Effective-Mass Theory of Carbon Nanotube Junctions

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(Received May 6, 1998)

Electronic states in junctions of nanotubes with different circumferences are studied in an effective-mass approximation. The junction is characterized by boundary conditions which mix wave functions associated with K and K' points. The wave functions obtained analytically at \( \varepsilon = 0 \) decay linearly with the distance from the thicker nanotube, showing that the conductance decays with the junction length in proportion to its third power.

KEYWORDS: graphite, carbon nanotube, junction, five- and seven-member ring, conductance, effective-mass theory

\[ \text{§1. Introduction} \]

Recent synthetic techniques have made it possible to obtain various carbon structures based on fullerenes. A carbon nanotube (CN) was first produced by means of the arc-discharge evaporation method.\(^1\) A CN is composed of coaxially rolled graphite sheets. A single-shell CN can be either a metal or a semiconductor depending on the circumferential length and the helical fashion. The purpose of this paper is to study electronic states in junctions consisting of two nanotubes with different diameters in a \( kp \) scheme.

Various energy band calculations have been performed.\(^2\)\textsuperscript{-12} It has been found that most characteristic properties are reproduced quite well in a \( kp \) method,\(^13,14\) which is effective in the study of effects of external fields such as a magnetic and electric field. In fact, it has been successful in the study of magnetic properties including the Aharonov-Bohm effect on the band gap,\(^15,16\) optical absorption spectra,\(^17,18\) and lattice instabilities in the presence and absence of a magnetic field.\(^19,20\)

Transport properties of CN’s were also studied in the \( kp \) scheme for a model of short-range scatterers. The conductivity calculated in the Boltzmann transport theory showed a large positive magnetoconductance.\(^21\) This positive magnetoconductance was confirmed by full quantum mechanical calculations in the case that the mean free path is much larger than the circumference length.\(^22\)

Effects of impurity scattering in CN’s were studied in detail and a possibility of complete absence of back scattering was pointed out and proved rigorously except for scatterers having a potential range smaller than the lattice constant.\(^23,24\)

A junction which connects tubes with different diameters through a region sandwiched by a pentagon-heptagon pair has been observed in the transmission electron microscope.\(^25\) Some theoretical calculations on CN junctions within a tight-binding model were reported, which imply that the conductance of junctions exhibit a universal power-law dependence on the ratio of the circumference of two nanotubes.\(^26\)\textsuperscript{-28} Effects of a magnetic field were studied also and intriguing dependence on the magnetic-field direction was predicted.\(^29,30\)

In this paper, we shall discuss electronic states of such junction systems in the \( kp \) scheme and clarify the origin of the universal behavior. In §2 a brief review is given on the effective-mass approximation. Boundary conditions for envelope functions are derived in §3. Wave functions in junctions are discussed in §4. Results of numerical calculations are presented in §5.

\[ \text{§2. Effective Mass Equation} \]

The structure of two-dimensional (2D) graphite sheet is shown in Fig. 1. Primitive translation vectors \( a \) and \( b \) are given by

\[
a = a e'_{x}, \quad b = a \left( -\frac{1}{2} e'_{x} + \frac{\sqrt{3}}{2} e'_{y} \right),
\]

where \( a \) is the lattice constant and \( e'_{x} \) and \( e'_{y} \) are unit vectors in the \( x' \) and \( y' \) directions fixed onto the graphite sheet. A unit cell contains two carbon atoms denoted as A and B. Three nearest neighbor A atoms around a B atom are located at

\[
\begin{align*}
\bar{r}_1 &= a \frac{1}{\sqrt{3}} e'_{y}, \\
\bar{r}_2 &= a \left( -\frac{1}{2} e'_{x} - \frac{1}{2 \sqrt{3}} e'_{y} \right), \\
\bar{r}_3 &= a \left( \frac{1}{2} e'_{x} - \frac{1}{2 \sqrt{3}} e'_{y} \right).
\end{align*}
\]

Two \( \pi \)-bands having approximately a linear dispersion crosses the Fermi level at K and K’ points whose wave vectors are given as

\[
\begin{align*}
K &= \frac{2 \pi}{a} \left( \frac{1}{3} e'_{x} + \frac{1}{\sqrt{3}} e'_{y} \right), \\
K' &= \frac{2 \pi}{a} \frac{2}{3} e'_{x}.
\end{align*}
\]

3542
The result is given by

\[ H F(r) = \varepsilon F(r), \]

with

\[
H = \begin{pmatrix}
0 & \gamma(k_x - ik_y) & 0 & 0 \\
\gamma(k_x + ik_y) & 0 & 0 & 0 \\
0 & 0 & 0 & \gamma(k_x - ik_y) \\
0 & 0 & \gamma(k_x + ik_y) & 0
\end{pmatrix},
\]

and

\[
F(r) = \begin{pmatrix}
P_A^K(r) \\
P_B^K(r) \\
P_A^{K'}(r) \\
P_B^{K'}(r)
\end{pmatrix}.
\]

§3. Boundary Conditions

3.1 Armchair nanotube

Let us consider a junction of two armchair nanotubes as illustrated in Fig. 2. We separate the junction into three regions, a thicker nanotube with circumference \( L_5 \), a junction region where the circumference \( L(y) \) varies along the axis direction chosen in the \( y \) direction, and a thinner nanotube with circumference \( L_7 \). We have \( L_5 = m_5 \sqrt{3} a \) and \( L_7 = m_7 \sqrt{3} a \) for chiral vectors given by

\[
L_5 = -m_5(a + 2b), \\
L_7 = -m_7(a + 2b),
\]

with integer \( m_5 \) and \( m_7 \). There is a five-member ring (whose position is denoted as \( R_5 \)) at the boundary of the thicker nanotube and the junction region and a seven-member ring (\( R_7 \)) at the boundary of the junction region and the thinner nanotube.

The tight-binding equation of motion at a site in the region denoted as \( a' \) in Fig. 2 gives the following relation between the amplitude at a site in the region \( b \) and that at a site in the region \( a' \) extrapolated from the junction region:

\[
\psi_A(R_A^{a'}) = \psi_B(R_B^{a'}), \\
\psi_B(R_B^{a'}) = \psi_A(R_A^{a'}),
\]

where

\[
R_A^{a'} = R - n(a - b) - \tau_3, \\
R_B^{a'} = R - n(a - b) - 2\tau_3,
\]

and

\[
R_A^{b'} = R - n(2a + b) + \tau_2, \\
R_B^{b'} = R - n(2a + b) + 2\tau_2,
\]

with integer \( n \). Obviously, we have

\[
R_A^{b'} = R(\pi / 3)(R_B^{a'} - R) + R, \\
R_B^{b'} = R(\pi / 3)(R_A^{a'} - R) + R,
\]

where \( R(\theta) \) is an operator corresponding to a rotation by angle \( \theta \) around \( R \) which is the vertex of the equilateral triangle formed by the boundaries of the junction region, i.e.,

\[
R(\theta) = \begin{pmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix}.
\]

Similarly, the tight-binding equation of motion at a site
in the region denoted as (b) in Fig. 2 gives the relation between the amplitude at a site in the region (a') and that at a site in the region (b') extrapolated from the junction region:

\[
\psi_A(R_A') = \psi_B(R_B'),
\]

\[
\psi_B(R_B') = \psi_A(R_A'),
\]

(3.7)

where

\[
R_A' = \rho - n(a - b) - a - \overline{a},
\]

\[
R_B' = \rho - n(a - b) - a + \overline{a},
\]

(3.8)

and

\[
R_A'' = \rho - n(2a + b) - a + \overline{b},
\]

\[
R_B'' = \rho - n(2a + b) - a - \overline{b},
\]

(3.9)

with integer \( n \). Again, we have

\[
R_A'' = \rho - n(a - b) - a + \overline{b} + \overline{a},
\]

\[
R_B'' = \rho - n(a - b) - a - \overline{b} + \overline{a},
\]

(3.10)

with

\[
R_A' = R(\pi/3)(R_B' - R) + R,
\]

\[
R_B' = R(\pi/3)(R_A' - R) + R.
\]

(3.12)

for all lattice points \( R_A \) and \( R_B \). In terms of the envelope functions, these conditions can be written explicitly as

\[
\exp(i\mathbf{k} \cdot R_A') F_A^K(R_A) + \phi^n \exp(i\mathbf{k} \cdot R_A') F_A^{K'}(R_A') = -\omega \phi^n \exp(i\mathbf{k} \cdot R_B) F_B^K(R_B) + \exp(i\mathbf{k} \cdot R_B) F_B^{K'}(R_B),
\]

(3.13)

and

\[
-\omega \phi^n \exp(i\mathbf{k} \cdot R_B') F_B^K(R_B') + \exp(i\mathbf{k} \cdot R_B') F_B^{K'}(R_B') = \exp(i\mathbf{k} \cdot R_A') F_A^K(R_A') + \phi^n \exp(i\mathbf{k} \cdot R_A') F_A^{K'}(R_A').
\]

(3.14)

In the following we shall choose the origin at \( R \), i.e., \( R = 0 \). Because \( R^{-1}(\pi/3)K = K' \), we have

\[
\exp(i\mathbf{k} \cdot R_A') = \exp(i\mathbf{k} \cdot R_B),
\]

\[
\exp(i\mathbf{k} \cdot R_B') = \exp(i\mathbf{k} \cdot R_A).
\]

(3.15)

Further, we have \( R^{-1}(\pi/3)K' = K - (4\pi/\sqrt{3}a)e_y' \). Noting that \( R_A = n_1a + n_2b - \overline{a} \) and \( R_B = n_1a + n_2b + \overline{a} \) with integers \( n_1 \) and \( n_2 \), we have

\[
\exp(i\mathbf{k} \cdot R_A') = \exp(i\mathbf{k} \cdot R_B),
\]

\[
\exp(i\mathbf{k} \cdot R_B') = \exp(i\mathbf{k} \cdot R_A).
\]

(3.16)

Because the envelope functions are slowly-varying functions, the conditions (3.13) and (3.14) are satisfied if and only if

\[
F[R(\pi/3)r] = T(\pi/3)F(r),
\]

(3.17)

with

\[
T(\pi/3) = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & \omega & 0 \\
0 & -1 & 0 & 0 \\
\omega & 0 & 0 & 0
\end{pmatrix}.
\]

(3.18)

It is straightforward to show that this should be modified into

\[
T(\pi/3) = \begin{pmatrix}
0 & 0 & 0 & \phi \psi(R) \\
0 & 0 & -\omega & 0 \\
0 & -\omega & 0 & 0 \\
\omega & 0 & 0 & 0
\end{pmatrix},
\]

(3.19)

with

\[
\phi \psi(R) = \exp[i(\mathbf{k} \cdot \mathbf{R}) \cdot \mathbf{R}].
\]

(3.20)

if \( R \) is not chosen at the origin, i.e., \( R \neq 0 \). Physical quantities do not depend on the choice of the origin and consequently on the phase \( \psi(R) \).

Consider the thicker nanotube. An equation of motion at a site in the region (c') gives the following conditions:

\[
\psi_A(R_A^{(c)}) = \psi_A(R_A^{(d)}),
\]

(3.21)

\[
\psi_B(R_B^{(c)}) = \psi_B(R_B^{(d)}),
\]

(3.22)

where \( \psi_A(R_A^{(c)}) \) is the extrapolated amplitude. Similarly, an equation of motion at a site in the region (d') gives

\[
\psi_A(R_A^{(d)}) = \psi_A(R_A^{(c)}),
\]

\[
\psi_B(R_B^{(d)}) = \psi_B(R_B^{(c)}),
\]

where \( \psi_B(R_B^{(d)}) \) is the extrapolated amplitude. Obvi-
ously, we have
\[ R_A^{(d)} = R_A^{(c)} + L_5, \]
\[ R_B^{(d)} = R_B^{(c)} + L_5. \]
(3.23)

Therefore, these boundary conditions can be generalized into
\[ \psi_A(R_A + L_5) = \psi_A(R_A), \]
\[ \psi_B(R_B + L_5) = \psi_B(R_B), \]
(3.24)
for all lattice points \( R_A \) and \( R_B \). By using the slowly-varying nature of the envelope functions, we get
\[ F(r + L_5) = U(L_5)F(r), \]
(3.25)
with
\[ U(L) = \begin{pmatrix}
  e^{iK \cdot L} & 0 & 0 & 0 \\
  0 & e^{iK \cdot L} & 0 & 0 \\
  0 & 0 & e^{iK' \cdot L} & 0 \\
  0 & 0 & 0 & e^{iK' \cdot L}
\end{pmatrix}. \]
(3.26)

The above becomes a simple periodic boundary conditions since \( \exp[iK \cdot L_5] = \exp[iK' \cdot L_5] = 1 \) for the armchair nanotube. This leads to the conclusion that the armchair nanotube is always metallic. Completely the same conclusions can be obtained for the thinner nanotube if we replace \( L_5 \) by \( L_7 \).

### 3.2 Zigzag nanotubes and generalizations

Figure 3 shows the structure of a junction consisting of two zigzag nanotubes. We have \( L_5 = m_5a \) and \( L_7 = m_7a \) for chiral vectors given by
\[ L_5 = -m_5a, \]
\[ L_7 = -m_7a. \]
(3.27)

with integer \( m_5 \) and \( m_7 \). The tight-binding equation of motion at a site in the region denoted as (a') and (b) in Fig. 3 gives the following relation:
\[ \psi_B(R_B^{(a)}) = \psi_A(R_A^{(b)}), \]
\[ \psi_A(R_A^{(d)}) = \psi_B(R_B^{(c)}), \]
(3.28)
with
\[ R_A^{(b)} = R(\pi/3)(R_B^{(a)} - R) + R, \]
\[ R_B^{(b)} = R(\pi/3)(R_A^{(d)} - R) + R. \]
(3.29)

By a proper extrapolation of the wave functions toward outside of the junction region, we can generalize the above boundary conditions into eq. (3.11) with eq. (3.12).

As a result, the boundary conditions for the envelope functions are exactly the same as those for the junction of armchair nanotubes, i.e., eq. (3.17) with eq. (3.18) or eq. (3.19).

The boundary conditions in the nanotube region are given by the same equation as in the armchair case, i.e., eq. (3.25). Only difference is that
\[ \exp[iK \cdot L_5] = \exp\left(-\frac{2\pi i\nu_5}{3}\right), \]
\[ \exp[iK' \cdot L_5] = \exp\left(\frac{2\pi i\nu_5}{3}\right), \]
(3.30)
with \( \nu_5 = 0 \) for a metallic case and \( \nu_5 = \pm 1 \) for a semiconducting case, where \( \nu_5 = 3M_5 + \nu_5 \) with integer \( M_5 \). The same is applicable to the thinner nanotube.

**Fig. 3** The structure of a junction consisting of two zigzag nanotubes having an axis parallel to each other.

**Fig. 4** The structure of a junction consisting of two nanotubes having an axis not parallel to each other (\( \theta \) is their angle).

Next, let us consider a junction having a more general structure. Figure 4 shows an example of such junctions. The junction is characterized by two equilateral triangles with a common vertex point and sides parallel to the chiral vectors of two nanotubes. For any site close to the upper boundary denoted as (a'), there exists a corresponding site near the lower boundary denoted as...
(+), obtained by a rotation around \( R \) by \( \pi/3 \). The relation between the amplitude of these points is also given by eq. (3.11) with eq. (3.12). As a result, the boundary conditions for the envelope functions are also given by eq. (3.17) with eq. (3.18) or eq. (3.19).

![Fig. 5 Schematic illustration of the topological structure of a junction of two carbon nanotubes with different diameter. In the nanotube regions, two cylinders corresponding to spaces associated with the \( K \) and \( K' \) points are independent of each other and completely decoupled. In the junction region, on the contrary, they are interconnected to each other.](image)

Figure 5 gives an illustration of the topological structure of the junction. In the nanotube regions, the \( K \) and \( K' \) points are completely decoupled and therefore belong to different subspaces. In the junction region they are interconnected to each other. In the junction region, the wavefunction \( F^K_A \) turns into \( F^K_B \) with an extra phase \( e^{-i0(R)} \) when being rotated once around the axis. After another rotation, it comes back to \( F^K_A \) with an extra phase \( \omega^{-1} = \exp(-2\pi i/3) \). On the other hand, \( F^K_B \) turns into \( F^K_A' \) with phase \( -\omega e^{-i0(R)} \) under a rotation and then into \( F^K_B' \) with phase \( \omega = \exp(2\pi i/3) \) after another rotation.

The above boundary conditions for nanotubes and their junctions have been obtained based on the nearest-neighbor tight-binding model. The essential ingredients of the boundary conditions lie in the fact that the 2D graphite system is invariant under the rotation of \( \pi/3 \) followed by the exchange between A and B carbon atoms. Therefore, the conditions given by eq. (3.17) with eqs. (3.18) or (3.19) are quite general and valid in more realistic models of the band structure.

The present method can be used also to obtain boundary conditions around a five- and seven-member ring schematically illustrated in Fig. 6. First, around the five-member ring, we note that

\[
T(5\pi/3)T(\pi/3) = T(2\pi) = 1. \tag{3.31}
\]

This immediately gives the conditions

\[
F[R(5\pi/3)r] = T(5\pi/3) F(r),
\]

\[
T(5\pi/3) = T^{-1}(\pi/3) = \begin{pmatrix}
0 & 0 & 0 & \omega^{-1}
0 & 0 & -1 & 0
0 & -\omega & 0 & 0
1 & 0 & 0 & 0
\end{pmatrix}. \tag{3.32}
\]

Around the seven member ring, on the other hand, we have

\[
F[R(7\pi/3)r] = T(7\pi/3) F(r),
\]

\[
T(7\pi/3) = T(\pi/3). \tag{3.33}
\]

![Fig. 6 The structure of a 2D graphite sheet in the vicinity of five- and seven-member ring.](image)

3.3 Symmetry

In the following we shall confine ourselves to a junction system consisting of two metallic nanotubes having an axis in the same direction. Extensions to more general cases will be discussed in a later publication. In the case of such symmetric systems, the \( k \cdot p \) equation has a special symmetry valid only in metallic nanotubes as is shown below. We choose the \( x \) axis as shown in Figs. 2 and 3 and consider transformation \( \Pi \) defined as

\[
\Pi : \begin{pmatrix}
F^K_A(x, y) \\
F^K_B(x, y) \\
F^K_A'(x, y) \\
F^K_B'(x, y)
\end{pmatrix} \rightarrow \begin{pmatrix}
+iF^K_B(-x, y) \\
-iF^K_A(-x, y) \\
+iF^K_A'(-x, y) \\
-iF^K_B'(-x, y)
\end{pmatrix}, \tag{3.34}
\]

i.e.,

\[
\Pi F(r) = P F(\Pi r), \tag{3.35}
\]

with

\[
P = \begin{pmatrix}
0 & i & 0 & 0 \\
-i & 0 & 0 & 0
\end{pmatrix}, \tag{3.36}
\]

and \( \Pi r = r' \) where \( r = (x, y) \) and \( r' = (-x, y) \). We have

\[
PH(k_x, k_y)P^{-1} = H(-k_x, k_y), \tag{3.37}
\]
which shows that \( \Pi \) commutes with the Hamiltonian \( \mathcal{H} \). Further, we have

\[
\Pi \mathbf{F}(\pi/3, r) = P F(\Pi r) \mathbf{F}(\pi/3, r) = PT^{-1}(\pi/3) P \mathbf{F}(\Pi r)
\]

(3.38)

which shows that \( \Pi \) commutes with the boundary conditions also in the junction region. In the nanotube region with chiral vector \( \mathbf{L} \), on the other hand,

\[
\Pi \mathbf{F}(r + L) = P \mathbf{F}(\Pi r - L) = P U(-L) \mathbf{F}(\Pi r) = P U(-L) P^{-1} \mathbf{F}(r)
\]

(3.39)

which shows that \( \Pi \) commutes with the boundary conditions only in metallic nanotubes where \( U(L) = 1 \). Because \( \Pi^2 \) is an identity, \( \Pi \) has eigenvalues \( p = \pm 1 \), which will be called ‘parity’ in the following. In metallic nanotubes, the states are classified by the parity.

The physical meaning of this symmetry is clear in armchair nanotubes (\( \eta = -\pi/2 \)). Under the transformation \( \Pi \), we have

\[
\psi_A(R) \rightarrow e^{iK \cdot R} \Pi F_A^K(R) + e^{\pi i/2} e^{iK' \cdot R} \Pi F_A^{K'}(R)
\]

\[
= e^{iK \cdot (R - \Pi R)} e^{iK \cdot \Pi R} F_B^K(\Pi R) + e^{\pi i/2} e^{iK' \cdot \Pi R} F_B^{K'}(\Pi R)
\]

\[
= -e^{\pi i/2} e^{iK \cdot \Pi R} F_B^K(\Pi R) + e^{iK' \cdot \Pi R} F_B^{K'}(\Pi R)
\]

\[
= \psi_B(\Pi R).
\]

(3.40)

where use has been made of \( R - \Pi R = (3n + 1) \pi \) with an integer \( n \). Similarly, we have \( \psi_B(R) \rightarrow \psi_A(\Pi R) \). Thus the transformation \( \Pi \) is nothing but a mirror reflection around the \( y \) axis. In other nanotubes including zigzag and those having a chirality, this symmetry is absent in the original discrete lattice, but is still present in the \( k \cdot p \) approximation.

In the remaining part of this section we shall confine ourselves to metallic nanotubes in which the envelope functions satisfy the conventional periodic boundary conditions. Consider the energy range \( 2\pi\gamma/L_5 < \varepsilon < -2\pi\gamma/L_5 \) where only a single band having a linear dispersion \( \varepsilon = \gamma k \) crosses the energy in both thicker and thinner nanotubes. For \( \varepsilon = \gamma k > 0 \), the right-going waves associated with the K and K’ points in the nanotube region are given by \( F_{n,K}^+(x, y) \) and \( F_{n,K'}^+(x, y) \) with

\[
F_{n,K}^+(x, y) = \begin{pmatrix} 1 \\ i \\ 0 \\ 0 \end{pmatrix} \frac{1}{\sqrt{2L}} e^{i k y} \quad (n = 0),
\]

(3.41)

\[
F_{n,K'}^+(x, y) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ -i \end{pmatrix} \frac{1}{\sqrt{2L}} e^{i k y} \quad (n = 0),
\]

where \( L = L_5 \) in the thicker nanotube and \( L = L_7 \) in the thinner nanotube, respectively. Similarly, the left-going waves associated with the K and K’ points in the nanotube region are given by \( F_{n,K}^-(x, y) \) and \( F_{n,K'}^-(x, y) \) with

\[
F_{n,K}^-(x, y) = \begin{pmatrix} 1 \\ -i \\ 0 \\ 0 \end{pmatrix} \frac{1}{\sqrt{2L}} e^{-i k y} \quad (n = 0),
\]

(3.42)

\[
F_{n,K'}^-(x, y) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ i \end{pmatrix} \frac{1}{\sqrt{2L}} e^{-i k y} \quad (n = 0).
\]

It is clear that \( F_{0,0}^{K,K'} \) and \( F_{0,0}^{K',K} \) have parity \( p = -1 \), while \( F_{0,0}^{K,K'} \) and \( F_{0,0}^{K',K} \) have parity \( p = +1 \). This shows that wavefunctions \( F_{0,0}^{K,K'} \) and \( F_{0,0}^{K',K} \) are decoupled and independent of each other. This means that the electron wave corresponding to the K point (or valley) is not reflected into the same K point but into the K’ point. Further, the transmitted wave has a component only in the valley corresponding to the incident wave. This explains the results of numerical calculations in a tightbinding model quite well.\(^{29}\)

This symmetry can be used to show the absence of back scattering from an impurity potential found quite recently for metallic nanotubes.\(^{23,24}\) Consider an external potential which is slowly varying in the scale of the lattice constant, its effect can be incorporated as a diagonal potential in the \( k \cdot p \) Hamiltonian. The diagonal potential does not cause scattering between the K and K’ points. When the potential is symmetric around the axis \( (x = 0) \), the transformation \( \Pi \) commutes with the Hamiltonian and therefore the back scattering in the same valley is prohibited, leading to the complete absence of the back scattering. Note, however, that this discussion based on the symmetry alone is limited to the case of symmetric potential, while previous discussions based on a time-reversal process are valid for any potentials.

\[\S 4. Wave Functions\]

In the following we shall restrict ourselves to the case \( \varepsilon = 0 \) in metallic nanotubes, for which analytic results can be obtained. In this case the Schrödinger equation leads to \( F_{A}^{K}(x, y) = F_{A}^{K}(z) \) and \( F_{B}^{K'}(x, y) = F_{B}^{K'}(z) \) with \( z = x + iy \). We have further \( F_{B}^{K}(x, y) = F_{B}^{K}(\bar{z}) \) and \( F_{B}^{K'}(x, y) = F_{B}^{K'}(\bar{z}) \). The solutions in the tube regions and in the junction region are determined by imposing the boundary conditions obtained in the previous section to these general solutions.

\[4.1 Tube region\]

Consider a nanotube with circumference \( L \). The right-going waves associated with the K and K’ points in the nanotube region consist of traveling waves given by
eq. (3.41) with \( k \rightarrow +0 \) and evanescent waves given by

\[
F_n^{K^+}(x, y) = \begin{pmatrix}
1 \\
0 \\
0 \\
1/\sqrt{L} \cdot e^{j \kappa(n)z}
\end{pmatrix} \quad (n > 0),
\]

\[
F_n^{K^-}(x, y) = \begin{pmatrix}
0 \\
1 \\
0 \\
1/\sqrt{L} \cdot e^{j \kappa(n)z}
\end{pmatrix} \quad (n < 0),
\]

\[
F_n^{K'^+}(x, y) = \begin{pmatrix}
0 \\
0 \\
1 \\
1/\sqrt{L} \cdot e^{j \kappa(n)z}
\end{pmatrix} \quad (n > 0),
\]

\[
F_n^{K'^-}(x, y) = \begin{pmatrix}
0 \\
0 \\
1 \\
1/\sqrt{L} \cdot e^{j \kappa(n)z}
\end{pmatrix} \quad (n < 0),
\]

with

\[
\kappa(n) = \frac{2 \pi n}{L}.
\]

Similarly, the left-going waves associated with the K and K’ points in the nanotube region consist of traveling waves given by eq. (3.42) and evanescent waves given by

\[
F_n^{K^-}(x, y) = \begin{pmatrix}
1 \\
0 \\
0 \\
1/\sqrt{L} \cdot e^{j \kappa(n)z}
\end{pmatrix} \quad (n > 0),
\]

\[
F_n^{K'^-}(x, y) = \begin{pmatrix}
0 \\
0 \\
1 \\
1/\sqrt{L} \cdot e^{j \kappa(n)z}
\end{pmatrix} \quad (n < 0),
\]

and

\[
F_n^{K'}(x, y) = \begin{pmatrix}
1 \\
0 \\
0 \\
1/\sqrt{L} \cdot e^{j \kappa(n)z}
\end{pmatrix} \quad (n > 0),
\]

\[
F_n^{K'}(x, y) = \begin{pmatrix}
0 \\
0 \\
1 \\
1/\sqrt{L} \cdot e^{j \kappa(n)z}
\end{pmatrix} \quad (n < 0),
\]

4.2 Junction region

As we have already seen, \( F_A^K \) and \( F_B^{K'} \) are functions of \( x = x + iy \) when \( \varepsilon = 0 \). Therefore, the boundary conditions for \( F_A^K \) and \( F_B^{K'} \) are given by

\[
F_A^K(\sqrt{\omega} z) = e^{i\psi(R)} F_B^{K'}(z),
\]

\[
F_B^{K'}(\sqrt{\omega} z) = e^{-i\psi(R)} F_A^K(z).
\]

We seek the solution of the form \( F_A^K(z) \propto z^{n_A} \) and \( F_B^{K'}(z) \propto z^{n_B} \). The substitution of these into the boundary conditions gives

\[
n_A = n_B = 3m + 1,
\]

with \( m \) being an integer. Similar relations are also obtained for \( F_B^J(z) \) and \( F_B^{K'}(z) \). We have

\[
F_m^{JA}(z) = \frac{1}{\sqrt{L_5}} \begin{pmatrix}
1 \\
0 \\
0 \\
(-)^m e^{-i\psi'}
\end{pmatrix} \left( \frac{\varepsilon}{L_5} \right)^{3m+1},
\]

and

\[
F_m^{JB}(z) = \frac{1}{\sqrt{L_5}} \begin{pmatrix}
1 \\
0 \\
0 \\
(-)^m e^{i\psi'}
\end{pmatrix} \left( \frac{\varepsilon}{L_5} \right)^{3m+1},
\]

with \( e^{-i\psi'} = \sqrt{\frac{\varepsilon}{\varepsilon}} e^{-i\psi(R)} \).

The amplitude of the above wavefunctions decays or grows roughly in proportion to \( y^{3m+1} \) with the change of \( y \). In particular, we have

\[
\int_{-L(y)/2}^{+L(y)/2} F_m^{JA} \cdot F_m^{JA} dz \propto \left( \frac{L(y)}{L_5} \right)^{6m+3}.
\]

This shows that the total squared amplitude integrated over \( x \) varies in proportion to \([L(y)/(L_5)^{3m+1}]\) with the change of \( L(y) = -(2/\sqrt{3})y \). In the case of an sufficiently long junction, i.e., for small \( L_7/L_5 \), the wavefunction is dominated by that corresponding to \( m = 0 \). This means that the conductance decays in proportion to \((L_7/L_5)^3\), explaining results of numerical calculations in a tight-binding model quite well.28-28

4.3 Symmetry

The wave functions are classified by the parity \( p \) (the eigenvalue of \( \Pi \)) as follows:

- Parity – even \( (p = +1) \)
  \( F_0^{K^-}, F_0^{K'^-} \)
  \( F_n^{K^+}(z) - iF_n^{K'^+}(z), F_n^{K'^+}(z) + iF_n^{K'}(z); \)
  \( F_n^{K^+}(z) - iF_n^{K^-}(z), F_n^{K^-}(z) - iF_n^{K'^-}(z); \)

- Parity – odd \( (p = -1) \)
  \( F_0^{K'^-}, F_0^{K'^-} \)
  \( F_n^{K^+}(z) + iF_n^{K'^+}(z), F_n^{K'^+}(z) - iF_n^{K'}(z); \)
  \( F_n^{K^+}(z) + iF_n^{K^-}(z), F_n^{K^-}(z) + iF_n^{K'^-}(z); \)

where \( n = 1, 2, \ldots \) and \( m = 0, \pm 1, \pm 2, \ldots \) .

4.4 Connecting Solutions

We put the right-going wave \( F_0^{K^+} \) from the left side of the junction (through the thicker tube). A part of the wavefunction is reflected back into the thicker tube region, while the rest is transmitted through the junction region into the thinner tube. To obtain the overall wavefunction of the system, we should connect these three types of solutions at the boundary \( y = y_5 \) and at \( y = y_7 \). For this purpose, it is sufficient to set the value of these functions equal on the boundaries, since
our Hamiltonian is linear in $k_x$ and $k_y$. Moreover, we can consider the odd-parity solutions only, because they are independent of the solutions of the opposite parity.

At $y = y_6$, the conditions are written as

$$F_0^{K^+} + \alpha_0^{K^+} - F_0^{K^-} + \sum_{n > 0} \alpha_n^{K^+} (F_n^{K^+}(z) - iF_n^{K^-}(z)) + \sum_{n > 0} \alpha_n^{K^-} (F_n^{K^-}(z) + iF_n^{K^+}(z)) = \sum_m A_m (F_m^{JA}(z) + iF_m^{JB}(z)),$$

(4.13)

with $z = x + iy_6$ and $\xi = x - iy_6$ ($-L_5/2 < x < +L_5/2$), where $\alpha_n^{K^+}$, $\alpha_n^{K^-}$, and $A_m$ are expansion coefficients.

At $y = y_7$, on the other hand, we have

$$\alpha_0^{K^+} F_0^{K^+} + \sum_{n > 0} \alpha_n^{K^+} (F_n^{K^+}(z) + iF_n^{K^+}(\xi)) + \sum_{n > 0} \alpha_n^{K^-} (F_n^{K^-}(z) - iF_n^{K^-}(\xi)) = \sum_m A_m (F_m^{JA}(z) + iF_m^{JB}(z)),$$

(4.14)

for $z = x + iy_7$ and $\xi = x - iy_7$ ($-L_7/2 < x < +L_7/2$).

We take the Fourier components of each side of eq. (4.13) and obtain the following set of linear equations for coefficients $\alpha$'s and $A$'s.

$$\sum_m A_m I_m,0 = \frac{1}{\sqrt{2}},$$

$$\sum_m (-1)^m A_m I_m,0 = \frac{1}{\sqrt{2}} e^{i\psi},$$

(4.15)

and

$$\sum_m A_m I_m,-n = 0,$$

$$\sum_m (-1)^m A_m I_m,-n = 0,$$

$$\sum_m A_m I_m,n = \alpha_n^{K^+},$$

$$\sum_m (-1)^m A_m I_m,n = \alpha_n^{K^-} e^{i\psi},$$

(4.16)

Similarly, we have from eq. (4.14)

$$\sum_m A_m I_m,0 \left( \frac{L_7}{L_5} \right)^{3m+3/2} = \frac{1}{\sqrt{2}} \alpha_0^{K^+},$$

$$\sum_m (-1)^m A_m I_m,0 \left( \frac{L_7}{L_5} \right)^{3m+3/2} = 0,$$

(4.17)

and

$$\sum_m A_m I_m,-n \left( \frac{L_7}{L_5} \right)^{3m+3/2} = \alpha_n^{K^+} e^{i\psi},$$

$$\sum_m (-1)^m A_m I_m,-n \left( \frac{L_7}{L_5} \right)^{3m+3/2} = 0,$$

(4.18)

In the above equations, we have defined

$$I_{m,n} = \int_{-1/2}^{+1/2} \left( \hat{y} + \frac{\sqrt{3}}{2} \right)^{3m+1} e^{2\pi im\hat{y}} dt.$$

(4.19)

In actual calculations, we have to limit the total number of eigenmodes in both nanotube and junction regions. In the junction region the wavefunction for $m \geq 0$ decays and that for $m < 0$ becomes larger in the positive $y$ direction. It is natural, therefore, that we retain a equal number of decaying and growing modes and have $-M \leq m \leq M-1$ when the number of different $m$'s is $2M$. The same is applicable to the nanotube region, and we have $-N \leq n \leq N$ for the Fourier series in the nanotube region. Then, the total number of coefficients is $2M + 2(2N + 1)$, while the total number of equations is $4(2N + 1)$. Therefore, the set of the equations has a unique solution if we set $M = 2N + 1$.

4.5 Two-Mode Approximation

An approximate expression for the transmission $T$ and reflection probabilities $R$ can be obtained by neglecting evanescent modes completely, i.e., by putting $N = 0$. In this case we have $M = 1$ corresponding to $m = 0$ and $-1$ and should consider only eqs. (4.15) and (4.17) with $A_0$ and $A_{-1}$. The solution gives

$$T = \frac{2 \frac{L_0^2 L_7}{(L_0^2 + L_7^2)^2}}{\pi \hbar},$$

$$R = \frac{\frac{L_0^2 - L_7^2}{(L_0^2 + L_7^2)^2}}{\pi \hbar},$$

(4.20)

They show the desired unitarity or the flux conservation, i.e., $T + R = 1$. Further, we have $T \rightarrow 1$ in the short junction ($L_7/L_5 \sim 1$) and $T \sim 4(L_7/L_5)^3$ in the long junction ($L_7/L_5 \ll 1$). Using Landauer’s formula\(^3\) the conductance of the junction is given by

$$G = 2 \frac{e^2}{\pi \hbar} T = \frac{8L_0^2 L_7^3}{(L_0^2 + L_7^2)^2},$$

(4.21)

where the factor two comes from the contribution of the K and K' points. Figure 7 compares this two-mode result with those obtained in a tight-binding calculation for metallic armchair and zigzag nanotubes.\(^3\) This simple analytic expression seems to overestimate the conductance slightly in the region $L_7/L_5 \sim 1/2$, but the overall agreement is surprisingly good.
§5. Numerical Results

In actual calculations, we cannot make $M$ and $N$ arbitrarily large because of the problem of the numerical accuracy due to the presence of both decaying and growing solutions in the junction region. In the following, we shall choose $M$ for a given value of $L_7/L_5$ in such a way that $(\sqrt{3}L_7/2L_5)^3 M < \delta$, where $\delta$ is a positive quantity much smaller than unity. With the decrease of $\delta$, the number of the modes included in the calculation increases.

Because cutoffs $M$ and $N$ have been introduced, the resulting transmission and reflection probabilities do not necessarily satisfy the flux conservation condition $T + R = 1$. In fact, the flux is conserved automatically only if the wave function is continuous at the boundary of a nanotube and the junction region. In the following we shall renormalize them so as to fulfill the flux conservation, i.e., $T \rightarrow T/(T + R)$ and $R \rightarrow R/(T + R)$. Note that the two-mode result mentioned in the previous section satisfies the conservation but is highly likely to be just exceptional.

The convergence of the results with the increase of the number of modes is expected to be slow because two wave functions satisfying different boundary conditions should be connected to each other. Further, the wavefunctions can be singular around a five- and seven-member ring. In fact, the conditions given by eq. (3.32) give immediately that $F_A \propto F_A^{KR} \propto \delta^3$ and $F_B \propto F_B^{KR} \propto \delta^3$ around the five-member ring where $\beta = (3m - 4)/5$ with $m = 0, 1, \ldots$. The lower bound of integer $m$ is determined by the condition that the probability amplitude does not diverge when being integrated. Similarly, the conditions given by (3.33) give that $F_A \propto F_A^{KR} \propto \delta^3$ and $F_B \propto F_A^{KR} \propto \delta^3$ around the seven-member ring where $\beta = (3m - 5)/7$ with $m = 0, 1, \ldots$. This shows that the wave function can have a singularity of the form $r^{-4/5}$ or $r^{-1/5}$ in the vicinity of a five-member ring and $r^{-5/7}$ or $r^{-2/7}$ in the vicinity of a seven-member ring, where $r$ is the distance from the defect position.

![Fig. 7](image_url) The conductance obtained in the two-mode approximation and tight-binding results of armchair and zigzag nanotubes versus the effective length of the junction region $(L_5 - L_7)/L_5$.

![Fig. 8](image_url) Calculated conductance versus the effective length of the junction region $(L_5 - L_7)/L_5$. The results are almost independent of the value of $\delta$.

![Fig. 9](image_url) Calculated $T + R$ (not renormalized) as a function of the effective length of the junction region $(L_5 - L_7)/L_5$ for various values of $\delta$. The total number of modes in the junction region is also shown.

Figure 8 shows some examples of calculated conductance for $\delta = 10^{-4}$ and $10^{-10}$. The results do not depend on $\delta$ except in the region $L_7/L_5 \sim 1/2$, where the transmission becomes slightly smaller first with the decrease
of $\delta$ and then gradually increases with the further decrease of $\delta$. The result for $\delta = 10^{-10}$ is closer to the tight-binding result. The dependence on the value of $\delta$ is extremely small and is not important at all.

Figure 9 shows the sum $T + R$ where $T$ and $R$ have not been renormalized. The sum deviates slightly from unity in the region $L_7/L_5 \sim 1/3$ but the deviation becomes smaller with the decrease of $\delta$. The convergence is slow because of the reasons mentioned above. The figure shows also the total number of modes in the junction region included in the calculation.

§6. Summary and Conclusion

We have obtained the boundary conditions for envelope functions in junctions of two carbon nanotubes with different circumferences. The boundary conditions mix wave functions associated with $K$ and $K'$ points in the junction region sandwiched by a five- and seven-member ring. The wavefunctions obtained analytically at $\varepsilon = 0$ decay linearly with the distance from the boundary with the thicker nanotube, showing that the conductance decays with the junction length in proportion to its third power, in agreement with results of numerical simulations.

Acknowledgments

The authors thank Professor Riichiro Saito, Dr. Takeshi Nakanishi, and Dr. Ryo Tamura for valuable discussion. This work was supported in part by Grant-in-Aid for Scientific Research from Ministry of Education, Science and Culture. Numerical calculations were performed in part on FACOM VPP500 in Supercomputer Center, Institute for Solid State Physics, University of Tokyo.

32) T. Nakanishi: (private communication).