Abstract for ISSP Summer School 2003 by T. Nakanishi (http://staff.aist.go.jp/t.nakanishi/index-e.html)

Electrical Conduction in Carbon Nanotubes

Takeshi Nakanishi

AIST, 1 Umezono, Tsukuba 305-8562, Japan

Carbon nanotubes (CNs) are new kinds of quantum wires topologically different from conventional wires fabricated at semiconductor heterostructures. Further, electronic states in the vicinity of the Fermi level are quite different from those of free electrons. In this talk a brief review is given of transport properties of CNs mainly from a theoretical point of view. The topics include an effective-mass description of electronic states, the absence of backward scattering except for scatterers with a potential range smaller than the lattice constant, a conductance quantization in the presence of lattice vacancies, and effects of topological defects.

In a two-dimensional graphite, a unit cell contains two carbon atoms denoted as A and B and two bands having approximately a linear dispersion cross the Fermi level at K and K' points of the first Brillouin Zone. Therefore, electronic states in the vicinity of the Fermi level are described by a four-component envelope function $\mathbf{F}(\mathbf{r})$. In the absence of an impurity, it satisfies Weyl's equation for neutrinos:[1]

$$\mathcal{H}_{0}\mathbf{F} = \varepsilon \mathbf{F}, \quad \mathcal{H}_{0} = \gamma \begin{pmatrix} 0 & k_{x} - ik_{y} & 0 & 0 \\ \hat{k}_{x} + i\hat{k}_{y} & 0 & 0 & 0 \\ 0 & 0 & 0 & \hat{k}_{x} + i\hat{k}_{y} \\ 0 & 0 & \hat{k}_{x} - i\hat{k}_{y} & 0 \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} F_{A}^{K} \\ F_{B}^{K} \\ F_{A}^{K'} \\ F_{B}^{K'} \end{pmatrix}$$

where γ is a band parameter, $\hat{\mathbf{k}} = (\hat{k}_x, \hat{k}_y)$ a wave-vector operators, F_A^K and F_B^K are the envelope functions at A and B site related to the K point, $F_A^{K'}$ and $F_B^{K'}$ are those for the K' point, the x axis is chosen in the circumference or chiral vector \mathbf{L} , and y in the axis direction.

An effective potential of an impurity is derived from a tight-binding model. When the potential range is smaller than the lattice constant, it has an off-diagonal matrix element between K and K' points comparable to the diagonal element. With the increase of the range, this off-diagonal element decreases rapidly and the diagonal element corresponding to neighboring A and B sites becomes identical. The crossover between these two regimes occurs around the range smaller than the lattice constant.



Fig. (a) Lattice structure of two-dimensional graphite sheet. η is the chiral angle. The coordinates are chosen in such a way that x is along the circumference of a nanotube and y is along the axis. (b) The first Brillouin zone and K and K' points. (c) The coordinates for a nanotube.

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When intervalley terms can be neglected and the diagonal effective potential is identical for A and B sites, the back scattering between states with +k and -k vanishes identically for the bands crossing the Fermi level in the absence of a magnetic field [2]. This leads to an extremely large conductivity or mean free path. The absence of the back scattering disappears in magnetic fields, giving rise to a huge positive magnetoresistance.

It has been proved that the Born series for back-scattering vanish identically [2]. This has been shown to be ascribed to Berry's phase which corresponds to a sign change of the wave function under a spin rotation of a neutrino-like particle in a two-dimensional graphite [3].

Effects of scattering by a vacancy in CNs have been studied [4]. A model potential used in the calculation is huge potentials on the vacancy, which is corresponding to the short-range potential. The conductance G at $\epsilon = 0$ is quantized and depends on the difference between numbers of removed site on each sublattice but independents of shape of the vacancy. For the fundamental examples, when a single carbon site (site A), two carbon sites in the nearest neighbor, and site A and three sites around it are removed, we have $G = e^2/\pi\hbar$, $2e^2/\pi\hbar$, and 0, respectively. In the presence of a magnetic field perpendicular to the tube axis, the conductance depends only on the field component in the direction of the vacancy.

A characteristic scatterer of CNs is a topological disorder, which is easily found in CN's but not in the conventional quantum wire of semiconductors. The observation of CN junctions consisting of CN's with different diameter has been reported. An essential feature of the structure is the topological disorder containing a pair of pentagonal and heptagonal ring defects in the otherwise hexagonal network. A universal power-law dependence on the ratio of their circumferences has been shown in the conductance [5].

In the presence of a magnetic field perpendicular to the tube axis, the amplitude of the electron wave function is localized around a certain position of CN determined by the field direction [1]. This enables a variation of the probability density at the position of the pentagonal and heptagonal ring.

Explicit conductance calculations are performed for junctions of two armchair nanotubes known to be always metallic [6]. The dependence on direction of the magnetic field shows in general that the conductance increases with the decreasing of the amplitude of the wavefunction on the pentagonal and heptagonal ring. Only exception is the case that the field is parallel to the pentagonal and heptagonal ring. In fact, the conductance is independent of the magnetic field in this case and surprisingly, the conductance depends only on the magnetic field component perpendicular to the pentagonal and heptagonal ring.

The author acknowledges the collaboration with T. Ando, M. Igami, and R. Saito.

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