Quantum Anomalies in Carbon Nanotubes

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A brief review is given on electronic and transport properties of carbon nanotubes mainly from a theoretical point of view. The topics include also a description of electronic states in a tight-binding model and in an effective-mass or $k \cdot p$ scheme. Transport properties are discussed including absence of backward scattering except for scatterers with a potential range smaller than the lattice constant, its extension to multi-bands cases, long-wavelength phonons and electron-phonon scattering, effects of lattice vacancies, and junctions together with topological defects.

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1. Introduction

Graphite needles called carbon nanotubes (CNs) have been a subject of an extensive study since discovery in 1991 [1,2]. A multi-wall CN is a few concentric tubes of two-dimensional (2D) graphite consisting of carbon atom hexagons arranged in a helical fashion about the axis. The diameter is usually between 20 and 300 Å and their length can exceed 1 µm. The distance of adjacent sheets or walls is larger than the distance between nearest neighbor atoms in a graphite sheet and therefore their electronic properties are dominated by those of a single layer CN. Single-wall nanotubes were produced in a form of ropes a few years later [3,4]. The purpose of this paper is to give a brief review of recent theoretical study on electronic and transport properties of carbon nanotubes.

Carbon nanotubes can be either a metal or semiconductor, depending on their diameters and helical arrangement. The condition can be obtained based on the band structure of a 2D graphite sheet and periodic boundary conditions along the circumference direction. It was first predicted by means of a tight-binding model ignoring effects of the tube curvature [5-14]. It is well reproduced in a $k \cdot p$ method or an effective-mass approximation [15]. The theoretical predictions have been confirmed by Raman experiments [16] and direct measurements of local density of states by scanning tunneling spectroscopy [17-19].

The $k \cdot p$ scheme has been used successfully in the study of wide varieties of electronic properties. Some of such examples are magnetic properties including the AB effect on the band gap [20], optical absorption spectra [21], exciton effects [22], lattice instabilities in the absence [23,24] and presence of a magnetic field [25], magnetic properties of ensembles of nanotubes [26], effects of spin-orbit interaction [27], junctions [28], vacancies [29], topological defects [30], and properties of nanotube caps [31].

Transport properties of CNs are interesting because of their unique topological structure. There have been reports on experimental study of transport in CN bundles [32] and ropes [33,34]. Transport measurements became possible for a single multi-wall nanotube [35-39] and a single single-wall nanotube [40-44]. Single-wall nanotubes usually exhibit large charging effects presumably due to nonideal contacts [45-49]. Almost ideal contacts were realized also [50].

In this paper we shall mainly discuss electronic states and transport properties of nanotubes obtained theoretically in the $k \cdot p$ method combined with a tight-binding model. It is worth mentioning that several papers giving general reviews of electronic properties of nanotubes were published already [51-56].

In section 2 electronic states in two-dimensional graphite are discussed in a nearest-neighbor tight-binding model and in the effective-mass scheme, and the presence of a topological anomaly is demonstrated. In section 3 electronic states in nanotubes are discussed. In section 4 the absence of backscattering in the presence of scatterers is discussed and the discussion is extended toward the presence of perfectly conducting channel when several bands coexist at the Fermi level. In section 5 a continuum model for phonons in the long-wavelength limit is introduced and effective Hamiltonian describing electron-phonon interaction is derived. In sections 6 and 7, a brief discussion is made on effects of lattice vacancies and the transport across junctions with topological defects, respectively. A short summary is given in section 8.

2. Two Dimensional Graphite and Neutrino

The structure of 2D graphite sheet is shown in Fig. 1. A unit cell contains two carbon atoms which are denoted by A and B. We have the primitive translation vectors $a = a(1,0)$ and $b = b(-(1/2), \sqrt{3}/2)$, and the vectors connecting between nearest neighbor carbon atoms $\overrightarrow{a} = a(0,1/\sqrt{3}), \overrightarrow{b} = b(-1/2, -1/2\sqrt{3})$, and $\overrightarrow{c} = a(1/2, -1/2\sqrt{3})$. The first Brillouin zone is given by a hexagon with two corner points K and K'. The corresponding wave vectors are given by $K = (2\pi/a)(1/3, 1/\sqrt{3})$ and $K' = (2\pi/a)(2/3, 0)$ for K and K' points, respective-
ly.

In a nearest-neighbor tight-binding model, the energy bands are given by

$$
\epsilon_{\pm}(\mathbf{k}) = \pm \gamma | \mathbf{k} | \exp \left[ \frac{i}{\hbar} \int_{0}^{l} \mathbf{F}(r) \cdot \mathbf{r} \right].
$$

The band structure is shown in Fig. 2. Near the K and K' point, we have $\epsilon_{\pm}(\mathbf{k}+\mathbf{K}) = \epsilon_{\pm}(\mathbf{k}+\mathbf{K}') = \pm \gamma \sqrt{k_x^2 + k_y^2}$ with $\gamma = \sqrt{3} \alpha \gamma_0 / 2$.

Essential and important features of electronic states become transparent when we use a $\mathbf{k} \cdot \mathbf{p}$ scheme in describing states in the vicinity of K and K' points. The effective-mass equation for the K point is given by

$$
\gamma (\mathbf{\sigma} \cdot \mathbf{k}) \mathbf{F}(r) = \epsilon \mathbf{F}(r), \quad \mathbf{F}(r) = \left( \mathbf{F}_A(r), \mathbf{F}_B(r) \right),
$$

where $\sigma = (\sigma_x, \sigma_y)$ is the Pauli spin matrix, $\gamma$ is a band parameter, $\mathbf{k} = -i \nabla$, and $\mathbf{F}_A$ and $\mathbf{F}_B$ represent the amplitude at two carbon sites A and B, respectively [15].

The above equation is same as Weyl's equation for a neutrino with vanishing rest mass and constant velocity independent of the wave vector. The energy becomes $\epsilon_{\pm}(\mathbf{k}) = \pm \gamma | \mathbf{k} |$ and the velocity is given by $| \mathbf{v} | = \gamma / \hbar$ independent of $\mathbf{k}$ and $\epsilon$. The density of states becomes $D(\epsilon) = \epsilon / 2 \pi \gamma^2$. Figure 3 shows the energy dispersion and the density of states.

An important feature is the presence of a topological singularity at $\mathbf{k} = 0$. A neutrino has a helicity and its spin is quantized into the direction of its motion. The spin eigen function changes its signature due to Berry's phase under a 2π rotation. Therefore the wave function acquires phase $-\pi$ when the wave vector $\mathbf{k}$ is rotated around the origin along a closed contour [57,58]. The signature change occurs only when the closed contour encircles the origin $\mathbf{k} = 0$ but not when the contour does not contain $\mathbf{k} = 0$. This topological singularity at $\mathbf{k} = 0$ causes a zero-mode anomaly in the conductivity [59,60].

A singularity at $\epsilon = 0$ manifests itself in magnetic fields even in classical mechanics. The equation of motion gives the cyclotron frequency $\omega_c = eBv^2 / \epsilon \hbar$, where $v$ is the electron velocity given by $| \mathbf{v} | = \gamma / \hbar$. The cyclotron frequency $\omega_c$ diverges and changes its signature at $\epsilon = 0$ [61]. In quantum mechanics $\hat{k}_x$ and $\hat{k}_y$ satisfy the commutation relation $[\hat{k}_x, \hat{k}_y] = -i / \hbar^2$, where $l$ is the magnetic length given by $\sqrt{ch / eB}$. Semiclassically, the Landau levels can be obtained as $\epsilon_n = \pm \sqrt{n + \frac{1}{2} (\sqrt{3} / \gamma)}$ with integer $n$ and an appropriate small correction $\delta$. Because of the uncertainty relation, $k^2 = 0$ is not allowed and there is no Landau level at $\epsilon = 0$. However, a full quantum mechanical treatment gives $\epsilon_n = \sqrt{|n|} \text{sgn}(n) \sqrt{\gamma^2 / 2}$, leading to the formation of Landau levels at $\epsilon = 0$.

We consider, for example, a system with scatterers with a potential range much smaller than the typical electron wavelength (which is actually infinite at $\epsilon = 0$) [62]. The relaxation time in the absence of a magnetic field becomes $\tau_0^{-1} = 2 \pi | \epsilon | W / \hbar$ with $W$ being a dimensionless parameter to characterize the scattering strength given by $W = n_i (\langle u_i \rangle^2 / 4) \pi^2$, where $u_i$ and $n_i$ are the strength and the concentration of scatterers, respectively, and $\langle \cdots \rangle$ means the average over impurities.

With the use of the Boltzmann transport equation, the transport relaxation time becomes $\tau(\epsilon) = 2 \pi n_0(\epsilon)$ and the conductivity $\sigma_0 = (e^2 / 2 \pi \hbar) W^{-1}$ independent of the Fermi level, i.e., nonzero even at $\epsilon = 0$ where the density of states vanishes.

In the presence of a magnetic field, the conductivity tensor $\sigma_{\mu\nu}$ with $\mu = x, y$ and $\nu = x, y$ is given by $\sigma_{xx} = \sigma_{yy} = \sigma_0 / (1 + (\omega \tau)^2)$ and $\sigma_{xy} = -\sigma_{yx} = -\sigma_0 \omega \tau / (1 + (\omega \tau)^2)$. Using the explicit expressions for $\omega_c$ and $\tau$, we have $\sigma_{xx} = \sigma_0 \epsilon^4 / (1 + \epsilon^4)$ and $\sigma_{xy} = -\sigma_0 \epsilon^2 / (1 + \epsilon^4)$, with $\epsilon = \sqrt{2} \pi \alpha l (\epsilon_F / e B)$, where $\epsilon_B$ is the magnetic energy defined by $\epsilon_B = \gamma / \hbar$. Because $\tau(\epsilon_F)^{-1} \propto | \epsilon_F |$, the dependence on the Fermi energy $\epsilon_F$ is fully scaled by $\epsilon_B$. Therefore, the conductivities exhibit a singular jump to zero at $\epsilon_F = 0$ from $\sigma_0$ for nonzero $\epsilon_F$ in the limit of the vanishing magnetic field $\epsilon_B \rightarrow 0$.

A singular behavior appears also in the dynamical conductivity [60]. In a relaxation-time approximation, the dynamical conductivity is calculated as

$$
\sigma(\omega) = \frac{e^2}{4 \hbar} \left( \frac{4}{\pi} \frac{\epsilon_F}{\hbar \omega + i [\hbar / \tau(\epsilon_F)]} + 1 \right)
+ \frac{1}{\pi} \ln \left( \frac{\hbar \omega + i [\hbar / \tau(\epsilon_F)]}{2 \epsilon_F} + 2 \epsilon_F \right).
$$

Because $\hbar / \tau(\epsilon) \propto | \epsilon |$, the frequency dependence is scaled by $\hbar \omega / \epsilon_F$. The scaling of the dynamical conductivity $\sigma(\hbar \omega / \epsilon_F)$ shows that $\sigma(\omega, \epsilon_F)$ exhibits a singular behavior at the point $(\omega, \epsilon_F) = (0, 0)$. The correct way is to let $\omega \rightarrow 0$ at each $\epsilon_F$, leading to a singular jump of the static conductivity to $e^2 / 8 \hbar$ at $\epsilon_F = 0$ from $\sigma_0$ for nonzero $\epsilon_F$.

A more refined treatment has been performed for the magnetoconductivity in a self-consistent Born approximation in which level-broadening effects are properly taken into account [59]. The result shows that the conductivity at $\epsilon_F = 0$ is given by $e^2 / \pi \hbar^2$, which is universal and independent of the scattering strength. The resulting conductivity varies smoothly across $\epsilon_F = 0$ but exhibits a sharp jump in the limit of weak scattering $(W \ll 1)$ from the Boltzmann result $\sigma_0$ for $\epsilon \neq 0$ down to $\sigma = e^2 / \pi \hbar^2$ at $\epsilon_F = 0$.

A similar calculation was performed quite recently for the dynamical conductivity [60]. Figure 4 shows an example of the results. The frequency dependence is scaled by $\hbar \omega / \epsilon_F$ as long as $\epsilon_F \neq 0$. When $\epsilon_F$ is very close to 0, however, the conductivity at $\omega = 0$ becomes small and the discrete jump present in the Boltzmann conductivity is removed. The energy scale causing this crossover behavior becomes smaller for weaker $W$ leading to a singular behavior of the dynamical conductivity in the weak scattering limit.

3. Carbon Nanotubes

Every structure of single tube CNTs can be constructed using the chiral vector $\mathbf{L} = n_1 a + n_2 b$ from a graphite sheet as shown in Fig. 1 (a). In another convention for the choice of primitive translation vectors, $\mathbf{L}$ is characterized by two integers $(n_1, n_1)$ with $n_1 = n_a - n_b$ and
$n_2 = n_b$ and the corresponding CN is often called an $(n_1, n_2)$ nanotube.

The wave function is written as a product of the neutrino wave function and the Bloch function at the K point in the k-p scheme. The Bloch function $\psi_K$ acquires a phase under translation, i.e., $\psi_K(r+L) = \psi_K(r) \exp(iK \cdot L)$. Therefore, the boundary conditions for the neutrino wave function becomes [15]

$$F(r+L) = F(r) \exp\left(-\frac{2\pi i \nu}{3}\right). \quad (3.1)$$

This corresponds to the presence of a fictitious Aharonov-Bohm (AB) magnetic flux along the axis determined by $L$. In the k-p scheme, therefore, electrons in a nanotube can be regarded as neutrinos on a cylinder surface with an AB flux.

The neutrino wave function is written as $F(r) \propto \exp[i\kappa_\nu(n)x + iky]$ with $\kappa_\nu(n) = (2\pi/L)(n - \nu/3)$, where the $x$ axis and $y$ axis are chosen in the circumference and axis direction, respectively, $n$ is an integer, and $k$ is the wave vector in the axis direction. The corresponding energy levels are

$$\epsilon^{(\pm)}(n, k) = \pm \gamma \sqrt{\kappa_\nu(n)^2 + k^2}, \quad (3.2)$$

where + and − stand for conduction and valence bands, respectively. Figure 5 shows a schematic illustration of the bands for $\nu = 0$ and +1. When $\nu = 0$, there are bands with a linear dispersion without a gap and CN becomes a metal, while when $\nu = \pm 1$, on the other hand, there is a nonzero gap and CN becomes a semiconductor. There is a one-to-one correspondence between the AB flux and the band gap. The effective-mass equation for the K’ point is obtained by replacing $\sigma_y$ by $-\sigma_y$ in Eq. (2.2) and the boundary conditions are obtained by the replacement $\nu$ by $-\nu$.

4. Absence of Backscattering

The topological singularity at $k = 0$ leads to the unique property of a metallic nanotube that there exists no backscattering and the tube is a perfect conductor even in the presence of scatterers [58,62]. In fact, it has been proved that the Born series for backscattering vanish identically [62]. Further, the conductance has been calculated exactly for finite-length nanotubes containing many impurities with the use of Landauer’s formula [63]. The absence of backward scattering has been confirmed by numerical calculations in a tight-binding model [64].

Backscattering corresponds to a rotation of the k direction by $\pm \pi$ (in general $(2n+1)\pi$ with integer $n$). In the absence of a magnetic field, there exists a time reversal process corresponding to each backscattering process. The time reversal process corresponds to a rotation of the k direction by $\pm \pi$ in the opposite direction. The scattering amplitudes of these two processes are same in the absolute value but have an opposite signature because of Berry’s phase. As a result, the backscattering amplitude cancels out completely. In semiconducting nanotubes, on the other hand, backscattering appears because the symmetry is destroyed by a nonzero AB magnetic flux.

An important information has been obtained on the mean free path in nanotubes by single-electron tunneling experiments [40,44]. The Coulomb oscillation in semiconducting nanotubes is quite irregular and can be explained only if nanotubes are divided into many separate spatial regions in contrast to that in metallic nanotubes [65]. This behavior is consistent with the presence of backscattering leading to a localization of the wave function. In metallic nanotubes, the wave function is extended in the whole nanotube because of the absence of backscattering. With the use of electrostatic force microscopy the voltage drop in a metallic nanotube has been shown to be negligible [66].

In a one-dimensional metal with linear bands, the Coulomb interactions are known to induce a breakdown of the Fermi liquid theory by causing strong perturbations. The resulting system is known as a Tomonaga-Luttinger liquid, which is predicted to show non-Fermi-liquid behavior such as the absence of Landau quasi-particles, spin-charge separation, suppression of the tunneling density of states, and interaction-dependent power laws for transport quantities. For armchair CN’s, in particular, there have been many theoretical works in which an effective low-energy theory was formulated and explicit predictions were made on various quantities like the energy gap at the Fermi level, tunneling conductance between the CN and a metallic contact, etc. [67-71]. Some experiments suggested the presence of such many-body effects [42,43,72].

In ref. 72, for example, the conductance of bundles (ropes) of single-wall CN’s are measured as a function of temperature and voltage. Electrical connections to nanotubes can be achieved by either depositing electrode metal over the top of the tubes (end contacted) or by placing the tubes on the top of predefined metal leads (bulk contacted). The measured differential conductance displays a power-law dependence on temperature \( \propto T^\alpha \) and applied bias \( \propto V^\alpha \), where \( T \) is the temperature and \( V \) is the voltage. The obtained different values of the power \( \alpha \) between two samples of bulk and end contacted roughly agree with the theoretical predictions on the exponent of the electron tunneling into the bulk and the end of the Tomonaga-Luttinger liquid.

When the Fermi level moves away from the energy range where only linear bands are present, interband scattering appears because of the presence of several bands at the Fermi level. Let $r_{\beta\alpha}$ be the reflection coefficient from a state with wave vector $k_\alpha$ to a state with $k_\beta \equiv -k_\alpha$ in a 2D graphite sheet. Here, $\beta$ stands for the state with wave vector opposite to $\beta$. Only difference arising in nanotubes is discretization of the wave vector. Apart from a trivial phase factor arising from the choice in the phase of the wave function, the reflection coefficients satisfy the symmetry relation [73]:

$$r_{\beta\alpha} = -r_{\alpha\beta}. \quad (4.1)$$

This leads to the absence of backward scattering $r_{\alpha\alpha} = -r_{\alpha\alpha} = 0$ in the single-channel case as discussed above. Define the reflection matrix $r$ by $[r]_{\alpha\beta} = r_{\alpha\beta}$. Then, we have $r = -r^T$, where $r^T$ is the transpose of $r$. In general we have det $P = \text{det} P$ for any matrix $P$. In metallic nanotubes, the number of traveling modes $n_c$ is always
given by an odd integer and therefore \( \det(-r) = -\det(r) \), leading to \( \det(r) = 0 \).

By definition, \( r_{\beta\alpha} \) represents the amplitude of an out-going mode \( \beta \) with wave function \( \psi_\beta(r) \) for the reflected wave corresponding to an in-coming mode \( \alpha \) with wave function \( \psi_\alpha(r) \). The vanishing determinant of \( r \) shows that there exists at least one nontrivial solution for the equation

\[
\sum_{\alpha=1}^{n} r_{\beta\alpha} a_\alpha = 0. \tag{4.2}
\]

Then, there is no reflected wave for the incident wave function \( \sum_{\alpha} a_\alpha \psi_\alpha(r) \).

Figure 6 shows some examples of the length dependence of the calculated conductance for different values of the energy. There are three and five traveling modes for \( 1 < \varepsilon L/2\pi\gamma < 2 \) and \( 2 < \varepsilon L/2\pi\gamma < 3 \), respectively. The arrows show the mean free path of traveling modes obtained by solving the Boltzmann transport equation (see below). The relevant length scale over which the conductance decreases down to the single-channel result is given by the mean free path.

Figure 7 shows an example of the conductivity obtained by solving the Boltzmann equation. The Boltzmann transport equation can be converted into the equation in terms of mean free path for each band in quasi-one-dimensional systems \([74, 75]\) and the conductivity becomes the sum of the mean free path of each band. The Boltzmann equation gives an infinite conductivity as long as the Fermi level lies in the energy range \(-1 < \varepsilon L/2\pi\gamma < +1\) where only the linear metallic bands are present. However, the conductivity becomes finite when the Fermi energy moves away from this energy range into the range where other bands are present. Further, the increase of the number of conducting modes gives no enhancement of electronic conduction, because the inter-band scattering becomes increasingly important than the number of conducting modes.

This conclusion is quite in contrast to the exact prediction that there is at least a channel which transports with probability unity, leading to the conclusion that the conductance is given by \( 2e^2/\pi\hbar \) independent of the energy for sufficiently long nanotubes. The difference originates from the absence of phase coherence in the approach based on a transport equation. In fact, in the transport equation scattering from each impurity is treated as a completely independent event after which an electron looses its phase memory, while in the transmission approach the phase coherence is maintained throughout the system.

Effects of inelastic scattering can be considered in a model in which the nanotube is separated into segments with length of the order of the phase coherence length and the electron looses the phase information after the transmission through each segment. Figure 8 shows some examples of calculated conductance for \( \varepsilon(2\pi\gamma/L)^{-1} = 1.5 \) with \( n_s = 3 \). As long as the length is smaller than or comparable to the inelastic scattering length \( L_B \), the conductance is close to the ideal value \( 2e^2/\pi\hbar \) corresponding to the presence of a perfect channel. When the length becomes much larger than \( L_B \), the conductance decreases in proportion to the inverse of the length. When \( L_B \) becomes comparable to the mean free path \( (\Lambda_0/L \sim 6 \) in the present case), the conductance becomes close to the Boltzmann result given by the dotted line.

5. Electron-Phonon Scattering

At nonzero temperatures, lattice vibrations usually constitute the major source of electron scattering and limit the resistivity. Among phonons, long-wavelength acoustic phonons consisting of twisting, stretching, and breathing modes as shown in Fig. 9 are most important. These modes can be treated by a continuum model \([76]\).

The potential-energy functional for displacement \( u = (u_x, u_y, u_z) \) is written as

\[
U[u] = \int dxdy \left( B(u_{xx} + u_{yy})^2 + \mu [(u_{xx} - u_{yy})^2 + 4u_{xy}^2] \right),
\]

with\[
\begin{align*}
\frac{u_{xx}}{R} + \frac{u_x}{R} &= \frac{\partial u_y}{\partial y}, \\
2u_{xy} - \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} &= 0
\end{align*}
\]

where the term \( u_z/R \) is due to the finite radius \( R = L/2\pi \) of the nanotube. The parameters \( B = \lambda + \mu \) and \( \mu \) denote the bulk modulus and the shear modulus for a graphite sheet \( (\lambda \text{ and } \mu \text{ are Lamé’s constants}) \). The corresponding kinetic energy is written as

\[
K[u] = \int dxdy \frac{M}{2} \left( (\dot{u}_x)^2 + (\dot{u}_y)^2 + (\dot{u}_z)^2 \right),
\]

where \( M \) is the mass density given by the carbon mass per unit area.

The phonon modes are specified by the wave vector along the circumference \( \chi(q) = 2\pi n/L \) and that along the axis \( q \), \( u(r) = u \exp[i\chi(q) x + iq\gamma] \). When \( n = 0 \) and \( \chi = 0 \), in particular, the eigen equation becomes

\[
M\omega^2
\begin{pmatrix}
u_x \\ u_y \\ u_z
\end{pmatrix}
= \begin{pmatrix} \mu q^2 & 0 & 0 \\ 0 & (B + \mu)q^2 - i(B - \mu)qR^{-1} & 0 \\ 0 & i(B - \mu)qR^{-1} & (B + \mu)R^{-2} \end{pmatrix}
\begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix},
\]

which has three eigen modes called twisting, stretching, and breathing modes.

The twisting mode is made of pure circumference-directional deformation and its velocity \( v_5 \) is equal to that of the TA mode of a graphite sheet \( \omega_T(q) = v_5 q \) with \( v_T = \sqrt{\mu/M} \). In the long wavelength limit \( q = 0 \), the radial deformation generates a breathing mode with frequency \( \omega_B = \sqrt{(B + \mu)/MR^{-1}} \), which is inversely proportional to the radius \( R \) of the CN. In the case \( |qR| \ll 1 \), the deformation in the nanotube-axis direction generates stretching modes. When \( \omega \ll \omega_B \), we have from the last equation of the above \( u_z \approx -iqR u_y(B - \mu)/(B + \mu) \). Upon substitution of this into the second equation, we have \( \omega_S = v_S q + v_5 q \sqrt{AB}/(B + \mu)M \). The velocity \( v_S \) is usually smaller than that of the LA mode of the graphite \( \sqrt{(B + \mu)/M} \).

This model is too simple when dealing with modes
with \( n \neq 0 \). In this case, we have to consider the potential energy due to nonzero curvature of the 2D graphite plane. The curvature energy is of the order of the fourth power of the wave vector and therefore is much smaller than \( U[\mathbf{u}] \) as long as \( q R \ll 1 \) for \( n = 0 \) and 1 but becomes appreciable only for \( n > 1 \). Figure 10 shows phonon dispersions calculated in this continuum model.

A long-wavelength acoustic phonon gives rise to an effective electron-phonon coupling

\[
H'_K = \begin{pmatrix} V_1 & V_2 \\ V_2^* & V_1 \\ \end{pmatrix},
\]

with

\[
V_1 = g_1(u_{xx} + u_{yy}), \quad V_2 = g_2e^{3i\eta}(u_{xx} - u_{yy} + 2iu_{xy}),
\]

where the diagonal term represents the conventional deformation potential and the second a small term due to a change in the distance between nearest neighbor carbon atoms. We have \( g_1 \sim 30 \) eV and \( g_2 \sim 1.5 \) eV and therefore \( g_1 > g_2 \).

The matrix elements for the backscattering between right-going \( |s+\rangle \) and left-going \( |s-\rangle \), where \( s = +1 \) for the conduction band and \( -1 \) for the valence band, is written as

\[
(s - |H'_K|s+) = -iReV_2.
\]

This means that the diagonal deformation-potential term does not contribute to the backward scattering as in the case of impurities and only the real part of the much smaller off-diagonal term contributes to the backward scattering. We have

\[
ReV_2 = g_2[\cos 3\eta(u_{xx} - u_{yy}) - 2\sin 3\eta u_{xy}].
\]

In armchair nanotubes with \( \eta = \pi/6 \), we have \( ReV_2 = -2g_2u_{xy} \) and only shear or twist modes contribute to the scattering. In zigzag nanotubes with \( \eta = 0 \), on the other hand, \( ReV_2 = g_2(u_{xx} - u_{yy}) \) and only stretching and breathing modes contribute to the scattering.

When a high-temperature approximation is adopted for phonon distribution function, the resistivity for an armchair nanotube is calculated as \( \rho(T) = (\hbar/e^2)R^{-1}(g_2^2kB T/2\gamma^2\mu) \), where \( \mu \) is the shear modulus. At temperatures much higher than the frequency of the breathing mode \( \omega_B \), the resistivity of a zigzag nanotube is same as \( \rho(T) \). At temperatures lower than \( \omega_B \), on the other hand, the breathing mode does not contribute to the scattering and therefore the resistivity becomes smaller than \( \rho(T) \). Because of the small coupling constant \( g_2 \) the absolute value of the resistivity is much smaller than that in bulk 2D graphite dominated by much larger deformation-potential scattering. The resistivity of an armchair CN is same as that obtained previously [77] except for a difference in \( g_2 \).

The mean free path \( \Lambda \) at high temperature is given by \( \Lambda = (\mu a^2/3k_B Tn^2\beta^2)L \). Using the parameters we obtain \( \Lambda \sim 600 \times L \) at room temperature. The mean free path is as large as 1 \( \mu \)m for thin armchair nanotubes with diameter \( \sim 1.5 \) nm and increases in proportion to \( L \). This means that a metallic CN becomes a one-dimensional ballistic conductor even at room temperature.

When the energy is outside of the region \(-1 < \varepsilon < (2\pi\gamma/L)^{-1} < +1 \) where only metallic linear bands are present, it is necessary to solve a Boltzmann transport equation taking scattering between bands into account [75,78]. Figure 11 shows obtained Fermi energy dependence of conductivity for metallic and semiconducting CN’s for \( g_1/g_2 = 10 \).

For metallic nanotubes, around \( \varepsilon \sim 0 \), the diagonal potential \( g_1 \) causes no backward scattering between two bands with linear dispersion, and smaller off-diagonal potential \( g_2 \) determines resistivity. However, when the Fermi energy becomes higher and the number of bands increases, \( g_1 \) dominates the conductivity due to interband scattering and the conductivity drops drastically. On the other hand, such a drastic change disappears for semiconducting CN’s and smaller conductivity compared to that of a metallic CN shows dominance of the diagonal potential independent of the Fermi energy.

6. Lattice Vacancies

So far, we have exclusively considered the case that scattering potential has a range larger than the lattice constant. When the range becomes smaller than the lattice constant, the effective potential for A and B sites in a unit cell can be different. In this case the scatterer becomes dependent on “pseudo-spin” and causes backscattering due to “pseudo-spin-flip scattering.” Further, it causes intervalley scattering between K and K’ points, which causes also backscattering and leads to nonzero resistance.

A typical example of such short-range and strong scatterers is a lattice vacancy. Effects of scattering by a lattice vacancy in armchair nanotubes have been studied within a tight-binding model [79,80]. It has been shown that the conductance at zero energy in the absence of a magnetic field is quantized into zero, one, or two times of the conductance quantum \( e^2/\pi h \) for a vacancy consisting of three B carbon atoms around an A atom, of a single A atom, and of a pair of A and B atoms, respectively [80]. Numerical calculations were performed for about \( 1.5 \times 10^5 \) different kinds of vacancies and demonstrated that such quantization is quite general [81]. This rule was analytically derived in a \( k\cdot p \) scheme later [29,82].

7. Junction and Topological Defects

A junction which connects CNs with different diameters through a region sandwiched by a pentagon-heptagon pair has been observed in the transmission electron microscope [2]. Some theoretical calculations on CN junctions within a tight-binding model were reported for junctions between metallic and semiconducting nanotubes and those between semiconducting nanotubes [83,84]. In particular tight-binding calculations for junctions consisting of two metallic tubes with different chirality or diameter demonstrated that the conductance exhibits a universal power-law dependence on the ratio of the circumference of two nanotubes [85]. The
\( \mathbf{k} \cdot \mathbf{p} \) scheme is ideal to clarify electronic states and their topological characteristics in such junction systems.

Figure 12 shows the development of a junction system onto a 2D graphite sheet [84]. We have a pair of a pentagon (\( \mathbf{R}_5 \)) and heptagon (\( \mathbf{R}_7 \)) ring, and \( \mathbf{L}_5 \) and \( \mathbf{L}_7 \) are the chiral vector of the thick and thin nanotube, respectively. Therefore, \( \mathbf{R}_5 - \mathbf{L}_5 \) and \( \mathbf{R}_7 - \mathbf{L}_7 \) are rolled on to \( \mathbf{R}_5 \) and \( \mathbf{R}_7 \), respectively. An equilateral triangle with a base connecting \( \mathbf{R}_5 \) and \( \mathbf{R}_5 - \mathbf{L}_7 \) and another with a base connecting \( \mathbf{R}_7 \) and \( \mathbf{R}_7 - \mathbf{L}_7 \) have a common vertex point at \( \mathbf{R} \). The angle between \( \mathbf{L}_5 \) and \( \mathbf{L}_7 \) is denoted as \( \theta \).

Boundary conditions can be derived by considering such a structure of the junction [86]. In the junction region, where any point on the development moves onto the corresponding point after making a rotation by \( \pi/3 \) around \( \mathbf{R} \) as shown in Fig. 12. Then, we have

\[
F(R_{\pi/3}r) = T_{\pi/3} F(r),
\]

\[
T_{\pi/3} = \begin{pmatrix}
0 & 0 & 0 & e^{i\psi(R)} \\
0 & 0 & -e^{-i\psi(R)} & 0 \\
0 & -e^{-i\psi(R)} & 0 & 0 \\
e^{-i\psi(R)} & 0 & 0 & 0
\end{pmatrix},
\]

with \( e^{i\psi(R)} = \exp[i(\mathbf{K}' - \mathbf{K}) \cdot \mathbf{R}] \), where \( \omega = \exp(2\pi i/3) \) and \( R_{\pi/3} \) describes a \( \pi/3 \) rotation around \( \mathbf{R} \). Because of the boundary conditions, states near the K and K’ point mix together in the junction region.

Under these boundary conditions, the Schrödinger equation can be solved analytically. An approximate expression for the transmission \( T \) and reflection probabilities \( R \) can be obtained by neglecting evanescent modes decaying exponentially into the thick and thin nanotubes [86]. The solution at \( \varepsilon = 0 \) gives \( T = 4L_5 L_7 / (L_5 + L_7)^2 \), \( R = (L_3 - L_5)^2 / (L_3 + L_5)^2 \). We have \( T \sim 4L_7 / L_5^3 \) in the long junction \( (L_7 / L_5 < 1) \). When they are separated into different components, \( T_{KK} = T \cos^2(3\theta/2) \), \( T_{KK'} = T \sin^2(\theta/2) \), \( R_{KK'} = 0 \), and \( R_{KK'} = R \), where the subscript KK means intravalley scattering within K or K’ point and KK’ stands for intervalley scattering between K and K’ points. As for the reflection, no intravalley scattering is allowed. Explicit calculations can be performed also for \( \varepsilon \neq 0 \) [87,88].

Junctions can contain many pairs of topological defects. Effects of three pairs present between metallic (6,3) and (9,0) nanotubes were studied [79], which shows that the conductance vanishes for junctions having a three-fold rotational symmetry, but remains nonzero for those without the symmetry.

A typical example of topological defects present in 2D graphite is a Stone-Wales defect, composed of two heptagon-pentagon pairs next to each other [89]. It is realized by bond alternation within four nearest honeycombs and is known to be energetically quasi-stable. An effective-mass Hamiltonian for a nonlocal Stone-Wales defect was derived by a procedure similar to that of impurities or short-range defects [30].

The resulting conductance exhibits two dips at a positive energy and a negative energy [90,30]. Except in the vicinity of the dips, the conductance is close to the ideal value \( 2e^2/h \). The two-dip structure corresponds to the case of a pair of vacancies at A and B sites although two dips lie at positions asymmetric around \( \varepsilon = 0 \). A Stone-Wales defect can be obtained by first removing a pair of neighboring A and B sites and then adding a pair in the perpendicular direction. The above result seems to show that the removal of a pair is likely to be more dominant than the addition of nonlocal transfer between neighboring sites.

8. Summary

In summary, a brief review has been given on electronic and transport properties of carbon nanotubes mainly from a theoretical point of view. The topics include a description of energy bands in a tight-binding model and in an effective-mass or \( \mathbf{k} \cdot \mathbf{p} \) scheme. In the latter scheme, electrons in nanotubes are regarded as neutrinos on cylinder surface with a fictitious Aharonov-Bohm flux passing through the cross section. The \( \mathbf{k} \cdot \mathbf{p} \) description is particularly useful for revealing extraordinary properties of metallic nanotubes. In fact, in metallic carbon nanotubes, there is at least a single channel transmitting through the system without backscattering independent of energy for scatterers with potential range comparable to or larger than the lattice constant. This channel is sensitive to inelastic scattering when several bands coexist at the Fermi level, however. This has been demonstrated in a model of an electron losing its coherence for a distance determined by a phase coherence length. Phonons cause backscattering at high temperatures, but effects are very weak and nanotubes are considered as ballistic conductors even at room temperature, because the strong deformation potential has no contribution. The effective-mass scheme is useful also for understanding effects of lattice vacancies, junctions, and topological defects.

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References


Figure Captions
Fig. 1. (a) The lattice structure of a 2D graphite sheet and various quantities. We shall consider the case that 0 ≤ η ≤ η. The zigzag nanotube corresponds to η = 0 and the armchair nanotube to η = π/6. (b) The coordinate system on cylinder surface.

Fig. 2. Calculated band structure of a two-dimensional graphite along K → Γ → M → K shown in the inset.

Fig. 3. The energy dispersion and density of states in the vicinity of K and K’ points obtained in a k·p scheme.

Fig. 4. An example of the dynamical conductivity calculated in the self-consistent Born approximation. ε0 is an arbitrary energy scale. After Ref. 60.

Fig. 5. Energy bands of a nanotube obtained in the effective-mass approximation for ν = 0 (left) and ν = +1 (right).

Fig. 6. An example of the length dependence of the calculated conductance. The arrows show the mean free path of traveling modes obtained by solving the Boltzmann transport equation. For lower three curves there are three bands with n = 0 and ±1 and for upper three curves there are five bands with n = 0, ±1, and ±2. The mean free path is same for bands with same |n| and decreases with the increase of |n|. After Ref. 73.

Fig. 7. An example of the energy dependence of the conductivity calculated using Boltzmann transport equation. The conductivity is infinite in the energy range −1 < εL/2πγ < +1 but becomes finite in the other region where there are several bands coexist at the Fermi level. The dashed line shows the density of states and thin solid lines show the contribution of each band to the conductivity (the lowest curve represents the contribution of m = 0, the next two m = ±1, . . . ). After Ref. 73.

Fig. 8. An example of the conductance in the presence of inelastic scattering as a function of the length for different values of the phase coherence length Lφ. After Ref. 73.

Fig. 9. Schematic illustration of long-wavelength phonons consisting of transverse twist modes and longitudinal stretching and breathing modes.

Fig. 10. Frequencies of phonons obtained in the continuum model.

Fig. 11. Fermi-energy dependence of conductivity for metallic (solid line) and semiconducting (broken line) CN’s with g1/g2 = 10 in units of σA(0) denoting the conductivity of an armchair CN with ε = 0. After Ref. 76.

Fig. 12. The structure of a junction consisting of two nanotubes having an axis not parallel to each other (θ is their angle).
Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5
0.0 1.0 2.0 3.0 4.0
0.0
0.5
1.0

\[ \frac{\omega(q)}{\omega_B(n)} \]

0.0 1.0 2.0 3.0 4.0

\[ \varepsilon \left( \frac{2\pi \gamma}{L} \right)^{-1} \]

\[ \frac{\sigma(\varepsilon)}{\sigma_A(0)} \]

\[ g_1/g_2 = 10 \]

\[ \text{Metal} \]

\[ \text{Semiconductor} \]

Fig. 10

Fig. 11

Fig. 12