Analysis of quantum conductance of carbon nanotube junctions
by the effective mass approximation

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Abstract

The electron transport through the nanotube junctions which connect the
different metallic nanotubes by a pair of a pentagonal defect and a heptagonal
defect is investigated by Landauer’s formula and the effective mass approx-
imation. From our previous calculations based on the tight binding model,
it has been known that the conductance is determined almost only by two
parameters, i.e., the energy in the unit of the onset energy of more than two
channels and the ratio of the radii of the two nanotubes. The conductance is
calculated again by the effective mass theory in this paper and a simple an-
alytical form of the conductance is obtained considering a special boundary
conditions of the envelop wavefunctions. The two scaling parameters appear
naturally in this treatment. The results by this formula coincide fairly well
with those of the tight binding model. The physical origin of the scaling law
is clarified by this approach.

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Since the discovery of the carbon nanotubes [1], they attract much interest as one dimensional conductor with nanometer size. It has been theoretically predicted that they become metallic or semiconducting according to the radius and the helicity of the honeycomb lattice forming the tubes. [2] Electronic devices with nanometer size might be available by using the metallic nanotubes as leads. Therefore we concentrate our discussion to the metallic nanotubes in this paper. Recently, it becomes possible to measure conductance of the individual nanotubes. [3] It is expected that such technological progress leads the realization of the nanometer devices.

The nanotubes can be combined naturally by introducing a pair of a pentagonal defect and a heptagonal defect as observed by Iijima. [4–8] Such defects are called disclinations and are necessitated to form various structures composed of curved surface of graphitic layer, for example, fullerenes, [9] minimal-surface structures [10], torus structures [11], cap structures at the end of the tube [12] and helical nanotubes [13]. The disclinations and their configurations have much influence in both of their geometrical structures and electronic structures. [14] Various remarkable examples have been reported on the crucial role of the disclination. However, it is still unclear that what are the essential physics governing their effects on the electronic states of nano-structures.

In the preceding papers, we calculated the conductances of the junctions between the two metallic nanotubes by using a tight binding model including only the $\pi$ orbitals. [5,6] Our calculations based on Landauer’s formula have revealed a remarkable scaling law; the conductances of the junctions are determined almost only by two parameters in a certain Fermi energy region. [5] Especially just at Fermi level of the undoped system, the conductance is almost determined only by the ratio of the circumference of the nanotubes. [6] The result indicates that only the size and shape of the junctions are necessary to determine their conductances. Therefore the helicity of the honeycomb lattice is not relevant to determine the conductance, so far as the junctions of the metallic nanotubes are concerned. It suggests that some continuum theory ignoring the atomic details but including only the size and shape of the junctions is valid, which would give some transparent viewpoint of the
scaling law.

Very recently, Matsumura and Ando proposed the effective mass approximations as one of such continuum theories. [15] They applied it to the electron transport of the nanotube junctions and made the physical meaning of the scaling law somewhat clear. But their discussion is limited just to the case of the fixed Fermi energy case of the undoped system and the conductance is not given as an analytical form, as far as we know. In this paper, their discussion is generalized to the systems with general Fermi levels. Furthermore, the final result of the conductance is represented by a closed analytical form which gives a transparent view points.

First of all, we explain the Bloch state of a monolayer graphite forming the single wall nanotube by a simple tight binding model and relate it to the effective mass theory. [16] Fig.1 shows the development map of the nanotube. The vector $\vec{R}$ represents the circumference of the tube. Two parallel lines perpendicular to $\vec{R}$ and parallel to the tube axis are connected with each other to form the tube. Here we use two pairs of the basic translation vectors $\{\vec{e}_1, \vec{e}_2\}$ and $\{\vec{e}_{1'}, \vec{e}_{2'}\}$, where $\vec{e}_{1'} = (\vec{e}_1 + \vec{e}_2)/\sqrt{3}$ and $\vec{e}_{2'} = \vec{e}_2 - \vec{e}_1$, to represent components of vectors on the development map. For example, the components of $\vec{R}$ in Fig.1 are represented as $(R_1, R_2) = (2, 5)$ and $(R_{1'}, R_{2'}) = (7\sqrt{3}/2, 1.5)$. In this paper, we concentrate our discussion to the metallic nanotube, so that only the tube of which $R_1 - R_2$ is an integer multiple of three is considered. [2] The four basic translation vectors have the same length which is about 0.25 nm and denoted by $a$ hereafter. The wavefunction can be represented by the Bloch state as $\psi_A(\vec{q}) = \exp(i(k_1q_1 + k_2q_2))\psi_A(0)$ for sublattice $A$ and $\psi_B(\vec{q} + \vec{\tau}) = \exp(i(k_1q_1 + k_2q_2))\psi_B(\vec{\tau})$ for sublattice $B$, where $\vec{\tau} = (\vec{e}_1 + \vec{e}_2)/3$, $\vec{q}$ is the position of the atom with integer components $q_1$ and $q_2$. When the metallic nanotube is not doped, i.e., the $\pi$ band is half filled, the Fermi energy locates at the $K$ and $K'$ corner points in the 2D Brillouin zone: corresponding wavenumbers $(k_1, k_2)$ are $(2\pi/3, -2\pi/3)$ and $(-2\pi/3, 2\pi/3)$, respectively. The corresponding energy position, i.e., the Fermi level of the undoped system, is taken to be zero hereafter. When the wavenumber $\vec{k}$ is near the corner point K, the wavenumber $\vec{k}'$ measured from the $K$ point, $(k'_1, k'_2) = (-2\pi/3 + k_1, 2\pi/3 + k_2)$,
is small so that the phase factors can be linearized as \( \exp(ik_1a) = w \exp(ik'_1a) \approx w(1 + ik'_1a) \) and \( \exp(ik_2a) = w^{-1} \exp(ik'_2a) \approx w^{-1}(1 + ik'_2a) \), where \( w = \exp(i2\pi/3) \). Then Schrödinger equation of a simple tight binding model for the Bloch state becomes

\[
E \psi_A(\vec{q}) = -i \gamma (wk'_2 + w^{-1}k'_1)a \psi_B(\vec{q} + \vec{\tau})
\]

and

\[
E \psi_B(\vec{q} + \vec{\tau}) = i \gamma (w^{-1}k'_2 + wk'_1)a \psi_A(\vec{q})
\]

Here \( \gamma \) is the hopping integral between the nearest neighboring sites, which is about \(-3\) eV. In this tight binding model, only the \( \pi \) orbital is considered and mixing between the \( \sigma \) and the \( \pi \) orbital caused by the finite curvature is neglected. By using \( \psi'_B(\vec{q}) = (-i)\psi_B(\vec{q} + \vec{\tau}) \) instead of \( \psi_B \), one can obtain

\[
E \psi_A(\vec{q}) = \frac{\sqrt{3}}{2} \gamma a(k'_{x'} - ik'_{y'}) \psi'_B(\vec{q}),
\]

and

\[
E \psi'_B(\vec{q}) = \frac{\sqrt{3}}{2} \gamma a(k'_{x'} + ik'_{y'}) \psi_A(\vec{q}),
\]

where \( k'_{x'} = (k'_1 + k'_2)/\sqrt{3} \) and \( k'_{y'} = k'_2 - k'_1 \). The solution of these equations shows the linear dispersion relation,

\[
|\vec{k}'| = \pm \frac{2E}{\sqrt{3}\gamma a}.
\]

For the one dimensional band which intersects the \( K \) point, the periodic boundary condition around the circumference is \( R_1k'_1 + R_2k'_2 = 0 \). From this condition, one can show that phase difference between \( A \) sublattice and \( B \) sublattice is represented by

\[
\psi'_B(\vec{q})/\psi_A(\vec{q}) = \pm i \exp(i\theta),
\]

where \( \theta \) is the angle of \( \vec{R} \) with respect to \( \vec{e}_{x'} \) measured anti-clockwise as shown Fig.1.

In the effective mass theory, the wavefunction is represented by \( F^K_{A,B}(\vec{q})w^{(q_1-q_2)} \), where \( F^K_{A,B} \) is the envelop wavefunction and \( w^{(q_1-q_2)} \) is the Bloch state wavefunction at the \( K \) point.
When the Fermi level $E_F$ is close to zero, the differential equation for $F_{A,B}^K$ is obtained from eq.(3) and eq.(4) along a parallel discussion by replacement $k'_x \rightarrow -i\partial_x$ and $k'_y \rightarrow -i\partial_y$ as below.

\[
(-\partial_y - i\partial_x)F_B^K = kF_A^K \quad (7)
\]

\[
(\partial_y - i\partial_x)F_A^K = kF_B^K \quad (8)
\]

Here $k = |\vec{k}'|$ and the isotropic linear dispersion relation (3) is used. When $\bar{F}_B^K = \exp(-i\theta)F_B^K$ is used instead of $F_B^K$, the above equations are transformed into

\[
(-\partial_y - i\partial_x)\bar{F}_B^K = kF_A^K \quad (9)
\]

and

\[
(\partial_y - i\partial_x)F_A^K = k\bar{F}_B^K \quad (10)
\]

where $(x, y)$ is defined by

\[
\partial_y - i\partial_x = (\partial_y - i\partial_x')\exp(-i\theta) \quad .
\]

The above transformation corresponds to the rotation of coordinate axes from $\{\vec{e}_x', \vec{e}_y'\}$ to $\{\vec{e}_x, \vec{e}_y\}$ by the angle $\theta$ anti-clockwise so that the $x$ axis is parallel to the circumference vector $\vec{R}$ as shown in Fig.1. In the following discussion, the $(x, y)$ coordinates are used and $\bar{F}_B^K$ is written simply as $F_B^K$ for simplicity. It can be seen from eq.(5) that the Bloch state wavefunction for the one dimensional band intersecting the $K$ point is represented by $(F_A^K, F_B^K) = (1, \pm i)$. The equations of the envelop wavefunctions $F_{A,B}^{K'}$ for the $K'$ corner point can be easily obtained in a similar way as

\[
(\partial_y - i\partial_x)F_B^{K'} = kF_A^{K'} \quad , (12)
\]

and

\[
(-\partial_y - i\partial_x)F_A^{K'} = kF_B^{K'} \quad . (13)
\]
Hereafter the envelop wavefunctions $F$’s are simply called the wavefunctions.

The wavefunction in the nanotube is given by the plane wave; $\exp(i(k_x x \pm k_y y))$. When the $x$ direction is taken to be parallel to the circumference of the tube, $k_x$ is quantized as $k_x(n) = 2\pi n/R$ and $k_y$ is given by $k_y(n) = \sqrt{k^2 - k_x(n)^2}$. Here $n$ is an integer representing a number of nodes around the circumference and $R$ is the circumference of the tube. When $k_y(n)$ is a real number, the channel $n$ is open and the corresponding wavefunction is extended, otherwise the channel is closed and the wavefunction shows exponential growth or decay. The number of the open channel is called the channel number. When the Fermi energy is zero, only the channel $n = 0$ is open, and therefore the channel number is kept two irrespective of $R$.

The electronic states near the Fermi energy for the undoped system ($E_F = 0$) govern the electron transport, so discussion in this paper is concentrated to this Fermi energy region where the channel number is kept two. In order to discuss the wavefunction in the junction part, the polar coordinates $(r, \theta)$ is useful. Its relation to the coordinate $(x, y)$ is usual one, i.e., $r = \sqrt{x^2 + y^2}$, $\tan \theta = y/x$. Fig. 2 is the development map of the nanotube junction where the coordinate $(x, y)$ is defined. A heptagonal defect and a pentagonal defect are introduced at A(=B) and C(=D), respectively. Therefore the indexes ‘7’ and ‘5’ are used to represent the thinner tube and thicker tube, respectively. The equilateral triangles ‘$\Delta OAB$’ and ‘$\Delta OCD$’ with bases ‘AB’ and ‘CD’ have common apex ‘O’, which is taken to be the origin of the coordinate $(x, y)$ in this paper. Then the wavefunction satisfies the wave equation $(z^2 \partial_z^2 - z \partial_z - \partial_\theta^2 - z^2)F = 0$, where $z = kr$. The solution is represented by Bessel functions $J_m$ and Neumann functions $N_m$ as

$$F = \sum_{m=-\infty}^{\infty} e^{im\theta}(c_m J_m(z) + d_m N_m(z)).$$

(14)

Matsumura and Ando have found that the wavefunction should satisfy the following boundary conditions in the junction part.

$$F^{K'}_A(z, \theta + \pi/3) = -F^K_B(z, \theta)$$

(15)
\[ F^K_B(z, \theta + \pi/3) = -\frac{1}{w} F^{'K}_A(z, \theta) \] (16)

\[ F^K_A(z, \theta + \pi/3) = F^K'_B(z, \theta) \] (17)

\[ F^{K'}_B(z, \theta + \pi/3) = w F^K_A(z, \theta) \] (18)

In these equations, \( w \equiv e^{2\pi i/3} \). From eq.(15) and eq.(16), terms in eq.(14) for \( F^{'K}_A \) and \( F^K_B \) are not zero only when \( m = 3l + 2 \) (\( l = \text{integer} \)). Because the open channel \( n = 0 \) has no node along the circumference, it is fitted to the components with smaller \( |m| \) in eq.(14) better than to those with larger \( |m| \). So we assume that one can neglect all the terms except those with \( l = 0 \) and \( l = -1 \) in eq.(14). Then the wavefunctions can be written as

\[ F^{K'}_A = e^{2i\theta} f_2(z) + e^{-i\theta} f_1(z), \] (19)

and

\[ F^K_B = -e^{2i(\theta + \pi/3)} f_2(z) - e^{-i(\theta + \pi/3)} f_1(z), \] (20)

where

\[ f_m(z) = c_m J_m(z) + d_m N_m(z) \quad (m = 1, 2). \] (21)

From eq.(15) and eq.(13), the other two wavefunction \( F^{K'}_B \) and \( F^K_A \) can be derived from \( F^{'K}_A \) and \( F^K_B \) as

\[ F^{K'}_B = -i e^{i\theta} \tilde{f}_2(z) + i e^{-2i\theta} \tilde{f}_1(z), \] (22)

\[ F^K_A = i e^{i(\theta + 2\pi/3)} \tilde{f}_2(z) - i e^{-i(2\theta + 2\pi/3)} \tilde{f}_1(z), \] (23)

where

\[ \tilde{f}_1(z) = c_1 J_2(z) + d_1 N_2(z), \]
\[ \tilde{f}_2(z) = c_2 J_1(z) + d_2 N_1(z), \] (24)
by using well known recursion formula of the Bessel functions and Neumann functions. It is easily confirmed that eq. (22) and eq. (23) satisfy the boundary conditions eq. (17) and eq. (18). The amplitude of the open channel in the tube, which is denoted by $\alpha$, is obtained from the wavefunctions in the junction part as

$$\alpha^K_{7\pm} = \frac{1}{\sqrt{2R_7}} \int_A^B dx (F^K_A \pm iF^K_B),$$  \hspace{1cm} (25)

and

$$\alpha^K_{5\pm} = \frac{1}{\sqrt{2R_5}} \int_C^D dx' (F^K_A \pm i \exp(i\phi)F^K_B),$$  \hspace{1cm} (26)

for the $K$ point. The indexes $+$ and $-$ mean directions along which the electronic waves propagate as shown in Fig. 2. $R_5$ and $R_7$ are the circumferences of the thicker tube and thinner tube, and $\phi$ is angle between 'AB' and 'CD' in the development map Fig. 2. Equations for the $K'$ points are obtained from eq. (25) and eq. (26) by replacing $i$ and $\phi$ with $-i$ and $-\phi$, respectively. To simplify the calculation, the integrations in the above equations are transformed as $\int_C^D dx' \rightarrow R_5 \int_{\frac{\pi}{6\pi-\phi}}^{\frac{\pi}{6\pi}} d\theta$ and $\int_A^B dx \rightarrow R_7 \int_{\frac{2\pi}{3\pi}}^{\frac{2\pi}{3\pi}} d\theta$. If the wavefunction in the junction varies slowly near $r = R_5$ and $r = R_7$ along the radial directions, this replacement can be allowed.

The relation among the amplitudes of the open channel in the thicker tube, $\bar{\alpha}_5 = ^t(\alpha^K_{5+}, \alpha^K_{5+}, \alpha^K_{5-}, \alpha^K_{5-})$, those in the thinner tube, $\bar{\alpha}_7 = ^t(\alpha^K_{7+}, \alpha^K_{7+}, \alpha^K_{7-}, \alpha^K_{7-})$ and the wavefunctions in the junction part, $\bar{c} = ^t(c_2, d_1, c_1, d_1)$ is summarized in the followings.

$$\bar{\alpha}_5 = \sqrt{R_5 P_5(\phi) ML(\phi)L(kR_5)}\bar{c}$$  \hspace{1cm} (27)

$$\bar{\alpha}_7 = \sqrt{R_7 P_7 ML(kR_7)}\bar{c},$$  \hspace{1cm} (28)

where $M$ are constant matrices as

$$M = \begin{pmatrix}
w & 0 & 0 & -\frac{\sqrt{3}}{2}i w \\
0 & \frac{\sqrt{3}}{2}w & i w & 0 \\
0 & -\frac{\sqrt{3}}{2} & i & 0 \\
-1 & 0 & 0 & -\frac{\sqrt{3}}{2}i \\
\end{pmatrix}.$$  \hspace{1cm} (29)
\(\Lambda(\phi)\) is a diagonal matrix, where \(\Lambda_{1,1} = \Lambda_{3,3} = \exp(-i\phi)\) and \(\Lambda_{2,2} = \Lambda_{4,4} = \exp(-2i\phi)\). \(P_T\) and \(P_5(\phi)\) are defined by eq.(25) and eq.(26), respectively. The matrix elements of \(L(z)\) are 
\(L_{11} = L_{33} = J_1(z), L_{12} = L_{34} = N_1(z), L_{21} = L_{43} = J_2(z)\) and \(L_{22} = L_{44} = N_2(z)\). The other matrix elements of \(L(z)\) are zero. The vector \(\vec{\alpha}_7\) is given by a linear transformation of \(\vec{\alpha}_5\) defined by eq.(27) and eq.(28). The transformation matrix \(T\) (i.e., \(\vec{\alpha}_7 = T\vec{\alpha}_5\)) includes three independent parameters, i.e., \(\beta \equiv R_7/R_5\), \(z_5 \equiv kR_5\) and \(\phi\). The parameter \(z_5\) is related to the Fermi Energy \(E_F\) as follows. When \(|k|\) is near zero, channel number is always two which is independent of the radius of the nanotubes. But as \(|k|\) increases, the channel number increases firstly in the thicker tube, when \(|k|\) exceeds \(k_c = 2\pi/R_5\). Owing to the linear dispersion relation eq.(5), \(z_5 = 2\pi k/k_c = 2\pi E_F/E_c\) holds where \(E_c\) is the threshold Fermi energy corresponding to \(k_c\). The transmission rates are calculated from the transfer matrix \(T\), and the conductance \(\sigma\) is obtained by Landauer’s formula as

\[
\sigma = \frac{24}{\{\beta \sum_{i=1}^{2} \sum_{j=1}^{2} (3/4)^{i-j} - 2 X_{i,j}^2\} + 6}
\]

where

\[
X_{i,j} = \pi z_5 \{ J_i(\beta z_5) N_j(z_5) - N_i(\beta z_5) J_j(z_5) \}.
\]

The obtained conductance has a remarkable feature that it does not depend on the angle \(\phi\). It is consistent with the scaling law with the two parameters \(E_F/E_c\) and \(\beta = R_7/R_5\) in Ref. [6]. When \(E_F = 0\), \(\sigma\) has a simpler form as

\[
\sigma = 8/(\beta^3 + \beta^{-3} + 2) .
\]

Eq.(32) is also fitted well to the numerical data in Ref. [5] which shows one parameter scaling law.

Fig.3 and Fig.4 show the comparison between the conductances obtained by the tight binding model and those by eq.(30) for the \((2i, 2i + 3)-(10, 13)\) junctions, where the same notation as that of Ref. [6] is used to specify the junctions. The horizontal axis is \(|E_F|\) with the unit of the absolute value of the hopping integral \(|\gamma|\). The figures are shown in the
energy range where the channel number is kept two, i.e., $|E_F| < E_c$. Agreement between the two is quite good. But difference is larger for positive Fermi energy than that for negative Fermi energies. This difference is explained as the effect of discreteness of the lattice as follows. The wavefunction tends to have opposite signs between neighboring sites when the Fermi energy is positive. But such alternating sign arrangements are not possible for the paths with odd number steps surrounding the odd membered ring defects. Such effects come from the discreteness of the lattice and can not be treated by the continuum model assumed in the the effective mass theory. It should be also noted that a drop of $\sigma$ near $E_F = E_c$ appears in the tight binding model, while it is not reproduced by eq.(30). It comes from the effects of the closed channel which are not included in eq.(30). As $E_F$ approaches $E_c$, the decay length of the closed channel $n = 1$ increases and becomes more extended so that it has more important role in the transport. When the values of $\beta = R_7/R_5$ approaches to unity 1, the conductance does not depend on $E_F$ taking the values close to the maximum value. As the parameter $\beta$ decreases, the conductance $\sigma$ near $E_F = 0$ decreases and peak structure appears at $E_F$ somewhat lower than $E_c$. When $\beta$ increases further, the height of the peak is lowered. The value of $z_5$ corresponding to the Fermi energy at the peak is about half of the first period of $J_2(z)$, and $3/4$ of that of $J_1(z)$ so that we speculate that the peak structures are formed by resonance of these radial wavefunctions. More detailed discussions will appear elsewhere.

In this paper, the scaling law of the conductance of the nanotube junctions previously found by the tight binding model can be reproduced and analyzed by the effective mass theory. It provides the analytical representation of the conductances and a clear physical interpretations. It can be also applied to various structures relating to the nanotubes.

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FIGURES

FIG. 1. Development map of the nanotube.

FIG. 2. Development map of the nanotube junctions. It is similar to that of Ref. 7. Lines 'EB' and 'FA' are parallel. Lines 'DG' and 'CH' are also parallel and their angle with respect to 'EB' and 'FA' is denoted by $\phi$. The lines 'EB','BD' and 'DG' are connected with the lines 'FA','AC' and 'CH', respectively. The rectangles 'EBAF' and 'DGHC' form the thinner tube and the thicker tube, respectively. 'BD' is the rotated 'AC' by angle of 60 degree and the quadrilateral 'ABDC' forms a junction part with a shape of a part of a cone. A heptagonal defect and a pentagonal defect are introduced at A(=B) and C(=D), respectively.

FIG. 3. The conductances of the junction between $(2i,2i+3)$ tube and $(10,13)$ tube for negative Fermi energy. Corresponding values of $i$ are attached to each graphs. The horizontal axes are the absolute value of the Fermi energy in units of the absolute value of the hopping integral $|\gamma| = -\gamma$. The hopping integral $\gamma$ is taken to be negative. They are calculated by eq.(30), and the tight binding model, each of which are represented by dotted lines and plots connected with solid lines.

FIG. 4. The same figure as Fig.2 for the positive Fermi energy.
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Conductance ($2e^2/h$)

$|E_F|$ (|$\mathcal{M}$|)