-voltage characteristic is

$$U(J) = JR + \alpha(H)J^2$$

and the rectification effect appears

[O. V. Kibis, Phys. Sol. State **43**, 2336 (2001)]
[E. L. Ivchenko and B. Spivak, Phys. Rev. B **66**, 155404 (2002)]

Magneto-chiral anisotropy in charge transport through single-walled carbon nanotubes

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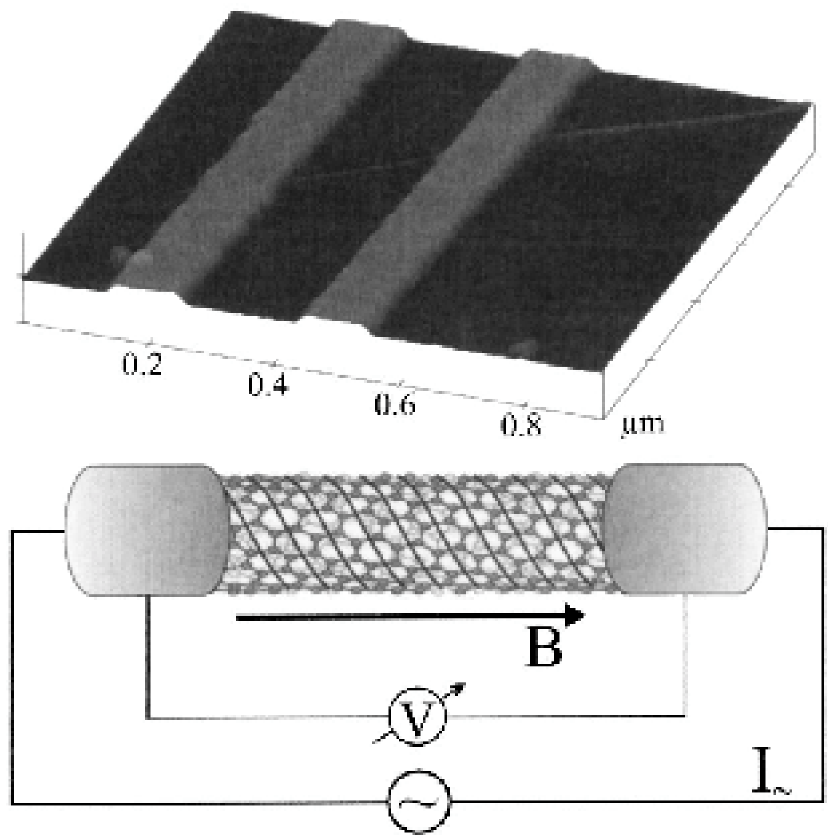
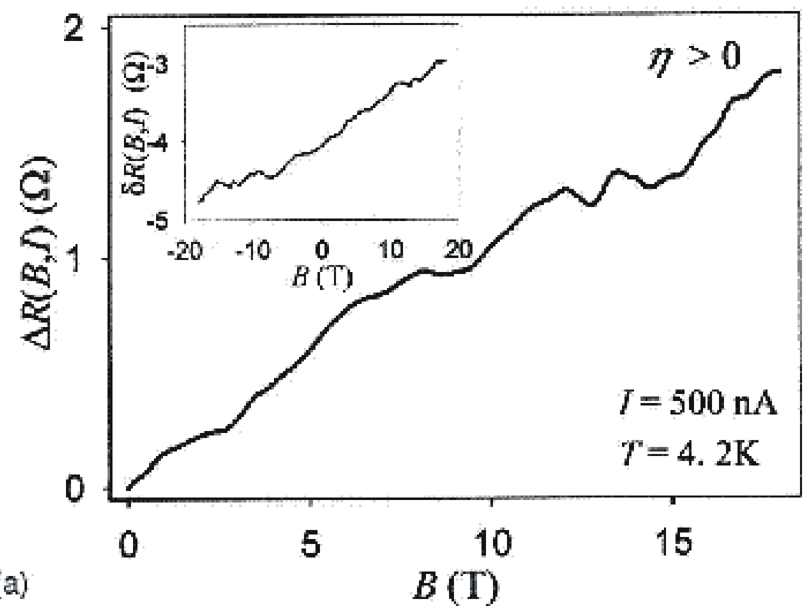
Carbon nanotubes are chiral molecular objects and therefore exist in two forms that are each other's mirror image. Many aspects of these fascinating new materials have recently been explored but their chirality has hardly been addressed. We have investigated the charge transport through individual single-walled carbon nanotubes in the presence of a magnetic field parallel to the tube axis. For most of the investigated tubes, a dependence of the resistance that is odd in both the magnetic field and in the current through the tube is observed. This effect is ascribed to the chirality of the nanotube and is called electrical magneto-chiral anisotropy. © *2002 American Institute of Physics.*
[DOI: 10.1063/1.1523895]

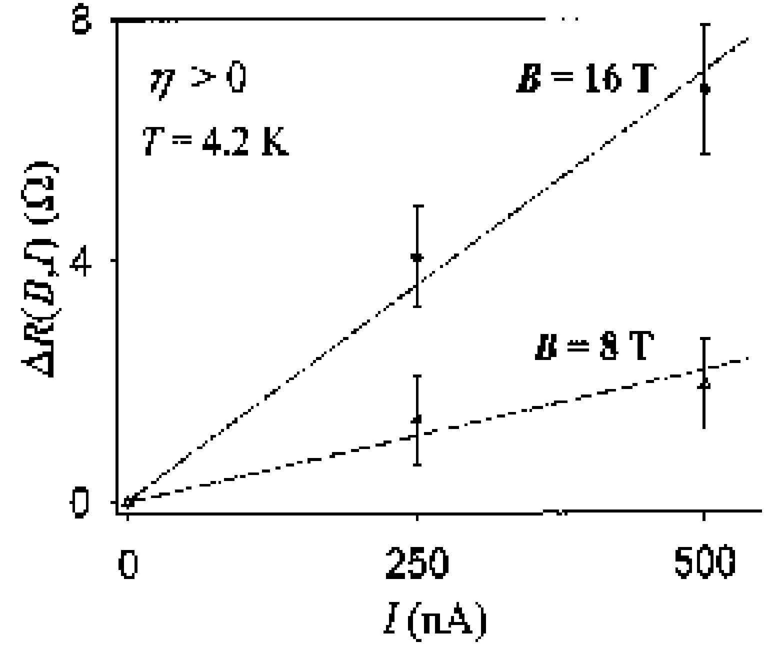
Experimental setup for studies of electron properties of carbon nanotubes in a magnetic field



J. Chem. Phys., Vol. 117, No. 24



(a)

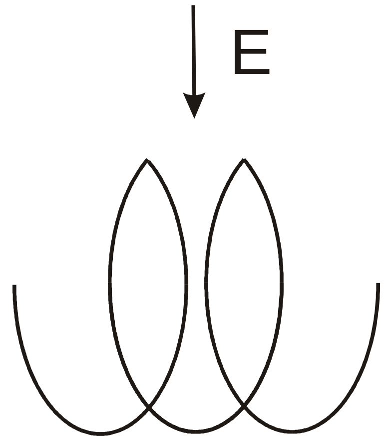


« For carbon nanotubes the odd power dependence on the magnetic field and the current was discovered in the theoretical works of Spivak *et al.*[17] and Kibis.[16] »

[V. Krstic, et al. J.Chem. Phys. 117, 11315 (2002)]

2. Electron properties of chiral nanotubes in an electric field

Helical one-dimensional conductor in a transverse electric field

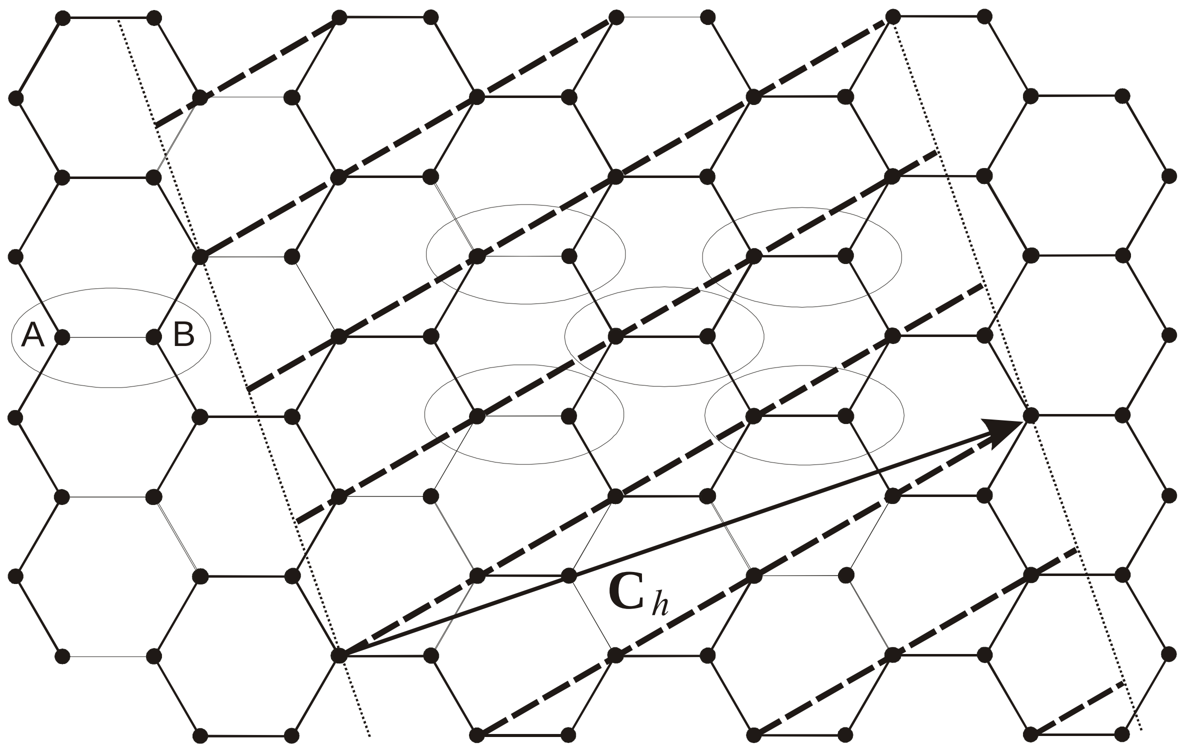


The potential electron energy along the helix

$$U(r) = qR\cos\left(\frac{2\pi r}{l}\right)$$

r is a coordinate along the helix line
l is the length of a single coil of the helix line
R is the radius of the helix

The helical one-dimensional electron motion takes place also in (n,1) carbon nanotubes:



The unrolled graphite sheet. By connecting the head and tail of the chiral vector we construct the nanotube having the crystal structure *(4,1)* . The dashed lines will then form a helix line on the nanotube wall.

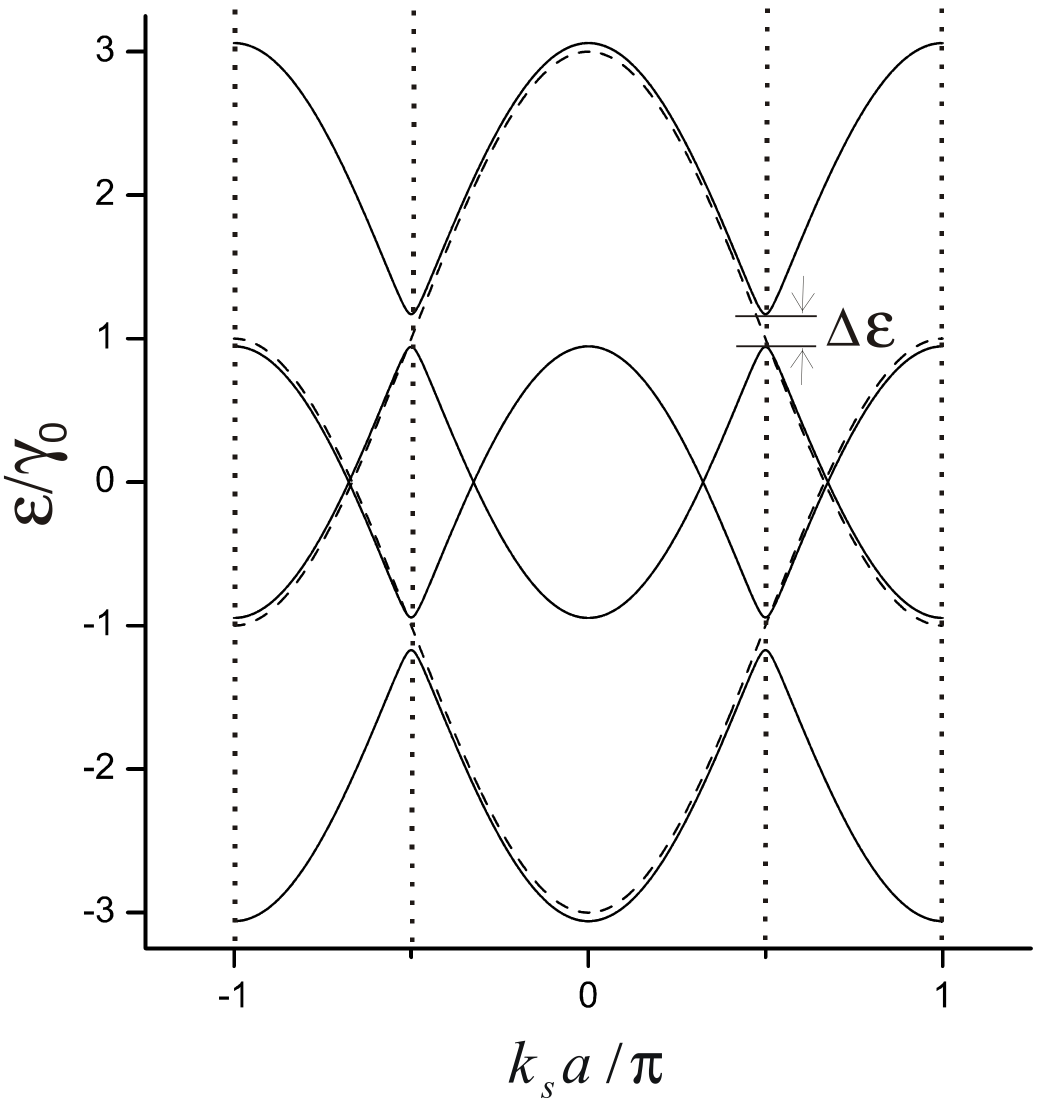
The electron energy in *(n,1)* carbon nanotubes depends only on the electron wave vector k_s along the helix line:

$$\varepsilon_j(k_s) = (-1)^j \gamma_0 \left[1 + 8\cos\left(\frac{n+1}{2}k_s a\right)\cos\left(\frac{nk_s a}{2}\right)\cos\left(\frac{k_s a}{2}\right)\right]^{1/2}$$

a is inter-atomic distance in the nanotube;

γ_0 is the overlap integral for electron wave functions between nearest atoms;

$j=1,2$ label valence and conduction bands



The Bragg gap opened by the electric field E

$$\Delta\varepsilon = \frac{\sqrt{3}Ea}{4\pi}$$

[O. V. Kibis, D. G. W. Parfitt, and M. E. Portnoi, *in press*]

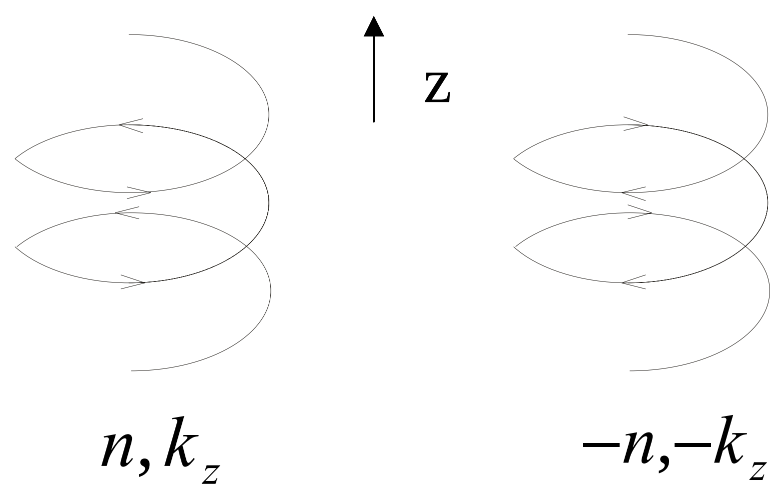
Electron energy spectrum of a *(1,1)* carbon nanotube in the presence of a transverse electric field (solid lines) and without the electric field (dashed lines).

3. Features of electron-photon interaction in chiral nanotubes

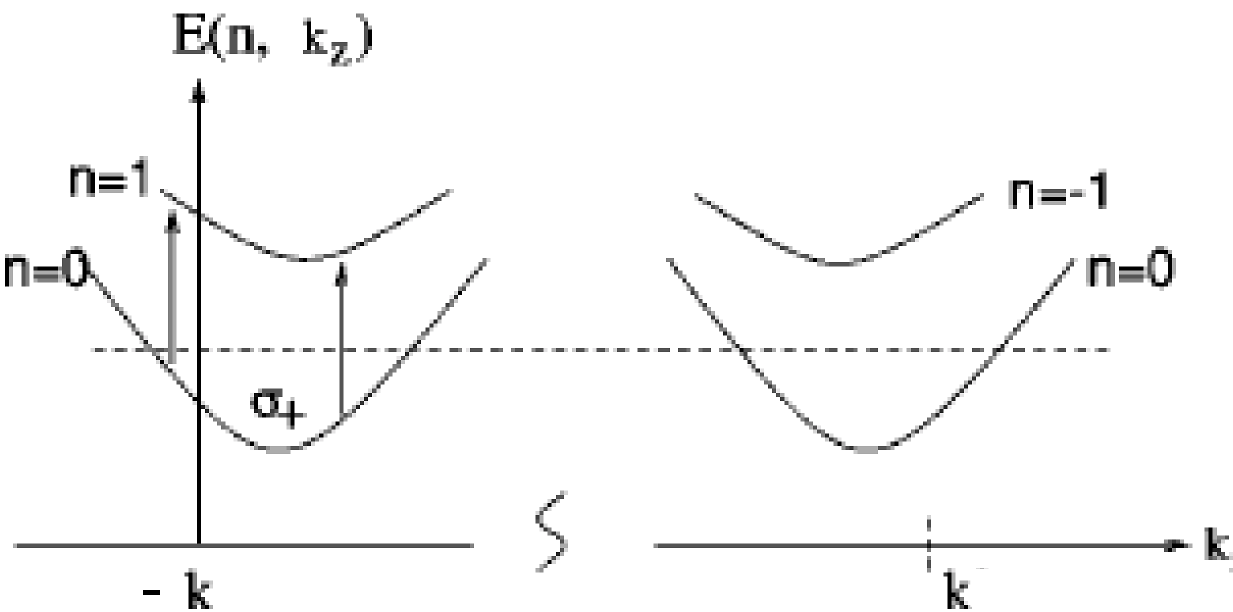
The helicoidal crystal structure of chiral carbon nanotubes results in the symmetry of electron energy spectrum

$$\varepsilon(n, k_z) = \varepsilon(-n, -k_z)$$

(n is the electron angular momentum along the nanotube axis, k_z is the electron wave vector along the nanotube axis)



Absorption of circularly polarized photons with angular momentum +1

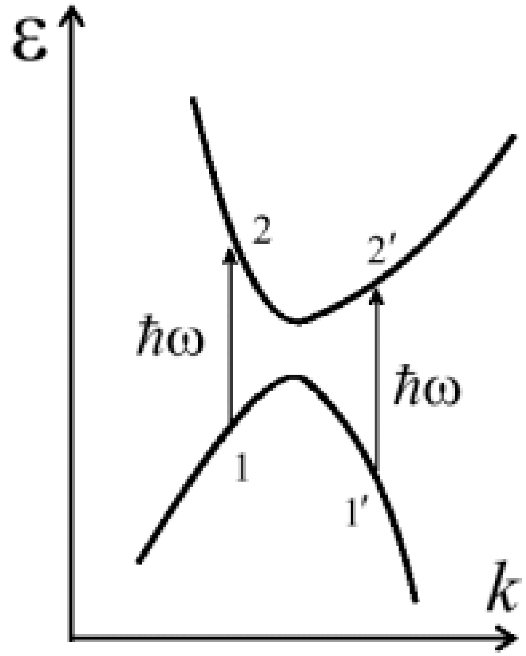


The scheme of direct inter-subband optical transitions between bands with $n=0$ and $n=1$. The dashed line corresponds to the level of the chemical potential in the conduction band.

Due to the asymmetrical distribution of photoexiting electrons in *k*-space, their summary velocity $\sum_i v_i \neq 0$ and photovoltaic effect appears

[O. V. Kibis and D. A. Romanov, Phys. Sol. State **37**, 69 (1995)]
[E. L. Ivchenko and B. Spivak, Phys. Rev. B **66**, 155404 (2002)]

Absorption of linearly polarized photons in a magnetic field



$$\varepsilon(\mathbf{k}) \neq \varepsilon(-\mathbf{k})$$

A structure of intersubband electron-photon transitions for chiral carbon nanotube having asymmetrical electron energy spectrum in the presence of photons with the energy $\hbar\omega$.

Due to the electron energy spectrum asymmetry the electron velocity along the nanotube axis

$$v(k) = \frac{1}{\hbar}\frac{d\varepsilon(k)}{dk}$$

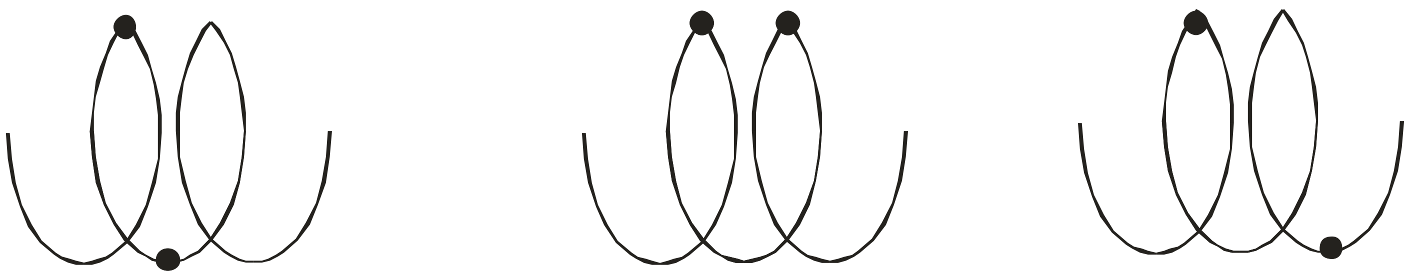
is also asymmetrical. Because of it the electrical current of photoexciting electrons along the nanotube axis

$$j \propto \sum_i v_i \neq 0$$

[O. V. Kibis, Physica E **12**, 741 (2002)], [E. L. Ivchenko and B. Spivak, Phys. Rev. B **66**, 155404 (2002)]

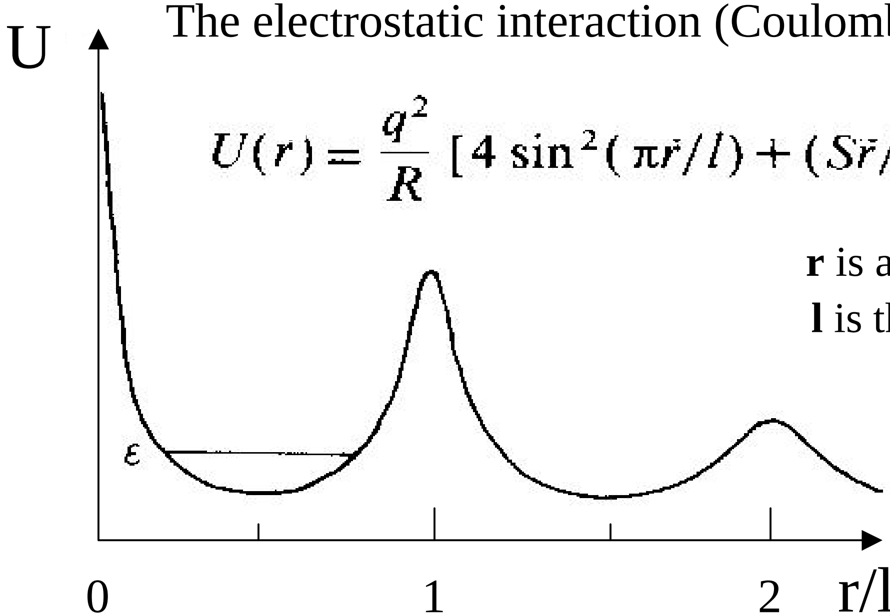
4. Features of electron-electron interaction in chiral one-dimensional structures

Two interacting electrons on a helix



The electrostatic interaction (Coulomb) potential $U = q^2 / r_0$

$$U(r) = \frac{q^2}{R}\left[4\sin^2(\pi r/l) + (Sr/Rl)^2\right]^{-1/2}$$



The electrostatic interaction potential.

r is a distance between two electrons along the helix line

l is the length of a single coil of the helix line

r_0 is a direct distance between two electrons

R is the radius of the helix

S is the pitch of the helix

The energy of ground bi-electron state is approximatelly

$$\varepsilon = q^2/2R + \tfrac{1}{2}\hbar\omega\,, \quad \omega = q/2(mR^3)^{1/2}$$

The life time of the electron pair is $\tau > \dfrac{4\hbar R}{q^2\pi}\exp[q\pi^2(Rm)^{1/2}/2\hbar]$

For $R \sim 100\,\mathring{A}$ we have a macroscopic life time $\tau \sim 10^{15}\,s$

Usual Coulomb interaction in a helical one-dimensional conductor leads to appearance of long lived electron pairs

[O. V. Kibis, Phys. Lett. A **166**, 393 (1992)]

Conclusions

The main consequences of chiral crystal structure for carbon nanotubes:

1. Conductivity oscillations in a magnetic field. The effect depends on chirality.

2. The asymmetrical electron energy spectrum results in rectification of electric current in a magnetic field.

3. Superlattice-like behavior of chiral nanotubes in a transverse electric field.

4. The photovoltaic effect.

5. The possibility of electron pairing due to the Coulomb electron interaction.