Band structures of periodic carbon nanotube junctions and their symmetries analyzed by the effective mass approximation

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The band structures of the periodic nanotube junctions are investigated by the effective mass theory and the tight binding model. The periodic junctions are constructed by introducing pairs of a pentagonal defect and a heptagonal defect periodically in the carbon nanotube. We treat the periodic junctions whose unit cell is composed by two kinds of metallic nanotubes with almost same radii, the ratio of which is between 0.7 and 1. The discussed energy region is near the undoped Fermi level where the channel number is kept to two, so there are two bands. The energy bands are expressed with closed analytical forms by the effective mass theory with some assumptions, and they coincide well with the numerical results by the tight binding model. Differences between the two methods are also discussed. Origin of correspondence between the band structures and the phason pattern discussed in Phys. Rev. B 53, 2114, is clarified. The width of the gap and the band are in inverse proportion to the length of the unit cell, which is the sum of the lengths measured along the tube axis in each tube part and along 'radial' direction in the junction part. The degeneracy and repulsion between the two bands are determined only from symmetries.

72.80.Rj,73.20.Dx,72.10.Fk
I. INTRODUCTION

Carbon nanotubes are one-dimensional structures formed by rolling up the honeycomb lattice of the monolayer graphite. Their radius and length are of nanometer and micrometer sizes, respectively. One of their interesting features, theoretically predicted and investigated experimentally, is that they become metallic or semiconducting according to the radius and the helicity of the honeycomb lattice forming the tubes. Especially metallic nanotubes are expected to be used as electric leads with nanometer size. Thus we concentrate our discussion to the metallic nanotubes in this paper.

A junction connecting different nanotubes can be formed without dangling bonds by introducing a pair of a pentagonal defect and a heptagonal defect. Such defects are called disclinations and are necessitated to form various structures composed of curved surface of graphitic layer, for example, fullerenes, minimal-surface structures, virus structures, cap structures at the end of the tube and helical nanotubes. The tight binding calculations show that the electronic states near the undoped Fermi level are drastically changed according to whether the Kekule patterns started from the different disclinations match with each other. The boundary between the mismatched Kekule patterns is called ‘phason line’ in Ref. 1 and the same word is used also in this paper. The Kekule pattern represents the periodicity of the Bloch states at the K and K’ corner points in the 2D Brillouin zone of the monolayer graphite, at which the Fermi level exists. It means that certain characters of the Bloch states remain, though the Bloch states themselves can not be the eigen states of the systems. In fact the electronic states of the junctions near the Fermi level can be described fairly well by the Bloch states multiplied by envelop functions as shown in this paper.

The way of tiling the honeycomb pattern on the nanotubes determines whether they are metallic or semiconducting. Adding only one atomic raw to a nanotube can change a metallic nanotube into a semiconducting one or vice versa. But once one knows whether the nanotube is semiconducting or metallic, necessary information to determine the electronic structures near the Fermi level is only about the size and the shape, i.e., one can forget detailed information about the honeycomb lattice such as the direction of the honeycomb row with respect to the tube axis. For example, the gap of the semiconducting tube is in inverse proportion to its radius because of the isotropic linear dispersion relation at the \( K \) and \( K' \) corner points. Another example is the conductances of the junction connecting two metallic nanotubes. It is determined almost only by the ratio of the circumferences of the nanotubes and the ratio \( |E/E_c| \), where \( E_c \) is threshold energy above which the channel number increases.

Both examples are independent of the helicity of the honeycomb lattice and suggest that some continuum theory ignoring the atomic details but including only the size and shape of the systems is effective. The continuum theory describing the envelope factors of the wave functions is known as the effective mass theory or the \( k \cdot p \) approximation. Purpose of this paper is to explain the origin of the correspondence between the band structures and the phason line of the periodic nanotube junctions by using this theory. Especially, whether the bands are degenerate or avoid each other is related to the symmetries as discussed in section 15. Furthermore dependence of the band structures on the size and the shape of the system is discussed in detail based on this theory.

II. EFFECTIVE MASS THEORY AND ITS APPLICATION TO THE SINGLE NANOTUBE JUNCTION

The single junction is discussed in this section, which provides a basis for the discussions of the periodic junctions. The expression is changed from that of our previous paper and other references to facilitate discussions. First of all, we explain the Bloch state of a monolayer graphite forming the single wall nanotube by the tight binding model and relate it to the effective mass theory. 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 vectors \( \{ \bar{e}_x, \bar{e}_y \} \) and \( \{ \bar{e}_x, \bar{e}_y \} \), where \( \bar{e}_x = (\bar{e}_1 + \bar{e}_2)/\sqrt{3} \) and \( \bar{e}_y = \bar{e}_2 - \bar{e}_1 \), 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 \( (R_x, R_y) = (7\sqrt{3}/2, 1.5) \). 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. The four vectors have the same length which is about 0.25 nm and denoted by \( a \) hereafter. The amplitudes of the wave function at \( \vec{q} = (q_1, q_2) \) and at \( \vec{q} + \vec{\tau} = (q_1 + 1/3, q_2 + 1/3) \) are represented by \( \psi_i(A, \vec{q}) \), respectively, with integer components \( q_1 \) and \( q_2 \).

The wave function \( \psi \) can be represented by the Bloch state as \( \psi_i(\vec{q}) = e^{i(k_1q_1 + k_2q_2)n}\psi_i(0) \) \((i = A, B)\). 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: the corresponding wave numbers (\( k_1a, k_2a \)) are \((2\pi/3, -2\pi/3)\) and \((-2\pi/3, 2\pi/3)\), respectively. The corresponding energy position, i.e., \( E \), the Fermi level of the undoped system, is taken to be zero hereafter. Near the undoped Fermi level, i.e., when the wavenumber \( k \) is near the corner point \( K \), the wavenumber \( k' \) measured from the \( K \) point, \( (k_1', k_2') = (k_1a - 2\pi/3, k_2a + 2\pi/3) \), is small so that the phase factors can be linearized as \( \exp(ik_1a) = w \exp(ik_1' a) \approx w (1 + ik_1' a) \) and \( \exp(ik_2a) = w^{-1} \exp(ik_2' a) \approx w^{-1} (1 + ik_2' a) \), where \( w \equiv \exp(2\pi i/3) \).
Then Schrödinger equation of a simple tight binding model for the Bloch state becomes

\[ E \psi_A(\vec{q}) = \frac{\sqrt{2}}{2} \gamma a (k_y' + ik_x') \psi_B(\vec{q}) \]  

and

\[ E \psi_B(\vec{q}) = \frac{\sqrt{3}}{2} \gamma a (k_y' - ik_x') \psi_A(\vec{q}) \]

where \( k_x' = (k_1 + k_2')/\sqrt{3} \) and \( k_y' = k_2' - k_1' \). Here \( \gamma (\approx -2.7 \text{ eV}) \) is the hopping integral between the nearest neighboring sites. 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. 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 \( R_1 k_1' + R_2 k_2' = 0 \). From this condition, one can show that phase difference between \( A \) sublattice and \( B \) sublattice is represented by

\[ \psi_B(\vec{q})/\psi_A(\vec{q}) = \pm \exp(i\eta) \]  

where \( \eta \) 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 wave function is represented by

\[ \psi_i(\vec{q}) = F_i^K(\vec{q}) w(q_1 - q_1) + F_i^{K'}(\vec{q}) w(q_2 - q_1) \quad (i = A, B). \]  

where \( F_i^K, F_i^{K'} \), \( w(q_1 - q_1) \), \( w(q_2 - q_1) \) are the envelop wave functions, the Bloch state wave function at the \( K \) point and that at the \( K' \) point, respectively. This definition of \( F_i's \) is different from that of our previous paper and other references by certain factors. The reason why this definition is used is that the representation of the time reversal operation \( I \) becomes simpler as

\[ I(F^K_A, F^K_B, F^{K'}_A, F^{K'}_B) = (-i\partial_y + \partial_x)F^K_B = kF^K_A \]  

\[ (-i\partial_y - \partial_x)F^K_A = kF^K_B \]  

Here \( k \equiv |\vec{k}'| \) and the isotropic linear dispersion relation \( \vec{K} \) is used. The equations of the envelop wave functions \( F^{K'}_{A,B} \) for the \( K' \) corner point can be easily obtained in a similar way as

\[ (i\partial_y + \partial_x)F^{K'}_B = kF^{K'}_A \]  

\[ (i\partial_y - \partial_x)F^{K'}_A = kF^{K'}_B \]  

Hereafter the envelop wave functions \( F's \) are often simply called the wave functions.

It can be seen from eq. (4) that the Bloch state wave function for the one dimensional band intersecting the \( K \) point is represented by the envelop wave functions \( (F^K_A, F^K_B, F^{K'}_A, F^{K'}_B) \) as

\[ \psi_{K\pm}(\vec{q}) = (e^{-i\eta /2}, \pm e^{i\eta /2}, 0, 0) \]  

where the upper sign and the lower sign represent the direction of the propagating waves. Here, positive direction is taken to be from the thicker tube to the thinner tube, as is shown in Fig. 2. From the propagating waves near the \( K \) point, the other propagating waves \( \psi_{K'\pm} \) are obtained by the time reversal operation \( I \) as

\[ \psi_{K'\pm} = I \psi_{K\mp} = (0, 0, e^{i\eta /2}, \mp e^{-i\eta /2}) \]  

Note that the direction of the propagation is reversed by the time reversal operation \( I \).

When the direction of \( x' = x(\text{R}) \) is taken to be parallel to the circumference of each tube as shown Fig. 2, \( k'_y' \) is quantized as \( k'_y(n) = 2\pi n/R \) 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 wave function is extended, otherwise the channel is closed and the wave function shows exponential grow 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 to two irrespective of \( R \).

The electronic states at the Fermi energy \( (E_F = 0) \) govern the electron transport for the undoped system, so discussion in this paper is concentrated to the energy region near zero where the channel number is kept to two. In order to discuss the wave function in the junction part, the polar coordinate \( (r, \theta) \) is useful. Its relation to the coordinate \( (x, y) \) is the 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 origin of the coordinate is defined. A heptagonal defect and a pentagonal defect
are introduced at $P_5(=Q_5)$ and $P_7(=Q_7)$, respectively. Thus from now on, the indices '7' and '5' are used to represent the thinner and the thicker tube, respectively. The equilateral triangles 'ΔOP_7Q_7' and 'ΔOP_5Q_5' with bases 'ΔP_7Q_7' and 'ΔP_5Q_5' have common apex $O$, which is taken to be the origin of the coordinate $(x,y)$ in this paper. Then the wave function satisfies the wave equation $(z^2\partial^2_z + z\partial_z + \partial^2_\theta + z^2)F = 0$, where $z = kr$. The solution is represented by Bessel functions $J_m$ and Neumann functions $N_m$ as

$$F = \sum_{m=-\infty}^{\infty} e^{im\theta} (c_m J_m(z) + d_m N_m(z)). \quad (13)$$

The boundary condition in the junction part is $\psi(r,\theta + \pi/3) = \psi(r,\theta)$. It is represented by

$$\psi_A(q_1, q_2) = \psi_B(q_1 + q_2, -q_1 - 1) \quad (14)$$

$$\psi_B(q_1, q_2) = \psi_A(q_1 + q_2 + 1, -q_1 - 1)$$

where $q = (q_1, q_2)$ is the position of arbitrary atoms in the junction part. Fig. 3 shows an example where $q_1 = q_2$, i.e., the points $B(2i, -i - 1)$ and $A(2i + 1, -i - 1)$ on line $OQ$ are transformed into $A(i, i)$ and $B(i, i)$ on line $OP$, respectively, under the rotation by $\pi/3$ with respect to the origin $O$. The angle $\theta$, i.e., the direction of $OQ$ can be taken arbitrary. In Fig. 3, it is taken to be parallel to the bond, i.e., $\theta = -\pi/3$, only to simplify the presentation.

From eq. (14) and eq. (3), the boundary conditions in the junction part are represented by

$$F_A^K'(z, \theta + \pi/3) = w F_A^K(z, \theta), \quad (15)$$

$$F_B^K(z, \theta + \pi/3) = w F_A^K'(z, \theta), \quad (16)$$

$$F_A^K(z, \theta + \pi/3) = \frac{1}{w} F_B^K(z, \theta), \quad (17)$$

$$F_B^K(z, \theta + \pi/3) = \frac{1}{w} F_A^K(z, \theta). \quad (18)$$

Similar boundary conditions are discussed by Matsumura and Ando. But the boundary conditions, eq. (14), eq. (13) and eq. (3) are different from those of Matsumura and Ando by certain factors due to the difference of the definition of $F_{A,B}^{K,K'}$. In these equations and hereafter, $w = e^{i2\pi/3}$. From eq. (13) and eq. (14), terms in eq. (14) for $F_A^K$ and $F_B^K$ are not zero only when $m = 3l + 2$ ($l$ = integer). Because the open channel $n = 0$ has no node along the circumference, it is better fitted to the components with smaller $|m|$ in eq. (14) 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) (Assumption I). Then the wave functions can be written as

$$F_A^{K'} = e^{i2\theta} f_2(z) + e^{-i\theta} f_1(z), \quad (19)$$

and

$$F_B^{K'} = e^{i2\theta} f_2(z) - e^{-i\theta} f_1(z), \quad (20)$$

where

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

From eq. (8) and eq. (9), the other two wave functions $F_B^K$ and $F_A^K$ can be derived from $F_A^{K'}$ and $F_B^{K'}$ as

$$F_B^K = -i\theta f_2(z) + e^{-i2\theta} f_1(z), \quad (22)$$

$$F_A^K = e^{i\theta} f_2(z) + e^{-i2\theta} f_1(z), \quad (23)$$

by using the 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. (8). The amplitude of the open channel in the tube, which is denoted by $\alpha$, is obtained from eq. (3) as

$$\alpha_{j \pm}^K = \frac{1}{\sqrt{2R_j}} \int_{Q_j}^{P_j} dx_j (e^{i\frac{2\pi}{3} R_j} F_A^K \pm e^{-i\frac{2\pi}{3} R_j} F_B^K) \quad (j = 5, 7), \quad (25)$$

for the $K$ point. The indices $+$ and $-$ mean directions in which the electronic waves propagate. $R_5$ and $R_7$ are the circumferences of the thicker tube and thinner tube. Path of integral is the straight line $F_j Q_j$, the angle of which is denoted by $\eta_j$ with respect to $x$ axis. Equations for $\alpha_{j \pm}^K$ are obtained from eq. (23) by replacing $\pm$ and $K$ in r. h. s with $\mp$ and $K'$, respectively. To simplify the calculation, the integrations in the above equations are transformed as

$$\int_{Q_j}^{P_j} dx_j \rightarrow R_j \int_{-\frac{5\pi + \eta_j}{3}}^{-\frac{\pi + \eta_j}{3}} d\theta. \quad (26)$$

If variation of the wave function along the radial directions is slow near $r = R_j$, this replacement can be allowed (Assumption II). The relation between the amplitudes of the open channel in each tube, $\hat{\alpha}_j = (\alpha_{j \pm}^K, \alpha_{j \mp}^K)$, and the coefficients representing the wave functions in the junction part, $\tilde{c} = (c_2, d_2, c_1)$, are summarized in the followings.

$$\hat{\alpha}_j = \sqrt{R_j} M L \Lambda(\eta_j) L(k R_j) \tilde{c}, \quad (27)$$

where $M$ is a constant matrix given by
\[
M = \begin{pmatrix}
-i & 0 & 0 & -\frac{\sqrt{3}}{2} \\
0 & -\frac{\sqrt{3}}{2} & -i & 0 \\
0 & -\frac{\sqrt{3}}{2} & i & 0 \\
i & 0 & 0 & -\frac{\sqrt{3}}{2}
\end{pmatrix}.
\] (28)

\[\Lambda(\eta)\] is a diagonal matrix, where \[\Lambda_{1,1} = \Lambda_{3,3} = e^{i\eta}\] and \[\Lambda_{2,2} = \Lambda_{4,4} = e^{2i\eta}\]. \[P(\eta)\] is defined by eq. (25) as

\[
P(\eta) = \begin{pmatrix}
e^{i\frac{\pi}{4}}, & e^{-i\frac{\pi}{4}}, & 0, & 0 \\
0, & 0, & e^{-i\frac{\pi}{4}}, & -e^{i\frac{\pi}{4}} \\
e^{i\frac{\pi}{4}}, & -e^{-i\frac{\pi}{4}}, & 0, & 0
\end{pmatrix}. \tag{29}
\]

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. From eq. (27), the relation between \(\beta\) (ratio between the radii) , \(\phi = \eta_1 - \eta_5\) (angle between the tube axes in the development map) and \(z \equiv kR_5\) as

\[
\left(\begin{array}{c}
\alpha_7^+ \\
\alpha_7^-
\end{array}\right) = \left(\begin{array}{c}
t_1, \\
t_2, \\
t_1, \\
t_2
\end{array}\right) \left(\begin{array}{c}
\alpha_5^+ \\
\alpha_5^-
\end{array}\right). \tag{30}
\]

where

\[
t_1 = h_+ \left(\begin{array}{c}
\cos(\frac{3}{2}\phi), \\
i \sin(\frac{3}{2}\phi)
\end{array}\right) \tag{31}
\]

\[
t_2 = h_- \left(\begin{array}{c}
\cos(\frac{3}{2}\phi), \\
i \sin(\frac{3}{2}\phi)
\end{array}\right). \tag{32}
\]

The factors \(h_+\) and \(h_-\) are represented by

\[
h_\pm = -\frac{1}{4}(X_{12} \mp X_{21}) + \frac{i}{2\sqrt{3}}(X_{11} \pm \frac{3}{4}X_{22}) \tag{33}
\]

where

\[
X_{ij} = \sqrt{3}\pi z\{J_i(\beta z)N_j(z) - N_i(\beta z)J_j(z)\}. \tag{34}
\]

The matrix in eq. (30) is called the transfer matrix of the junction, denoted by \(T_s\), hereafter. We assume here that evanescent waves can be neglected. (Assumption III) It can be easily confirmed that \(T_s\) in eq. (30) satisfies the time reversal symmetry and unitarity (See Appendix I). The parameter \(\alpha\) is related to the Fermi energy \(E_F\) as follows. When \(|k|\) is near zero, channel number is always two 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. (3), \(|z| = 2\pi k/k_c = 2\pi E_F/E_c\) holds where \(E_c\) is the threshold Fermi energy corresponding to \(k_c\). The transmission rates are calculated from the transfer matrix, and the conductance \(\sigma\) is obtained by Landauer’s formula as

\[
\sigma = 2|h_s|^2 = \frac{24}{\left\{\sum_{j=1}^2 \sum_{j=1}^2 (3/4)^{j-2} X_{ij}^2 \right\} + 6}. \tag{35}
\]

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. (34). Agreement between the two methods is fairly good. When \(\beta \sim 1\), \(\sigma\) is almost constant with a value near 2 in units of \(2e^2/h\). As \(\beta\) decreases, peak structures appear at \(E\) slightly below \(E_c\). The former case, \(\beta \sim 1\), is treated mainly in the following sections. In this case, \(\sigma\) is almost the same as that of \(E_F = 0\), which is

\[
\sigma = 8/(\beta^3 + \beta^{-3} + 2). \tag{36}
\]

Eq. (34) reproduces well the numerical results in Ref. (34).

### III. Band Structures of the Periodic Nanotube Junctions

From now on, \(a\) which is the length of the translation vectors \(\vec{e}_1, \vec{e}_2,\) and \(\frac{\sqrt{3}}{2}\gamma\), which is the hopping integral between the nearest neighbors multiplied by \(\frac{\sqrt{3}}{2}\), are taken to be units of the length and the energy, respectively. So \(a\) and \(\frac{\sqrt{3}}{2}\gamma\) are omitted in the following expressions. Fig. (3) shows the unit cell of the periodic junctions, which is composed by the two equivalent nanotube junctions, where one of the junctions is rotated by \(\pi\) with respect to the other. The unit cell in the development map is determined by four vectors: the circumference of the thicker tube \(R_5 = (m_5, n_5)\), that of the thinner tube \(R_7 = (m_7, n_7)\), the vector connecting the two pentagons in the thicker tube part, \(L^{(5)} = (L_1^{(5)}, L_2^{(5)})\) and that connecting the two heptagons in the thinner tube part \(L^{(7)} = (L_1^{(7)}, L_2^{(7)})\). The components of these vectors are referred to \((\vec{e}_1, \vec{e}_2)\), so that all of them are integers. In our discussion they can be taken arbitrary integers, so far as both of \(m_7 - n_7\) and \(m_5 - n_5\) are multiples of three. The transmission matrix \(T_s\) is determined by eq. (30) \(\sim\) eq. (34), using \(R_j = |R_j| = \sqrt{m_j^2 + n_j^2 + m_j n_j}\) \((j = 5, 7)\), and \(\cos \phi = (m_5 m_7 + n_5 n_7 + 2(m_5 n_7 + m_7 n_5))/(|R_5 R_7|)\). The transfer matrix of the unit cell \(T_p\) is obtained by combining the two identical transfer matrices of the junction, \(T_s\). Fig. (4) is a schematic view of this combination. The scattering occurs as \(\vec{a}_7^L = T_s \vec{a}_7^R\) in the left junction and \(\vec{a}_5^R = T_s \vec{a}_5^L\) in the right junction. Here superscripts \(L\) and \(R\) mean the the coordinate systems, origins of which are the left heptagon and the right heptagon , respectively. The coordinate system \(L\) is transformed to \(R\) with the rotation by \(\pi\) and the translation \(L^{(7)}\). Therefore the coordinates \(q^L\) and the sublattices \((A, B)\) of \(L\) are transformed to those of \(R\) as

\[
(q^R, \psi_B^R(q^R)) = (\psi_B^L(q^L), \psi_A^L(q^L)) \tag{37}
\]
As is known from eq. (11) and eq. (12), the Bloch state wave function corresponding to $\alpha_{L,7}^L$ and $\alpha_{L,7}^R$ is

$$\langle \psi_A^L(q^-), \psi_B^L(q^-) \rangle = (e^{\pm i n/2} + e^{\pm i n/2}) e^{i \tilde{q} \cdot \tilde{r}} u^\pm (\tilde{q}^1 - \tilde{q}^2) \alpha_{L,7}^L$$

(38)

and that corresponding to $\alpha_{L,7}^R$ and $\alpha_{L,7}^R$ is

$$\langle \psi_A^R(q^+), \psi_B^R(q^+) \rangle = (e^{\pm i n/2} + e^{\pm i n/2}) e^{-i \tilde{q} \cdot \tilde{r}} w^\pm (\tilde{q}^1 - \tilde{q}^2) \alpha_{L,7}^R$$

(39)

where the upper signs and the lower signs correspond to $K$ and $K'$, respectively. From eq. (37), eq. (38), and eq. (39), the relation between $\alpha_{L,7}^L$ and $\alpha_{L,7}^R$ is obtained as

$$\frac{\alpha_{L,7}^R}{\alpha_{L,7}^L} = \exp(i k_7^5 \cdot \tilde{L}^{(7)}) \begin{pmatrix} w^{l_7} & 0 \\ 0 & -w^{-l_7} \end{pmatrix} \frac{\alpha_{L,7}^L}{\alpha_{L,7}^R}$$

(40)

where $l_7 \equiv L_1^{(7)} - L_2^{(7)}$. In the same way,

$$\frac{\alpha_{L,7}^R}{\alpha_{L,7}^L} = \exp(i k_7^5 \cdot \tilde{L}^{(5)}) \begin{pmatrix} w^{l_5} & 0 \\ 0 & -w^{-l_5} \end{pmatrix} \frac{\alpha_{L,7}^L}{\alpha_{L,7}^R}$$

(41)

where $l_5 \equiv L_1^{(5)} - L_2^{(5)}$. Since $w^3 = 1$, $l_i$ can take either values of 0, or $\pm 1$ (mod 3). In order to visualize the integer $l_i$, the Kekule pattern with thick bonds and thin bonds are drawn in the development map so that the pentagons and the heptagons have only thin bonds as shown in Fig. 1. Domain boundary caused by mismatch of the pattern, which is called ‘the phonon line’ according to Ref. 13 occurs in the thicker tube (thinner tube) only when $l \pm 1$ ($l \equiv 1, \pm 1$). The reason for this correspondence is that the Bloch states at the $K$ and $K'$ corner points have the same periodicity as that of the Kekule pattern. Note that we do not intend here that the Kekule pattern represents the bond alternation. In this paper, the Kekule pattern is used only to show the periodicity of the Bloch states at the $K$ and $K'$ corner points.

The $2 \times 2$ diagonal matrices in equations (38) and (41) are denoted by $A_5$ and $A_7$, respectively. Then the transfer matrix of the unit cell, $T_p$, is obtained as

$$T_p = \begin{pmatrix} T_1 & T_2 \\ T_2 & T_1 \end{pmatrix}$$

(42)

where

$$T_1 = A_5^{1/2} (t_1 \Lambda_7 t_1^{-1} - t_2 \Lambda_7^{-1} t_2) A_5^{1/2}$$

$$T_2 = A_5^{1/2} (t_1 \Lambda_7^{-1} t_2 - t_2 \Lambda_7 t_1) A_5^{1/2}$$

(43)

Above equations (43) show that $t^* T_1 = T_1$ and $t^* T_2 = -T_2^*$. It means that

$$T_p^{-1} = T_p^*$$

(44)

where eq. (34) in Appendix is used. If $\tilde{x}$ is an eigen vector of $T_p$ with an eigen value $\lambda$, i.e., $T_p \tilde{x} = \lambda \tilde{x}$, it is also the eigen vector of $(T_p + T_p^{-1})/2 = \text{Re}(T_p)$ with the eigen value $\frac{1}{2} (\lambda + 1/\lambda)$. When $\lambda = \exp(i k(p))$ with a real value of $k(p)$, $k(p)$ is the Bloch wavenumber of the periodic junctions. The Bloch wavenumber $k(p)$ is obtained from the eigen value of the real matrix $\text{Re}(T_p)$ as $\cos(k(p)) = \frac{1}{2} (\lambda + 1/\lambda)$. Furthermore $\text{Re}(T_p)$ can be block diagonalized as

$$\begin{pmatrix} 1/2 (1, 1) & \text{Re}(T_1), \text{Re}(T_2) \\ 0 & \text{Re}(T_1), \text{Re}(T_2) \end{pmatrix}$$

(45)

The eigen values of $\text{Re}(T_p)$ can be represented by those of $\text{Re}(T_1 + T_2)$ or those of $\text{Re}(T_1 - T_2)$. After all, the dimension of the matrix which has to be diagonalized can be made half. Since in this paper the Fermi energy region is considered where the channel number is kept to two, the dimension of $\text{Re}(T_1 + T_2)$ is two. The two energy bands of the periodic junctions, $k^+(p)$ and $k^-(p)$, are obtained as

$$\cos(k^+(p)) = \frac{1}{2} \left( x_{11} + x_{22} \pm \sqrt{(x_{11} - x_{22})^2 + 4x_{21}^2 - 4y_{21}^2} \right)$$

(46)

where $x_{ij} = \text{Re}(T_1)_{ij}$ and $y_{ij} = \text{Re}(T_2)_{ij}$.

We have to discuss $\Lambda$, and $T_p$ further to obtain the dispersion relation. As for the phases of $\Lambda$, $k_i^0 \cdot \tilde{L}^{(i)} = EL_i$, where $\tilde{L}_i$ is the length of $L^{(i)}$ measured along each tube axis direction, i.e., $\tilde{L}_i \equiv |\tilde{L}^{(i)} \times \tilde{R}_i|/|\tilde{R}_i| (i = 5, 7)$. It is because $k_i^0 \cdot \tilde{R}_5 = 0$ and $k_i^0 \cdot \tilde{R}_7 = 0$, that is to say, $k_5^0$ and $k_7^0$ are parallel to each tube axis for the metallic nanotubes. For the discussion of $T_*$, the phases $p_\pm$ of $h_\pm$ in eq. (33) are defined by $h_+ = \sqrt{1/\tau} \exp(ip_+)$, and $h_- = -\sqrt{1/\tau} \exp(ip_-)$. As seen from eq. (35) and unitarity, $T$ and $R$ are the transmission rate and the reflection rate per channel, respectively. $T$ determines the Landauer’s formula conductance $\sigma$, as $\sigma = 2T$ in units of $2e^2/h$. When the tubes have almost the same radius, $0.7R_5 < R_7 < R_5$, expressions about $T$ and $p_\pm$ become simple, so the discussions in the followings are concentrated on this case. In this case, the transmission rate $T$ is almost constant value irrespective of $z = 2\pi E/E_c$. Therefore eq. (36) is used instead of eq. (34) in the following discussions. The transmission coefficient $T$ is almost constant near unity, i.e., $T \sim 1$ and $R \ll 1$. When $1 > R_7/R_5 > 0.7$, the range of $T$ is confined in $1.0 > T > 0.76$. Fig. 2 shows the quantities that $(p_{s}(z_{j+1}) - p_{s}(z_{j}))/|\Delta z|$ vs. $R_7/R_5$, where $\Delta z = \pi/5$, $z_{j} = j \Delta z$, $j = 0, 1, \cdots, 9$. They represent $\frac{\partial p_{s}}{\partial z}$, for

$$0 < z < 2\pi$$

i.e., $|E| < E_c$ ($z = 2\pi E/E_c = R_5 E$). When
$R_7/R_5 \geq 0.7$, the ten plots of each $R_7/R_5$ show almost the same value. It means that the phases $p_\pm$ are almost proportional to $E$. Fig. 7 shows that the gradients of $p_\pm$ are very close to $1 - R_7/R_5$, while those of $p_-$, denoted by $q$, are almost constant between $-0.1$ and $-0.05$. Therefore when $R_7/R_5 > 0.7$ and $|E| < E_c$, approximate expressions can be obtained as

\[
p_1 \sim (R_5 - R_7)E, \quad p_2 \sim gR_5 E \quad (g = -0.1 \sim -0.05).
\]  

(47)

The following two combinations of the gradients of phases determine the band structures. One is $\Omega_+ \equiv L_5 + L_7 + 2R_5 - 2R_7$ and the other is $\Omega_- \equiv L_5 - L_7 + 2gR_5$. The former is the length of the unit cell, which is defined as the sum of the four lengths, two of which are those of the tubes measured along each tube axis and the other two are those of the junctions measured along the ‘radial’ direction.

When there is no phason line in the thinner tube, $l_7 = 0$, we obtain

\[
\cos(k^{(p)}_{\pm}) = \frac{1}{T} \cos(\Omega_+E \pm \frac{2}{3}\pi l_5) - \frac{R}{T} \cos(\Omega_-E \pm \frac{2}{3}\pi l_5).
\]

(48)

On the other hand, when there is no phason line in the thicker tube, $l_5 = 0$, the following is obtained,

\[
\cos(k^{(p)}_{\pm}) = \frac{1}{T} \cos(\Omega_+E \pm \frac{2}{3}\pi l_7) - \frac{R}{T} \cos(\Omega_-E \pm \frac{2}{3}\pi l_7).
\]

(49)

Fig. 8 shows the comparison of the band structures calculated by equations (48), (49) and the tight binding model for case (a) where there is no phason line, i.e., $l_5 = l_7 = 0$, and for case (b) where there are the phason lines in only one side of the tubes, i.e., $l_5 = \pm 1, l_7 = 0$ or $l_5 = 0, l_7 = \pm 1$. The Fermi level comes at the highest energy of the negative energy bands. The results by the two different methods agree fairly well with each other, especially for the two bands nearest to the Fermi level. The two bands are degenerate in case (a), while they cross near $k^{(p)} = 2\pi/3$ in case (b). The latter shows that the system becomes metallic in case (b). But there is a significant difference between the results by the two methods in case (a). The gap appears at $E = 0$ in the tight binding model, while it does not appear in eq. (48) and eq. (49). Because existence of this gap determines whether the system is metallic or semiconducting, this difference cannot be neglected.

To investigate the origin of this difference, we have to compare the transfer matrix obtained by the tight binding model with the one obtained by eq. (48)~eq. (54). For the transmission rate $T$, agreement between the two methods is good, as is already seen in the preceding section. The ratios between the matrix elements of $t_1$ and $t_2$ is almost the same in the two method, as will be discussed in the next section. Therefore the cause of this difference must exist in the phase factors, $p_{\pm}$. We do not get complete explanations about this discrepancy yet. But some features can be found as below. The phase factors obtained by the tight binding model are written as $p_+ = \chi_+ (R_5 - R_7)E + \epsilon_+$ and $p_- = \chi_- gR_5 E + \epsilon_-$, where $\chi_{\pm}$ and $\epsilon_{\pm}$ represent the difference from eq. (47). Fig. 9 shows $\chi_+$ as a function of the absolute value of the angle, $|\phi|$. The number of calculated junctions is 274 as explained in the figure caption. The values of $\chi_+$ are almost unity in most of the cases, but it increases when $R_7/R_5$ approaches unity and $|\phi|$ is near $\pi/6$. Though it causes a change of the gradient of the dispersion, it does not affect existence of the gap. The range of the ratio $\chi_-$ is about $0 < \alpha_- < 1$, and it does not affect the existence of the gap, either. Fig. 10 shows intercepts $\epsilon_{\pm}$ as a function of $R_5 - R_7$. The intercept of $p_+$ is almost constant with the values near $0.03\pi$, but that of $p_-$, denoted by $\epsilon_-$, approaches zero as $R_5 - R_7$ increases. Thus we speculate that the nonzero intercept $\epsilon_-$ comes from the effects of discreteness of the lattice and it causes the gap as is shown below.

The second term in eq. (48) and eq. (49) can be considered almost constant with respect to $E$ compared to the first term, when $\Omega_+ \gg \Omega_-$, which is valid for the periodic junctions with $L_7, L_5 >> |g|R_5$. Therefore the argument in the second cosine term can be substituted with $2\epsilon_-$. Then one can see that the r. h. s. of eq. (48) and eq. (49) become larger than unity near $E = 0$, and the gap opens at $k^{(p)} = 0$. The width of the gap $W_g$ is estimated as

\[
W_g \sim 2\arccos(T + R\cos (2\epsilon_-))/\Omega_+.
\]

(50)

If $\epsilon_-$ is common, $W_g$ increases as $T$ decreases, and is in inverse proportion to the length of the unit cell, $\Omega_+$.

Next, the periodic junctions in which the both kinds of tubes have the phason lines is discussed. The discussions only for $l_5l_7 = 1$ are necessary, since those for $l_5l_7 = -1$ can be easily obtained from it by substitution $\phi \rightarrow \pi/3 - \phi$. When $l_5l_7 = 1$, the dispersion relation obtained by the effective mass theory is

\[
\cos(k^{(p)}_{\pm}) = \frac{1}{T} \cos(\Omega_+E) \cos(\delta_{\pm}) - \frac{R}{T} \cos(\Omega_-E) \cos(\delta_{\pm}) \pm \frac{1}{T} \sqrt{Y} \quad \text{51}
\]

where

\[
Y = \sin^2(\Omega_+E) \sin^2(\delta_+) + R^2 \sin^2(\Omega_-E) \sin^2(\delta_-)
\]

\[
= \frac{9}{8} R^2 \sin^2 (3\phi) \cos\{(\Omega_+ - \Omega_-)E\} \cos\{(\Omega_+ + \Omega_-)E\} + 1, \quad \text{52}
\]

\[
\cos(\delta_{\pm}) = \frac{1}{4} \pm \frac{3}{4} \cos (3\phi) \quad \text{53}
\]

Fig. 11 shows an example of the band structures calculated by the tight binding model and those calculated
by eq. (51). Agreement between the two methods is also satisfactory in this case. There are two types of the gap at $E = 0$. The gap opens when $Y$ becomes negative and the r. h. s. in eq. (54) becomes a complex number. It is denoted by type $I$. The gap of the other type, denoted by $II$, occurs when the r. h. s. in eq. (51) becomes larger than unity. The gap of type $I$ appears at nonzero $k^{(p)}$ while that of type $II$ appears at $\Gamma$ point, i.e., $k^{(p)} = 0$, as is seen in Fig. 13 (a) and (b), respectively. The band structures with the gap of type $II$ are similar to those for $l_5 = l_7 = 0$ shown in Fig. 8 (a).

By neglecting the $R^2$ term in $Y$ and expanding $Y$ with respect to $E$, the width of the gap of type $I$, denoted by $W_g^I$, can be approximated as

$$W_g^I \approx \frac{2 \sin \left(\frac{2\phi}{\Omega} \right)}{\Omega} \sqrt{6R(1 + \cos^2(2\epsilon_-))/(4 - 3 \cos^2 \left(\frac{3}{2} \phi \right))}$$

(54)

Due to the gap of type $I$, the HOMO band and the LUMO band avoid each other when $k^{(p)} \neq 0, \pi$. It is related to the symmetry as will be discussed in the next section. When $\phi$ approaches zero, $W_g^I$ also approaches zero and the band structures become similar to those for $l_5 = 0, l_7 = \pm 1$ or $l_5 = 0, l_5 = \pm 1$ which is shown in Fig. 8 (b). As $\phi$ approaches $\pi/3$, the gap of type $II$ appears instead of type $I$. Its width at $\phi = \pi/3$, denoted by $W_g^{II}$, is evaluated for $-\pi < 2\epsilon_- < 0$ by

$$W_g^{II} \approx 2 \arccos(T - R \cos(2\epsilon_- + \pi/3))/\Omega_+$$

(55)

Here the correction caused by the tight binding model $\cos(2\epsilon_-)$ is included in eq. (54) and eq. (55). The gap width is again in inverse proportion to the length of the unit cell, $\Omega_+$. By using Taylor expansion, $\arccos(1-x) \approx \sqrt{2x}$ for $0 < x \ll 1$, eq. (53) can be approximated further as

$$W_g^{II} \approx 2\sqrt{R(2 + 2 \cos(2\epsilon_- + \pi/3))/\Omega_+}$$

(56)

The common factor $\sqrt{R}$ in eq. (54) and eq. (56) can be written by using eq. (48) as $\sqrt{R} = \sqrt{1 - T} \approx \frac{3}{2}(1 - R_7/R_5)$. Thus relation between the gap width and the ratio of the circumferences $R_7/R_5$ is almost linear. When $\epsilon_-$ is near zero, eq. (54) approaches eq. (49) as $\phi$ approaches $\pi/3$. It means that even when $\phi$ is close to $\pi/3$ so that type of the gap becomes $II$, eq. (54) can be used approximately as the gap width. In Fig. 12 the solid line shows $W_g^I(\phi)/W_g^I(\pi/3) = 2 \sin(3\phi/2)/\sqrt{4 - 3 \cos^2(3\phi/2)}$ as a function of $\phi$. It can be seen that the gap increases as $\phi$ approaches $\pi/3$. The dotted line shows that for $l_5l_7 = -1$, which is obtained from the solid line for $l_5l_7 = 1$ by reversing the horizontal axis.

IV. DISCUSSIONS BASED ON SYMMETRIES

In this section, we discuss what can be said by considering only the symmetry of the junctions without solving the effective mass equations. To discuss the symmetry, the scattering matrix $S$ is used. Symmetric properties of $S$ and its relation to the transfer matrix are summarized in the Appendix. The scattering matrix $S$ determines the outgoing waves for the incoming waves as

$$S = \begin{pmatrix} a_+ & b_+ \\ a_- & b_- \end{pmatrix}$$

where $a_+ = (a_+^c, a_+^s) \text{ and } a_- = (a_-^c, a_-^s)$, each component of which is defined in eq. (22). Note that the order of $K$ and $K'$ is reversed between $a_+$ and $a_-$. Consider the operation $Q_1$ defined as $Q_1(F_A^K, F_B^K, F_A^{K'}, F_B^{K'}) = (-F_B^K, F_A^K, -F_B^{K'}, F_A^{K'})$. The amplitude $\alpha$ is transformed by this operation $Q_1$ as

$$Q_1 \alpha_\pm = \pm \begin{pmatrix} 0, 1 \\ 1, 0 \end{pmatrix} \alpha_\pm \equiv \pm \sigma_1 \alpha_\pm$$

(58)

Since the effective mass theory equations (51), (52), (53), and the boundary conditions (15), (16), (17), (18) are invariant under the operation $Q_1$,

$$- \sigma_1 r_j \sigma_1 = r_j \quad (j = 5, 7)$$

(59)

$$\sigma_1 t \sigma_1 = t$$

(60)

Eq. (59) means that $r_j$ is antisymmetric. On the other hand, $r_j$ is symmetric owing to time reversal symmetry. So $r_j$ is diagonal. From eq. (59), eq. (60) and unitarity of $S$, one can write $r_j$ and $t$ as

$$r_j = \sqrt{R} e^{i \theta_j} \begin{pmatrix} 1, 0 \\ 0, -1 \end{pmatrix} \quad (j = 5, 7),$$

(61)

and

$$t = \sqrt{T} e^{i(\theta_5 + \theta_7)} \begin{pmatrix} \cos(f), i \sin(f) \\ i \sin(f), \cos(f) \end{pmatrix},$$

(62)

where $R$ and $T = 1 - R$ are the reflection rate and the transmission rate, while $\theta_j$ and $f$ are certain real values. The meaning of $f$ is discussed in the following.

Consider operation $Q_2$ shown in Fig. 13, where the thinner tube part is fixed, but the thicker tube part is rotated by $\pi/3$ in the development map. Under the operation $Q_2$, the upper development map is transformed into the lower development map, where the angle of the circumference of the thicker tube increases by $\pi/3$ as $\theta_5 \rightarrow \theta_5 + \pi/3$. Then the angle between the two tube axes defined by $\eta_7 - \eta_5$ decreases by $\pi/3$ as $\phi' = \phi - \pi/3$. The two development maps in Fig. 13 correspond to an identical junction. The difference is only how to draw the cutting line on the honeycomb plane of the junction. Therefore the $S$ matrix of the upper development map becomes
the same as that of the lower one after an unitary transformation corresponding to the operation \(Q_2\). Following the same discussions as those for the boundary conditions \([13]\), \([16]\), \([17]\) and \([18]\), \((F_A^K, F_B^K, F_A'K, F_B'K)\)|\(\theta + \pi/3\) = \((\frac{1}{w}F_B^K, wF_A^K, wF_B^K, \frac{1}{w}F_A'K)\)\(|\theta\). By using it and \(\eta_5 = \eta_5 + \pi/3\) in eq. \([25]\),

\[
Q_2\alpha_{5\pm} = \pm i\sigma_1\tilde{\alpha}_{5\pm}
\]

while \(Q_2\tilde{\alpha}_{7\pm} = \tilde{\alpha}_{7\pm}\). From this symmetry, one can derive

\[
\begin{align*}
    r_5(\phi - \pi/3) &= -\sigma_1r_5(\phi)\sigma_1 \\
    t(\phi - \pi/3) &= -i\sigma_1t(\phi)
\end{align*}
\]

which leads

\[
f(\phi) = f(0) + \frac{3}{2}\phi.
\]

Lastly, we consider the coordinate transformation from the right-handed coordinate to the left handed coordinate \(Q_3\), \((x, y) \to (-x, y)\). It causes \(\eta_j \to -\eta_j\), \(\phi \to -\phi\), and exchange between the sublattices,

\[
Q_3(F_A^K, F_B^K, F_A'K, F_B'K) = (F_B^K, F_A^K, F_B'K, F_A'K),
\]

so that

\[
Q_3\alpha_{\pm} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \alpha_{\pm} \equiv \sigma_2\alpha_{\pm}.
\]

The result deduced from it is

\[
\begin{align*}
    r_j(-\phi) &= \sigma_2r_j(\phi)\sigma_2 \\
    t(-\phi) &= \sigma_2t(\phi)\sigma_2
\end{align*}
\]

which indicates that \(f(0) = 0\) in eq. \([63]\). The transfer matrix obtained from the above discussions has the same form as eq. \([31]\) and eq. \([32]\). Here it should be noted that these results can not be applied strictly to the scattering matrix when higher order terms of \(k\cdot p\) are included in the effective mass equations, which make the equations to be variant under the operation \(Q_1\). Thus the invariance under the operation \(Q_1\) holds within the linear approximation with \(\vec{k}\). Fig. 14 show how the \(Q_1\) invariance is accurate for the \(S\) matrix calculated by the tight binding model. It shows values of \(\text{Im}(t_{21}/t_{11})\) as a function of \(\phi\). The range of the indices of junctions \((m_5, n_5) - (m_7, n_7)\) and that of the energy are the same as those of Fig. 3 and Fig. 11. It can be seen that these plots coincide with \(\tan(3\phi/2)\) quite well. The other ratios between the matrix elements obtained by the tight binding model also coincide with those of eq. \([31]\) and eq. \([32]\) fairly well: \(|\frac{r_{12}}{t_{11}}| < 0.1, |\frac{t_{12}}{t_{11}}| < 0.2, |\frac{r_{21}}{r_{11}}| < 0.1, \text{ and } |\text{Re}(\frac{t_{21}}{t_{11}})| |\frac{r_{12}}{t_{11}}| < 0.2\) for the 274 junctions in Fig. 14.

The ratios between the matrix elements of the scattering matrix is determined in this way. But as for the factors \(h_{\pm}\), what can be known from the above discussions is only that they are periodic even functions of \(\phi\) with the period \(\pi/3\). One has to solve the effective mass equations to get more information on them. But there is an important result obtained solely from the argument of the symmetries. As is shown in the preceding sections, the two bands \(k^{(p)}_+\) and \(k^{(p)}_-\) are degenerate when neither of the two tubes has the phason line. On the other hand, the two band avoid each other when \(\phi \neq 0\) \((\phi \neq \pi/3)\) and both of the two tubes have the phason lines \(l_5l_7 = 1\) \((l_5l_7 = -1)\). From eq. \([25]\), these can be explained as below. The origin of the degeneracy in the former case is that both of \(\text{Re}(T_1)\) and \(\text{Re}(T_2)\) are diagonal and \(\text{Re}(T_{11}) = \text{Re}(T_{22})\). The origin of the repulsion between the bands in the latter case is that \(\text{Re}(T_2)\) has nonzero off-diagonal elements. These origins can be shown only from the results in this section without solving the effective mass equations.

V. SUMMARY AND CONCLUSION

The band structures of the periodic junctions composed by the two kinds of metallic nanotubes are considered by combining the transfer matrix of the single junction, \(T_s\). The transfer matrix \(T_s\) is obtained in an analytical form by the effective mass equations with assumptions I, II and III. The region of energy is \(|E| < E_c\), where \(E_c\) is the threshold energy above which more than two channels open. By combining the \(T_s\)’s, the dispersion relation of the periodic junctions is also obtained analytically. Discussions are concentrated to the case when the two tubes have almost the same radius, i.e., \(0.7 < R_5/R_7 < 1\). In this case, the transmission rate \(T\) per channel is near one and almost constant with respect to the energy. Agreement between the band structures by the effective mass theory and those by the tight binding model is satisfactory. Correspondence between the phason lines and the band structures near undoped Fermi level discussed in Ref.13 appears naturally. When there is no phason line (case i), the degenerate bands appear. When only one of the two kinds of tubes has the phason lines (case ii), the two bands cross with each other near \(k = 2\pi/3\). But in case (i), there is a significant difference between the results of the two methods. The gap appears at \(k = 0\) in the tight binding model, while it does not appear in the effective mass equations. The origin of this difference is that the values of the phase factors \(p_-\) at \(E = 0\) are different between the two methods. But explanation for it is not enough yet. In these two cases (i) and (ii), the angle between the two tube axes, \(\phi\), does not influence the band structures. But when both kinds of tubes have the phason lines, the band structures depend on \(\phi\) as follows (case iii). When \(l_5l_7 = 1\) \((l_5l_7 = -1)\), the gap width increases and the corresponding wave number changes from \(k^{(p)}_+ \simeq 2\pi/3\) to \(k^{(p)}_- = 0\), as \(\phi\) increases from 0 to \(\pi/3\) (decreases from \(\pi/3\) to 0). The width of the bands and the gap near the undoped Fermi level is in inverse proportion to the length of the unit cell which is defined as the sum of the four lengths, two of which are those of the tubes measured along each tube axis and the
other two are those of the junctions measured along the ‘radial’ direction, i.e., $R_5 - R_7$. It is also found that the ratio between the matrix elements of the transfer matrix $T_s$ is determined only by the symmetries. By using only the symmetries and without solving the effective mass equations, the degeneracy of the bands for case (i) and the gap at $k \neq 0$ for case (iii) can be derived.

In this paper, it is found that the effective mass theory is very useful to analyze the electronic states near the undoped Fermi levels. Though the discussions is limited to some type of the periodic nanotube junctions, similar phenomena have been found in other systems. One of the examples is another type of the periodic nanotubes composed by only one kind of the tube. Another example is pairs of disclinations in the monolayer graphite. These electronic states can be also classified according to the phason line pattern. We expect that similar discussions can be applied also to these cases.

**ACKNOWLEDGMENT**

We wish to thank K. Akagi. We would like to thank H. Matsumura and T. Ando for their useful suggestions. This work has been supported by the Core Research for Evolutional Science and Technology (CREST) of the Japan Science and Technology Corporation(JST).

**APPENDIX**

We consider the junction between a left lead 1 and a right lead 2 in the absence of magnetic field. When there is no magnetic field, the Hamiltonian $H$ can be taken to be real $H^* = H$. In this case, if $\psi$ is a stationary state, $H \psi = E \psi$, $\psi^*$ is also a stationary state, $H \psi^* = E \psi^*$. The direction of the probability flow of $\psi^*$ is opposite to that of $\psi$. In each lead, the propagating wave is represented by $\sum_{j=1}^{N_i} (\psi_j^{(i)})^* + \psi_j^{(i)}$ for the lead $i$ ($i = 1, 2$). Here the $j$’th left going wave $\psi_j^{(i)*}$ is taken to be complex conjugate of $j$’th right going wave $\psi_j^{(i)}$. They are normalized so that the probability flow is represented by $|\bar{x}_+^{(i)}|^2 - |\bar{x}_-^{(i)}|^2$ in each lead. The integer $N_i$ is the number of the extended state in each tube and called the channel number. By solving the Schrödinger equation, the outgoing wave $x_{out} \equiv \bar{t}^\dagger (\bar{x}_{1-}, \bar{x}_{2+})$ is determined by the incoming wave $x_{in} \equiv \bar{t}^\dagger (\bar{x}_{1+}, \bar{x}_{2-})$ by the scattering matrix $S$ as

$$x_{out} = S x_{in} ,$$

where

$$S = \begin{pmatrix} r_1, & t' \\ t', & r_2 \end{pmatrix}$$

In eq. (69), $r_1$ and $r_2$ are an $N_1 \times N_1$ matrix and an $N_2 \times N_2$ matrix, respectively, and they show the reflection rate. On the other hand, the block matrices $t$ and $t'$ show the transmission rate. The conservation of the probability flow $|\bar{x}_{in}|^2 = |\bar{x}_{out}|^2$ guarantees that $S$ is unitary, that is to say,

$$S^\dagger = S^{-1} .$$

In the absence of the magnetic field, the complex conjugate of the wave function represented by eq. (68) is also a stationary state. It is represented by $\bar{x}_{in} = S \bar{x}_{out}$, which means that

$$S^* = S^{-1} .$$

From eq. (70) and eq. (71), one can know $S$ is a symmetry matrix $S = S$, which means that $r_1 = t^{-\dagger} r_1$, $r_2 = t^{-\dagger} r_2$ and $t' = t^{-\dagger} t$. Here attention should paid when the base wave functions are unitary transformed, $\bar{x}_{\pm}^{(i)} = U_{\pm}^{(i)} \bar{x}_{\pm}^{(i)}$. For arbitrary unitary matrices $U_{\pm}^{(i)}$, eq. (70) holds in the representation $\bar{x}_{\pm}$. In contrast to it, eq. (71) holds only when $U_{\pm}^{(i)} = U_{\pm}^{(i)}$.

When the two leads have the same channel number, i.e., $N_1 = N_2$, one can consider the transfer matrix $T$ instead of the scattering matrix $S$. By the transfer matrix, the propagating wave in the lead 2, $\bar{x}_{2} \equiv \bar{t}^\dagger (\bar{x}_{2+}, \bar{x}_{2-})$, is determined by that in the lead 1, $\bar{x}_{1} \equiv \bar{t}^\dagger (\bar{x}_{1+}, \bar{x}_{1-})$ as

$$\bar{x}_{2} = T \bar{x}_{1} ,$$

where

$$T = \begin{pmatrix} t_{11}, & t_{12} \\ t_{21}, & t_{22} \end{pmatrix} .$$

From the time reversal symmetry, one can show $t_{11} = t_{22} \equiv t_1$ and $t_{21} = t_{12} \equiv t_2$ by the similar discussion to that about $S$. Conservation of the probability flow is represented by $t_1^t t_1 - t_2^t t_2 = 1$ and $t_1^t t_2 - t_2^t t_1 = 0$. From these, the inverse matrix of $T$ is

$$T^{-1} = \begin{pmatrix} t_1^t, & -t_2^t \\ -t_2^t, & t_1^t \end{pmatrix} .$$

The relation between $S$ and $T$ is represented as

$$t_1 = (1/t)^*$$

$$t_2 = -(1/t) r_1$$

FIG. 1. Development map of the nanotube.
FIG. 2. Development map of the nanotube junctions. It is similar to that of Ref. [2]. The lines ‘EP’ , ‘P+P’ , ‘P−G’ are connected and become identical with the lines ‘FQ’ , ‘Q−Q’ , and ‘Q+H’, respectively. The rectangles ‘EP’ and ‘P−G’ form the thinner tube and the thicker tube, respectively. ‘P−G’ is the rotated ‘Q−Q’ by angle of 60 degrees and the quadrilateral ‘P+P−Q Q’ forms a junction part with a square of a part of a cone. A heptagonal defect and a pentagonal defect are introduced at P= Q ( =Q5) and P= Q ( =Q7), respectively. The circumference s and lines is the unit cell of this periodic junctions becomes incommensurate. An area between the two dotted lines is the unit cell of this periodic junctions.

FIG. 3. An example of π/3 rotation. B′ and A′ indicates the B lattice and A lattice with their positions 2i e− (i +1) e and 2i e− (i +1) e , respectively. They are aligned along the line OQ which is parallel to the bonds. The angle between the line OP and the line OQ is π/3. The points A and B are aligned along the line OP and their positions are i e + i e . By the rotation π/3 with respect to the point O, the points B′ and A′ are transformed into the points A and B, respectively.

FIG. 4. Landauer’s formula. Conductances calculated by the tight binding model and those by the effective mass theory. The former is shown by plots and the latter is shown by solid lines. It can be seen that agreement between them is good. The horizontal axis is the energy in units of the absolute value of the hopping integral, |γ| = γ. (a) R= (1, 10), R= (3, 12), L(5) = (4, -5) and L(5) = (6, -3). R= R ≃ 0.766 and φ = ±0.034π. l= l= 0, i.e., neither of the two tubes has the phason line. (b) R= (7, 1), R= (6, 3), L(5) = (3, -2) and L(5) = (0, -3). R/ R ≃ 0.951 and φ ≃ 0.07π. l = -1 and l = 0, i.e., only the thinner tube has the phason line.

FIG. 5. Development map of the periodic junction. The positions of the pentagonal defects and heptagonal defects are denoted by symbols 5 and 7, respectively. The circumspheres of the thicker tube and the thinner tube are represented by vectors R and R. The upper bold line is connected with the lower bold lines so that the points connected by the circumspheres become identical. Vectors connecting the two pentagonal defects and the two heptagonal defects in each tube part are denoted by L(5) and L(7), respectively. The four vectors R, R, L(5) and L(7) determine the bond network of the periodic junction treated in this paper uniquely. In this figure, R = (2, 5), R = (1, 4), L(5) = (4, -4) and L(7) = (3, -3). In this figure, the thicker tube has the phason line represented by the dotted line where the Kekule pattern becomes incommensurate. An area between the two dotted lines is the unit cell of this periodic junctions.

FIG. 6. Schematic view of combination of two equivalent junctions to form the unit cell of the periodic junctions.

FIG. 7. The gradients , for 0 < z < 2π, i.e., |E| < Ec = 2π/ Ec = R, E. They are evaluated with , which corresponds to the length of the junction part. The horizontal axis is the ratio of the circumstances, R= R. The gradients are almost same as 1 - R/R , while are almost constant between -0.1 and -0.05. As a reference, the solid line representing 1 - R/R is shown.

FIG. 8. The band structures of the periodic junctions for one of the two kinds of tubes has no phason line. The vertical axis is the energy in units of the absolute value of the hopping integral, |γ| = γ. (a) R = (1, 10), R = (3, 12), L(5) = (4, -5) and L(5) = (6, -3). R= R ≃ 0.766 and φ = ±0.034π. l= l= 0, i.e., neither of the two tubes has the phason line. (b) R = (7, 1), R = (6, 3), L(5) = (3, -2) and L(5) = (0, -3). R/ R ≃ 0.951 and φ ≃ 0.07π. l = -1 and l = 0, i.e., only the thinner tube has the phason line.

FIG. 9. Gradients at z = 0 where z = k R = 2ER/(√3|γ|) calculated by the tight binding model and normalized by those obtained by the effective mass theory, i.e., (1 - R/R ). They are denoted by and plotted for 274 junctions. The horizontal axis is absolute values of the angle φ between the two tube axes in the development map in units of π. The range of the indices of the tubes, (m, n), of the calculated junctions is 1 ≤ min(m, n) ≤ 8 and |m - n| = 3i, i = 0 ~ 3 which satisfy 1 > R/R > 0.7. The error bar indicates that maximum and minimum of the for each junction in the energy region |E/γ| < 0.1. That is to say, it represents deviation from the linearity in this energy region. To evaluate this error bar, the scattering matrices for 9 different energies equally spaced in this energy region are calculated about each junction. Open diamond plots, closed circle plots, and open square plots correspond to 1 > R/R ≥ 0.95, 0.95 > R/R ≥ 0.9 and 0.9 > R/R ≥ 0.7, respectively.

FIG. 10. Values of the phases p± at E = 0 divided by π calculated by the tight binding model. They correspond to the intercepts e± divided by π. In the effective mass theory, they are zero. The range of the calculated junctions is same as that of Fig. 11. The horizontal axis is difference between the circumference of thicker tube and that of the thinner tube, R3 - R5, which corresponds to the length of the junction part.
FIG. 11. The band structures of the periodic junctions for both of two kinds of tubes have the phason lines. The vertical axis is the energy in units of the absolute value of the hopping integral. \(|\psi| \equiv -\gamma\). (a) \(R_1 = (10, 1), R_2 = (7, 7), L^{(7)} = (6, -5)\) and \(L^{(5)} = (13, -6)\). \(R_1/R_2 \approx 0.869\) and \(\phi \approx 0.14\pi\). \(l_1 = -1\) and \(l_2 = 1\). (b) \(R_1 = (6, 6), R_4 = (7, 7), L^{(7)} = (4, 2)\) and \(L^{(5)} = (10, -3)\). \(R_1/R_4 \approx 0.857\) and \(\phi = 0\). \(l_1 = -1\) and \(l_2 = 1\).

FIG. 12. The dependence of the gap width on the angle \(\phi\) scaled by its maximum value when both of the two kinds of tubes have the phason lines. It is approximately represented by \(2\sin(3\phi/2)/\sqrt{4 - 3\cos^2(3\phi/2)}\) as discussed in the text. The solid line and the dotted line correspond to the cases \(l_1l_2 = 1\) and \(l_1l_2 = -1\), respectively.

FIG. 13. The operation \(Q_2\) which fixes the thinner tube part but rotates the thicker tube part by \(\pi/3\) in the development map. The upper development map is transformed into the lower one under the operation \(Q_2\). These two development maps correspond to the identical junction, denoted by the (2, 2) - (2, 5) junction.

FIG. 14. Imaginary part of \(t_{21}/t_{11}\) as a function of angle between the two tube axes \(\phi\). The ranges of the junctions and energies are same as those of Fig. 11. They are fitted well by \(\tan(\frac{1}{2}\phi)\) represented by the solid line.

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22 The position of the Fermi level can not be known by the effective mass theory because it can not treat the bands far from \(E = 0\). It is the tight binding calculations that show that it comes at the highest energy of the negative energy bands.
23 One to one correspondence between the junction and its development map holds when the range of \(\phi\) is taken to be \(\phi_0 < \phi < \phi_0 + \pi/3\). Otherwise there are multiple different development maps representing a same junction, where \(\phi\) is different by a multiple of \(\pi/3\).
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