Effectiv-Mass Theory of Carbon Nanotubes with Vacancy

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Effects of impurities with a strong and short-range potential are studied in carbon nanotubes within a $k$-$p$ scheme. The calculated conductance approaches those obtained for nanotubes with a lattice vacancy when the strength of the potential is sufficiently large. The conductance at $\epsilon = 0$ is analytically shown to be quantized into zero, one, and two times of the conductance quantum $e^2/\pi h$ depending on the difference in the number of vacancies at A and B sublattices in nanotubes with a sufficiently large diameter.

KEYWORDS: graphite, carbon nanotube, vacancy, conductance, effective-mass theory

§1. Introduction

A carbon nanotube (CN) is composed of concentric tubes of rolled two-dimensional (2D) graphite sheets, on which hexagons are arranged in a helical fashion about the axis. The diameter of each tube ranges from 20 to 300 Å and the maximum length exceeds 1μm. Single-wall nanotubes having a diameter lying between 7 and 16 Å can be synthesized also. The purpose of this paper is to study effects of a strong and short-range perturbation including lattice vacancies in a $k$-$p$ scheme.

Various calculations have been performed to predict energy bands. It has been found that their characteristic properties are reproduced in a $k$-$p$ method. The $k$-$p$ scheme is quite powerful in the study of effects of external fields such as magnetic and electric fields. In fact, it has been successful in the study of magnetic properties including the Aharonov-Bohm effect on the band gap, optical absorption spectra, and lattice instabilities in the presence and absence of a magnetic field.

Transport properties of CN’s are interesting because of their unique topological structure. There have been some reports on experimental study of transport in CN bundles. Quite recently, measurements of magnetotransport of a single nanotube became possible. The tunneling at a finite-length CN and a connection of different CN’s were calculated. The conductivity was calculated in a constant-relaxation-time approximation. A calculation of the conductance of armchair nanotubes with a single vacancy was reported also.

The conductivity of CN’s was previously calculated using a Boltzmann transport equation and in Landaue’ approach for a model of short-range scatterers. The results were shown to have a close connection with transport in a 2D graphite sheet. In a previous paper, effects of impurity scattering in CN’s were studied in detail and the absence of backward scattering was predicted and proved rigorously except for scatterers having a potential range smaller than the lattice constant. This intriguing fact was related to Berry’s phase acquired by a rotation in the wave vector space in the system described by a $k$-$p$ Hamiltonian which is same as Weyl’s equation for a neutrino.

The conductance was calculated in a tight-binding model and the result confirmed the absence of backward scattering when the potential is sufficiently small, i.e., the maximum value is smaller than the typical width of the conduction and valence bands. A quantized conductance was observed in a multi-wall nanotube.

Quite recently, effects of scattering by a vacancy were studied in metallic armchair nanotubes in the presence and absence of a magnetic field. The conductance was shown to be quantized into zero, one, and two times of the conductance quantum $e^2/\pi h$ depending on the type of the vacancy. In this paper we shall extend a $k$-$p$ scheme so as to discuss effects of strong and localized potentials including those of lattice vacancies and present analytic derivation of the intriguing conductance quantization in the presence of vacancies.

§2. Effective-Mass Approximation

2.1 Hamiltonian

The structure of a 2D graphite is shown in Fig. 1 together with the first Brillouin zone and the coordinates system to be used in the following. A unit cell contains two carbon atoms denoted as A and B. In a 2D graphite, two bands having approximately a linear dispersion cross the Fermi level (chosen at $\epsilon = 0$) at K and K’ points of the first Brillouin Zone. The wave vectors of the K and K’ points are given by $K = (2\pi/a)(1/3,1/\sqrt{3})$ and $K’ = (2\pi/a)(2/3,0)$. 

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An eigenstate of the Hamiltonian is written as
\[ \mathcal{H} F(r) = \varepsilon F(r), \]
with
\[ \mathcal{H} = \mathcal{H}_0 + V, \]
where
\[ \mathcal{H}_0 = \begin{pmatrix} KA & KB & K' A & K' B \\ 0 & \gamma(\hat{k}_x - i\hat{k}_y) & 0 & 0 \\ 0 & 0 & 0 & \gamma(\hat{k}_x + i\hat{k}_y) \\ 0 & 0 & \gamma(\hat{k}_x - i\hat{k}_y) & 0 \end{pmatrix}, \]
and
\[ F(r) = \begin{pmatrix} F^K (r) \\ F^{K'} (r) \end{pmatrix}, \]
with
\[ F^K (r) = \begin{pmatrix} F^{KA} (r) \\ F^{KB} (r) \end{pmatrix}, \quad F^{K'} (r) = \begin{pmatrix} F^{K'A} (r) \\ F^{K'B} (r) \end{pmatrix}. \]

Here, \( F^{KA} \) and \( F^{KB} \) describe the amplitude at an A and B site, respectively, for the component at the K point, and \( F^{K'A} \) and \( F^{K'B} \) describe that for the K' point.

For the discussion of scattering from short-range scatterers localized at several lattice points, it is more convenient to choose the representation in which the (4,4) matrix Hamiltonian is rewritten as
\[ \mathcal{H}_0 = \begin{pmatrix} KA & K' A & KB & K' B \\ 0 & 0 & \gamma(\hat{k}_x - i\hat{k}_y) & 0 \\ 0 & 0 & 0 & \gamma(\hat{k}_x + i\hat{k}_y) \\ \gamma(\hat{k}_x + i\hat{k}_y) & 0 & 0 & 0 \\ 0 & 0 & \gamma(\hat{k}_x - i\hat{k}_y) & 0 \end{pmatrix}. \]

An eigenstate of the Hamiltonian is written as
\[ F_{snk}(r) = \frac{1}{\sqrt{AL}} f_{snk} \exp[i\kappa(n)x + iy], \]
where \( A \) is the length of the nanotube, \( s = +1 \) denotes a conduction band, \( s = -1 \) a valence band, \( k \) is the wave vector in the direction of the axis, and \( \kappa(n) \) is that in the circumference direction, i.e.,
\[ \kappa(n) = \frac{2\pi n}{L}, \]
with an integer \( n \) and the circumference \( L \). The four-component eigenvector \( f_{snk} \) is normalized as \( |f_{snk}| = 1 \) and satisfies
\[ \mathcal{H}_0(nk) f_{snk} = \varepsilon_{snk} f_{snk}, \]
with
\[ \mathcal{H}_0(nk) = \begin{pmatrix} 0 & \gamma(\kappa(n) - ik) & 0 & 0 \\ 0 & 0 & \gamma(\kappa(n) + ik) & 0 \\ 0 & \gamma(\kappa(n) + ik) & 0 & 0 \\ 0 & \gamma(\kappa(n) - ik) & 0 & 0 \end{pmatrix}, \]
and
\[ \varepsilon_{snk} = 8\gamma \sqrt{\kappa(n)^2 + k^2}. \]

For an impurity localized at a carbon A site \( r_j \), we have\(^{32}\)
\[ V(r) = V_j \delta(r - r_j), \]
with
\[ V_j = \begin{pmatrix} u_j & 0 \\ 0 & 0 \end{pmatrix}, \]
where
\[ \Phi_j^A = \begin{pmatrix} 1 & e^{i\phi_j^A} \\ e^{-i\phi_j^A} & 1 \end{pmatrix}, \]
with
\[ \phi_j^A = (K' - K) \cdot r_j + \eta. \]

Here, \( \eta \) is the chiral angle shown in Fig. 1. Define further a vector \( a_j \) as
\[ a_j = \begin{pmatrix} a_j K \\ a_{jK'} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\phi_j^A/2} \\ e^{-i\phi_j^A/2} \end{pmatrix}, \]
which satisfies
\[ (a_j, a_j) = a_j^\dagger a_j = 1, \quad a_j K' = a_{jK'}^*. \]
Then, we have
\[ \Phi_j^A = 2a_j a_j^+. \]
have

$$V_j = \begin{pmatrix} 0 & 0 \\ 0 & w_j \Phi_j \end{pmatrix},$$

(2.19)

where

$$\Phi_j = \begin{pmatrix} \frac{1}{e^{i\omega_j}} & e^{i\omega_j} \\ e^{i\omega_j} & \frac{1}{e^{i\omega_j}} \end{pmatrix},$$

(2.20)

with

$$\phi_j = (K' - K) \cdot r_j - \eta + \frac{\pi}{3}.$$  

(2.21)

In terms of a vector \( b_j \) defined as

$$b_j = \begin{pmatrix} b_{j1} \\ b_{j2} \end{pmatrix} = \begin{pmatrix} 1 \\ \sqrt{2} \end{pmatrix} \begin{pmatrix} e^{i\omega_j}/2 \\ e^{-i\omega_j}/2 \end{pmatrix},$$

(2.22)

we have

$$\Phi_j = 2b_j b_j^\dagger.$$  

(2.23)

### 2.2 Scattering matrix

In terms of a \( T \) matrix defined by

$$T = V + V \frac{1}{\varepsilon - H_0 + \ii} V + V \frac{1}{\varepsilon - H_0 + \ii} V + \ldots,\quad (2.24)$$

the scattering matrix can be written formally as

$$S = S^{(0)} + S^{(1)},$$

(2.25)

with

$$S^{(0)}_{\alpha\beta} = \delta_{\alpha\beta},$$

(2.26)

and

$$S^{(1)}_{\alpha\beta} = -i \frac{A}{h\sqrt{|v_{\alpha}v_{\beta}|}} T_{\alpha\beta},$$

(2.27)

where \( v_\alpha \) and \( v_\beta \) are the velocity of channels \( \alpha \) and \( \beta \).

The matrix element is written as

$$(\alpha | V_j | \beta) = f_{\alpha}^+ V_j f_{\beta} \frac{1}{AL} \exp[-i(\kappa_\alpha - \kappa_\beta) x_j - i(k_\alpha - k_\beta) y_j],$$

(2.28)

where \((x_j, y_j)\) is the position of the impurity, \( f_{\alpha} \) is the eigenvector for the state \( \alpha \) with energy \( \varepsilon_\alpha \), wave vector in the axis direction \( k_\alpha \), and that in the circumference direction \( \kappa_\alpha = n_\alpha (2\pi/L) n_\alpha \) with integer \( n_\alpha \). The \( T \) matrix is expanded as

$$T = T^{(1)} + T^{(2)} + T^{(3)} + \ldots,$$

(2.29)

with

$$(\alpha | T^{(1)} | \beta) = \sum_j f_{\alpha}^+ V_j f_{\beta} \frac{1}{AL} \exp[-i\kappa_\alpha x_j - i\kappa_\beta y_j],$$

(2.30)

$$(\alpha | T^{(2)} | \beta) = \sum_{\gamma} \sum_j f_{\alpha}^+ V_j f_{\gamma} \frac{1}{AL} \exp[-i\kappa_{\gamma} x_j - i\kappa_\beta y_j] \times \frac{1}{\varepsilon - \varepsilon_\gamma + \ii} \sum_{j'} f_{\gamma}^+ V_{j'} f_{\beta} \exp[-i\kappa_\gamma x_{j'} - i\kappa_\beta y_{j'}],$$

(2.31)

$$(\alpha | T^{(3)} | \beta) = \sum_{\gamma\gamma'} \sum_j f_{\alpha}^+ V_j f_{\gamma} \frac{1}{AL} \exp[-i\kappa_{\gamma} x_j - i\kappa_{\gamma'} y_j] \times \frac{1}{\varepsilon - \varepsilon_\gamma + \ii} \sum_{j'} f_{\gamma}^+ V_{j'} f_{\beta} \exp[-i\kappa_{\gamma'} x_{j'} - i\kappa_\beta y_{j'}] \times \frac{1}{\varepsilon - \varepsilon_{\gamma'} + \ii} \sum_{j''} f_{\beta}^+ V_{j''} f_{\beta} \exp[-i\kappa_{\beta} x_{j''} - i\kappa_\beta y_{j''}],$$

(2.32)

where \( \kappa_{\alpha\beta} \equiv \kappa_{\alpha} - k_{\beta}, k_{\alpha\beta} \equiv k_{\alpha} - k_{\beta}, \) etc. In the lowest order Born approximation, the \( T \) matrix is given by eq. (2.30), which shows that the effective potential is essentially given by the sum of the potential of each impurity.

We note the relation:

$$\sum_{\gamma} f_{\gamma} \frac{1}{\varepsilon - \varepsilon_\gamma + \ii} f_{\gamma}^+ = \sum_{nk} \left[ \varepsilon - H_0(nk) + \ii \right]^{-1}. \quad (2.33)$$

Then, the second order term becomes

$$\sum_{jj'} f_{\delta}^+ \frac{1}{AL} V_j G_{jj'}(\varepsilon + \ii) \frac{1}{AL} V_{j'} f_{\beta} \times \exp(-i\kappa_\alpha x_j - i\kappa_\beta y_j) \exp(i\kappa_\beta x_{j'} + i\kappa_\beta y_{j'}),$$

(2.34)

where

$$G_{jj'}(\varepsilon + \ii) \equiv G(r_j - r_{j'}, \varepsilon + \ii) = \sum_{nk} \left[ \varepsilon - H_0(nk) + \ii \right]^{-1} \exp[i\kappa(n) x_{j'} + i\kappa y_{j'}],$$

(2.35)

with

$$x_{j'} = x_j - x_{j'}, \quad y_{j'} = y_j - y_{j'}.$$  

(2.36)

Similarly, the third order term is given by

$$\sum_{jj''} f_{\delta}^+ \frac{1}{AL} V_j G_{jj''}(\varepsilon + \ii) \frac{1}{AL} V_{j''} G_{jj'''}(\varepsilon + \ii) \frac{1}{AL} V_{j'''} f_{\beta} \times \exp(-i\kappa_\alpha x_j - i\kappa_\beta y_j) \exp(i\kappa_\beta x_{j'} + i\kappa_\beta y_{j'}).$$

(2.37)

By repeating similar procedures up to an infinite order, we obtain the \( T \) matrix

$$(\alpha | T | \beta) = \sum_{ij} f_{\alpha}^+ T_{ij} f_{\beta} \exp[-i\kappa_\alpha x_i - i\kappa_\alpha y_i] \times \exp[i\kappa_\beta x_{j'} + i\kappa_\beta y_{j'}],$$

(2.38)

where

$$T_{ij} = \left[ \left( 1 - \frac{1}{AL} V G(\varepsilon + \ii) \right) \left( \frac{1}{AL} V \right) \right]_{ij},$$

(2.39)

with \( V_{j'''} = V_j \delta j'''. \)

The equation for \( T_{ij} \) is given by

$$T_{ij} = \frac{1}{AL} V_i \delta_{ij} + \frac{1}{AL} V_i \sum_k G(r_i - r_k, \varepsilon + \ii) T_{kj}.$$  

(2.40)

Effects of multiple scattering from a single impurity can exactly be taken into account by replacing eq. (2.40) by

$$T_{ij} = \frac{1}{AL} V_i \delta_{ij} + \frac{1}{AL} V_i \sum_{k \neq i} G(r_i - r_k, \varepsilon + \ii) T_{kj}.$$  

(2.41)

We then have

$$T_{ij} = \frac{1}{AL} V_i \delta_{ij} + \frac{1}{AL} V_i \sum_{k \neq i} G(r_i - r_k, \varepsilon + \ii) T_{kj}.$$  

(2.42)

with

$$V_i = \left[ 1 - \frac{1}{AL} V_i G(\varepsilon + \ii) \right]^{-1} V_i.$$  

(2.43)

In the following, we shall confine ourselves to the
case that
\[-\frac{2\pi\gamma}{L} < \varepsilon < \frac{2\pi\gamma}{L} .\]  
(2.44)
For this energy range, the eigen vectors are given by
\[f_{K\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ \pm i \end{pmatrix}, \quad f_{K'-\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad f_{K''\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ \mp i \end{pmatrix},\]  
(2.45)
and the velocity is given by \(|v| = \gamma/h\). We can write the scattering matrix as
\[S = \begin{pmatrix} r_{KK} & r_{KK'} & t_{KK} & t_{KK'} \\ r_{KK'} & r_{KK'} & t_{KK'} & t_{KK'} \\ t_{KK} & t_{KK'} & r_{KK'} & r_{KK'} \\ t_{KK'} & t_{KK'} & r_{KK'} & r_{KK'} \end{pmatrix},\]  
(2.46)
where \(t\)'s and \(r\)'s are transmission and reflection coefficients, respectively. When all impurities are localized in a region smaller than the circumference and \(|\varepsilon| \ll 2\pi\gamma/L\), in particular, eq. (2.38) can be replaced by
\[(\alpha|T|\beta) = f_+^\dagger T_S f_\beta \exp[-i(\kappa_{\alpha} - \kappa_{\beta})x_0 - i(\kappa_{\alpha} - \kappa_{\beta})y_0],\]  
(2.47)
with
\[T_S = \sum_{ij} T_{ij},\]  
(2.48)
where \(r_0 = (x_0, y_0)\) is the center-of-mass of all the impurities.

2.3 Green’s functions

The Green’s function is explicitly given by
\[G(x, y, \varepsilon + i0) = \frac{A}{2\pi} \int dk \sum_n f_+^\dagger[n, k] e^{i\varepsilon n x + ik y} (\varepsilon + i0)^2 - \gamma^2 |\kappa(n)|^2 + k^2] \\
\times \begin{pmatrix} \varepsilon & 0 & \gamma |\kappa(n) - ik| \\ 0 & \varepsilon & 0 \\ \gamma |\kappa(n) + ik| & 0 & \varepsilon \end{pmatrix},\]  
(2.49)
where we have introduced a cutoff function \(f_c[n, k]\) defined by
\[f_c[n, k] = \frac{k^2}{k^2 + |\kappa(n)|^2 + k^2},\]  
(2.50)
in order to extract the contribution from states in the vicinity of the Fermi level. The cutoff wave vector \(k_c\) is determined by the condition that the cutoff wave length \(2\pi/k_c\) should be comparable to the lattice constant \(a\), i.e., \(2\pi/k_c \approx a\). We introduce a cutoff integer \(n_c\) by \(k_c = 2\pi n_c/L\), i.e., \(\kappa(n_c) \approx k_c\) or \(n_c \approx L/a\). The Green’s function is written as
\[G = -\frac{i\gamma}{2\gamma} \begin{pmatrix} g_0 & 0 & g_1 \\ 0 & g_0 & 0 \\ g_1 & 0 & g_1 \end{pmatrix},\]  
(2.51)
where
\[g_0(x, y) = \frac{i\gamma}{\pi} \int dk \sum_n f_c[n, k] \frac{\varepsilon e^{i\kappa(n)x + ik y}}{(\varepsilon + i0)^2 - \gamma^2 |\kappa(n)|^2 + k^2}],\]  
\[g_1(x, y) = \frac{i\gamma}{\pi} \int dk \sum_n f_c[n, k] \frac{\gamma |\kappa(n) - ik| e^{i\kappa(n)x + ik y}}{(\varepsilon + i0)^2 - \gamma^2 |\kappa(n)|^2 + k^2}],\]  
(2.52)
and \(\tilde{g}_1(x, y) = g_1(x, -y)\). We immediately see that
\[g_0(-x, y) = g_0(x, -y) = g_0(-x, -y) = g_0(x, y),\]  
\[g_1(-x, -y) = -g_1(x, y),\]  
(2.53)
which leads to \(g_1(0, 0) = 0\).

The off-diagonal Green’s function appears only between matrix elements of impurities and therefore in the form
\[a_{ij}^\dagger \begin{pmatrix} g_1(r_{ij}) & 0 \\ 0 & \tilde{g}_1(r_{ij}) \end{pmatrix} b_j = (a_i, b_j) \tilde{g}_{ij}^{AB},\]  
(2.54)
with \(r_{ij} = r_i - r_j\), where
\[\tilde{g}_{ij}^{AB} = \frac{1}{2} \left[ g_1(r_{ij}) e^{-i(\phi^A - \phi^B)/2} + \tilde{g}_1(r_{ij}) e^{i(\phi^A - \phi^B)/2} \right] \times (a_i, b_j)^{-1},\]  
(2.55)
and \((a_i, b_j) = a_i^\dagger b_j\). This means that we can always use \(\tilde{g}_{ij}^{AB}\) for the off-diagonal Green’s function describing the propagation from a B site at \(r_j\) to an A site at \(r_i\). It should be noted that \((a_i, b_j) = a_i^\dagger b_j\) is real.

In the energy range (2.44), we have
\[g_0(x, y) = \varepsilon e^{i(\varepsilon/\gamma)/|y|},\]  
\[-2i\varepsilon + \sum_{n=1}^{\infty} \cos[\kappa(n)|x|] \left( \exp[-\sqrt{\kappa(n)^2 - (\varepsilon/\gamma)^2}/|y|] - \exp[-\sqrt{\kappa(n)^2 + k_c^2}/|y|] \right),\]  
(2.56)
and
\[g_1(x, y) = -i\text{sgn}(y) \left[ \varepsilon e^{i(\varepsilon/\gamma)/|y|} - e^{-k_c/|y|} \right] + 2 \sum_{n=1}^{\infty} \left[ \frac{\kappa(n) \sin[\kappa(n)|x|]}{\sqrt{\kappa(n)^2 - (\varepsilon/\gamma)^2}} - i\text{sgn}(y) \cos[\kappa(n)|x|] \right] \times \exp\left[ -\sqrt{\kappa(n)^2 + k_c^2}/|y| \right] \times \exp\left[ -\sqrt{\kappa(n)^2 + k_c^2}/|y| \right],\]  
(2.57)
with
\[\text{sgn}(y) = \begin{cases} +1 & (y > 0) \\ 0 & (y = 0) \\ -1 & (y < 0) \end{cases}\]  
(2.58)
At \(\varepsilon = 0\), in particular, we have
\[g_0(x, y) = 1,\]  
(2.59)
and
\[g_1(x, y) = -i\text{sgn}(y) \left[ 1 - e^{-k_c/|y|} \right] + 2 \sum_{n=1}^{\infty} \left[ \frac{\kappa(n) \sin[\kappa(n)|x|]}{\sqrt{\kappa(n)^2 + k_c^2}} - i\text{sgn}(y) \cos[\kappa(n)|x|] \right] \exp\left[ -\kappa(n)/|y| \right] \times \exp\left[ -\sqrt{\kappa(n)^2 + k_c^2}/|y| \right] \times \exp\left[ -\sqrt{\kappa(n)^2 + k_c^2}/|y| \right].\]  
(2.60)
The above shows that
\[\tilde{g}_1(x, y) = g_1(x, y)^*,\]  
(2.61)
and consequently
\[ \tilde{g}^{AB}_{ij} = \text{Re} \left[ g_1(r_{ij}) e^{-i(\phi_1^i - \phi_1^j)/2} (a_i, b_j)^{-1} \right], \quad (2.62) \]
i.e., \( \tilde{g}^{AB}_{ij} \) is real as well as \( g_0 \). When \(|y| \gg 2\pi/k_c\), we can neglect terms containing cutoff \( k_c \) and have
\[ g_1(x, y) = \frac{\cos[\pi(x+iy)/L]}{\sin[\pi(x+iy)/L]}, \quad (2.63) \]
This expression is not singular at \( y=0 \) except when \( x \sim 0 \) and therefore valid in the whole \((x, y)\) plane except in the vicinity of the origin, i.e., \(|r| \lesssim 2\pi/k_c\). In particular, we have \( g_1(\pm L/2, y) = 0 \) for \( y = 0 \) and \( g_1(x, y) \to -i \text{sgn}(y) \) for \(|y| \gg L/\pi \) at \( x = 0 \).

Figure 2 shows \( G_{KA,KB}(x, y) = (-i\lambda/2\gamma)g_1(x, y) \) obtained numerically for several values of the cutoff \( n_c \). The Green’s function is singular in the vicinity of \( r = 0 \) as has been discussed above and the singularity is cutoff by the distance \( r_c \sim \delta L/n_c \), where \( \delta \sim 0.2 \). This value is smaller than the cutoff distance \( a \sim L/n_c \), showing that the approximate expression with infinite cutoff, eq. (2.63) for \( \varepsilon = 0 \) for example, can be used in actual calculations. For impurities localized within a distance of a few times of the lattice constant, the off-diagonal Green’s function becomes extremely large. This singular behavior will be shown in §3 to be the origin of the peculiar dependence of the conductance on the difference in the number of vacancies at A and B sublattices.

Near \( \varepsilon = \pm 2\pi \gamma/L \) the Green’s functions diverge in proportion to \( [(2\pi \gamma/L)^2 - \varepsilon^2]^{-1/2} \). In fact, we have
\[ g_0(x, y) \sim -\text{sgn}(\varepsilon) \frac{\sqrt{2i} \cos(2\pi x/L)}{\sqrt{1 - |\varepsilon|(L/2\pi \gamma)}} \quad (2.64) \]
and
\[ g_1(x, y) \sim \frac{\sqrt{2} \sin(2\pi x/L)}{\sqrt{1 - |\varepsilon|(L/2\pi \gamma)}} \quad (2.65) \]
For a small distance, i.e., \(|x/L| \ll 1 \), the divergence at \( \varepsilon = \pm 2\pi \gamma/L \) is much stronger for the diagonal Green’s function than for the off-diagonal Green’ function, i.e., \(|g_0^{-1}g_1| \ll 1\) near \( \varepsilon = \pm 2\pi \gamma/L \) in contrast to \(|g_0^{-1}g_1| \gg 1\) in the other energy range. The energy corresponding to this crossover approaches \( \varepsilon = 2\pi \gamma/L \) with the increase of the circumference. This shows that a singular energy dependence appears in the conductance for closely spaced impurities located at both A and B sublattices in the vicinity of \( \varepsilon = \pm 2\pi \gamma/L \), as will be demonstrated in §3 and §4.

![Fig. 2](image-url)

**Fig. 2** The off-diagonal Green’s function for (a) \( y=0 \) and for (b) \( x=0 \) for several values of \( n_c \). The vertical arrows show the value of the cutoff distance \( L/n_c \).

At \( r = 0 \), the diagonal Green’s function is written as
\[ g_0(0, 0) = 1 - ig_0''(\varepsilon), \quad (2.66) \]
with
\[ g_0''(\varepsilon) = 2\pi \sum_{\varepsilon < \varepsilon < \varepsilon} \left( \frac{1}{\sqrt{\varepsilon^2 \kappa(n)^2 - \varepsilon^2}} - \frac{1}{\sqrt{\varepsilon^2 \kappa(n)^2 + \gamma^2 k_c^2}} \right). \quad (2.67) \]
The imaginary part \( g_0''(\varepsilon) \) is a monotonic function of \( \varepsilon \) in the energy range (2.44) and behaves as
\[ g_0''(\varepsilon) \approx 2\chi \frac{\epsilon L}{2\pi \gamma}, \quad (2.68) \]
with
\[ \chi = \sum_{n=1}^{\infty} \left( \frac{1}{n} - \frac{1}{\sqrt{n^2 + n^2}} \right) \approx \ln n_c, \] (2.69)
for \( |\varepsilon (L/2\pi\gamma)| \ll 1 \) and
\[ g_0''(\varepsilon) \approx \operatorname{sgn}(\varepsilon) \sqrt{\frac{2}{1 - |\varepsilon (L/2\pi\gamma)|}}, \] (2.70)
for \( \varepsilon \approx \pm 2\pi\gamma / L \).

### 2.4 T matrix

The Green’s function becomes diagonal for \( r = 0 \) and therefore the renormalized impurity potential for an A site, for example, by taking into account multiple scattering, becomes
\[ u_j \Phi_j^A \to \left( 1 - \frac{1}{AL} g_0 \right)^{-1} u_j \Phi_j^A = \frac{\gamma L}{i g_0} \Phi_j^A, \] (2.71)
where \( g_0 \equiv g_0(0, \varepsilon + i0) \) for simplicity. Use has been made of \( (\Phi_j^A)^A = 2^A \Phi_j^A \), which follows immediately from eq. (2.18), and \( \zeta = [1 + (2i \bar{u} g_0)^{-1} \varepsilon ]^{-1} \) with \( \bar{u} = u_{j}/2\gamma L \). This shows that due to the multiple scattering from a single impurity the potential strength \( u_j \) is renormalized into \( \zeta \gamma L/ig_0 \).

When impurities are separated into those at A and B sublattices, we have
\[ T_{ij}^{AA} = \frac{1}{AL} \zeta \gamma L \Phi_j^A \delta_{ij} + \frac{1}{AL} g_0 \left( \frac{1}{2\gamma} \right) g_0(r_{ik}) T_{ij}^{AA}, \] (2.72)
\[ T_{ij}^{BA} = \frac{1}{AL} g_0 \left( \frac{1}{2\gamma} \right) g_0(r_{ik}) T_{ij}^{BA}, \] (2.73)
\[ T_{ij}^{BB} = \frac{1}{AL} g_0 \left( \frac{1}{2\gamma} \right) g_0(r_{ik}) T_{ij}^{BB}, \] (2.74)
and
\[ T_{ij}^{AB} = \frac{1}{AL} g_0 \left( \frac{1}{2\gamma} \right) g_0(r_{ik}) T_{ij}^{AB}, \] (2.75)
where \( T_{ij}^{AA} \), etc. are a \( (2, 2) \) matrix.

In the following we shall confine ourselves to the case that the strength of all the impurities is the same and given by \( u \), i.e., \( u_{ij} = u \). In this case, an examination of perturbation series with respect to the impurity potential reveals that the T matrices can be written as
\[ T_{ij}^{AA} = \frac{1}{AL} \zeta \gamma L \left( 2a_i a_j^* t_{ij}^{AA} \right), \]
\[ T_{ij}^{BA} = \frac{1}{AL} \zeta \gamma L \left( 2b_i b_j^* t_{ij}^{BA} \right), \]
\[ T_{ij}^{BB} = \frac{1}{AL} \zeta \gamma L \left( 2b_i b_j^* t_{ij}^{BB} \right), \]
\[ T_{ij}^{AB} = \frac{1}{AL} \zeta \gamma L \left( 2a_i a_j^* t_{ij}^{AB} \right), \]
where
\[ \zeta = \frac{1}{1 + (2i \bar{u} g_0)^{-1}} \frac{1}{i g_0(i\varepsilon) + (2\bar{u})^{-1}}, \] (2.77)
Note that \( \zeta \to 1 \) in the limit \( \bar{u} = u/2\gamma L \to 0 \). Then, we have
\[ t_{ij}^{AA} = \delta_{ij} - \zeta g_0^{-1} \sum_{k, \alpha} g_0(r_{ik}) a_i^* a_k t_{ij}^{AA}, \]
\[ t_{ij}^{BA} = -\zeta g_0^{-1} \sum_{k, \alpha} g_0(r_{ik}) b_i^* b_k t_{ij}^{BA}, \] (2.78)
\[ t_{ij}^{BB} = -\zeta g_0^{-1} \sum_{k, \alpha} g_0(r_{ik}) b_i^* b_k t_{ij}^{BB}, \] (2.79)
and
\[ t_{ij}^{AB} = -\zeta g_0^{-1} \sum_{k, \alpha} g_0(r_{ik}) a_i^* a_k t_{ij}^{AB}, \]
and
\[ t_{ij}^{AB} = -\zeta g_0^{-1} \sum_{k, \alpha} g_0(r_{ik}) a_i^* a_k t_{ij}^{AB}. \]

In the case of a finite number of impurities, these linear equations can be solved numerically and the T matrix can be calculated explicitly.

In the following analytical treatment, we shall confine ourselves further to the case that impurities are located in an area with size much smaller than the circumference length. In this case, we can make the replacement \( g_0(r_{ik}) \to g_0 \) and the above set of equations is further reduced to
\[ t_{ij}^{AA} = \delta_{ij} - \zeta \sum_{k, \alpha} a_i^* a_k t_{ij}^{AA} - \zeta g_0^{-1} \sum_{k, \alpha} g_{ik} a_i^* b_k t_{ij}^{BA}, \]
\[ t_{ij}^{BA} = -\zeta \sum_{k, \alpha} b_i^* b_k t_{ij}^{BA} - \zeta g_0^{-1} \sum_{k, \alpha} g_{ik} b_i^* a_k t_{ij}^{AB}, \]
\[ t_{ij}^{BB} = -\zeta \sum_{k, \alpha} b_i^* b_k t_{ij}^{BB} - \zeta g_0^{-1} \sum_{k, \alpha} g_{ik} b_i^* a_k t_{ij}^{AB}, \]
\[ t_{ij}^{AB} = -\zeta \sum_{k, \alpha} a_i^* a_k t_{ij}^{AB} - \zeta g_0^{-1} \sum_{k, \alpha} g_{ik} a_i^* b_k t_{ij}^{BA}. \] (2.80)

Here, we can use eq. (2.62) for \( \bar{g}^{AB} \) and \( \bar{g}^{BA} \) because the phase factor \( \exp(iy_k/\gamma) \) can be replaced by unity when \( |y| \ll L \) and the energy is in the range (2.44). Further,
we can use eq. (2.47) and we just need the sum of $T_{ij}$.

Define the following matrices:

$$
t^{AA} = (t^{AA}_{ij}), \quad t^{BA} = (t^{BA}_{ij}),
$$

$$
t^{BB} = (t^{BB}_{ij}), \quad t^{AB} = (t^{AB}_{ij}),
$$

$$A = (A_{ij}), \quad B = (B_{ij}), \quad \Gamma^{AB} = (\Gamma^{AB}_{ij}), \quad \Gamma^{BA} = (\Gamma^{BA}_{ij}),$$

with

$$A_{ij} = a_i^+ a_j, \quad B_{ij} = b_i^+ b_j,$$

$$\Gamma^{AB}_{ij} = \gamma^{AB}_{ij} a_i^+ b_j, \quad \Gamma^{BA}_{ij} = \gamma^{BA}_{ij} b_i^+ a_j.$$  

(2.81)

Let $N_A$ be the number of impurities at $A$ sites and $N_B$ that at $B$ sites. Then, $t^{AA}$ and $A$ are an $(N_A, N_A)$ matrix, $t^{BB}$ and $B$ are an $(N_B, N_B)$ matrix, $t^{AB}$ and $\Gamma^{BA}$ are an $(N_A, N_B)$ matrix, and $t^{AB}$ and $\Gamma^{BA}$ are an $(N_A, N_B)$ matrix. We have

$$\begin{align}
(1-\zeta+\zeta A)t^{AA} &= 1 - \zeta \delta_{ij} \Gamma^{AB} t^{BA}, \\
(1-\zeta+\zeta B)t^{BB} &= 1 - \zeta \delta_{ij} \Gamma^{BA} t^{AB}, \\
(1-\zeta+\zeta B)t^{BA} &= -\zeta \delta_{ij} \Gamma^{BA} t^{AB}, \\
(1-\zeta+\zeta A)t^{AB} &= -\zeta \delta_{ij} \Gamma^{AB} t^{BA}.
\end{align}$$

(2.83)

It should be pointed out that

$$A = (a_1 a_2 \cdots a_{N_A})^+ (a_1 a_2 \cdots a_{N_A}),$$

$$B = (b_1 b_2 \cdots b_{N_B})^+ (b_1 b_2 \cdots b_{N_B}).$$

(2.84)

(2.85)

Further, both $A$ and $B$ are real symmetric matrices.

The sum of $T_{ij}$ can be written in general as

$$T_S = \begin{pmatrix} T^{AA} & T^{AB} \\ T^{BA} & T^{BB} \end{pmatrix},$$

(2.86)

where $T^{AA}$, $T^{AB}$, $T^{BA}$, and $T^{BB}$ are $(2, 2)$ matrices, given by

$$T^{AA} = \begin{pmatrix} t^{AA} & t^{BA} \\ t^{KA} & t^{KK} \end{pmatrix}, \quad T^{AB} = \begin{pmatrix} t^{AB} & t^{BA} \\ t^{KB} & t^{KK} \end{pmatrix},$$

$$T^{BA} = \begin{pmatrix} t^{BA} & t^{AB} \\ t^{KB} & t^{KK} \end{pmatrix}, \quad T^{BB} = \begin{pmatrix} t^{BB} & t^{BA} \\ t^{KB} & t^{KK} \end{pmatrix}.$$  

(2.87)

Then, the reflection coefficients are given by

$$r_{KK} = -\frac{A}{2\gamma} (T^{AA}_{KK} - T^{BB}_{KK} + i T^{AB}_{KK} + i T^{BA}_{KK}),$$

$$r_{KK'} = -\frac{A}{2\gamma} (T^{AA}_{KK} - T^{BB}_{KK} - i T^{AB}_{KK} - i T^{BA}_{KK}),$$

$$r_{K'K'} = -\frac{A}{2\gamma} (T^{AA}_{KK} + T^{BB}_{KK} - i T^{AB}_{KK} - i T^{BA}_{KK}),$$

$$r_{K'K} = -\frac{A}{2\gamma} (T^{AA}_{KK} + T^{BB}_{KK} + i T^{AB}_{KK} + i T^{BA}_{KK}),$$

(2.88)

and the transmission coefficients are given by

$$t_{KK} = 1 - \frac{A}{2\gamma} (T^{AA}_{KK} + T^{BB}_{KK} + i T^{AB}_{KK} - i T^{BA}_{KK}),$$

$$t_{K'K'} = 1 - \frac{A}{2\gamma} (T^{AA}_{KK} + T^{BB}_{KK} - i T^{AB}_{KK} + i T^{BA}_{KK}),$$

$$t_{K'K} = 1 - \frac{A}{2\gamma} (T^{AA}_{KK} - T^{BB}_{KK} - i T^{AB}_{KK} + i T^{BA}_{KK}),$$

$$t_{KK'} = 1 - \frac{A}{2\gamma} (T^{AA}_{KK} - T^{BB}_{KK} + i T^{AB}_{KK} - i T^{BA}_{KK}).$$

(2.89)

The similar expressions are obtained for $r'_{KK}$, etc. and $t'_{KK}$, etc.

§3. Examples

3.1 Impurities at same sublattices

Consider a single impurity with strength $u$ at an $A$ site $r_1$ illustrated in Fig. 3(a). In this case, we have $t^{AA} = 1$ and $t^{AB} = t^{BA} = t^{BB} = 0$, which leads to $T^{AA} = T^{BB} = 0$ and

$$T^{AA} = \frac{\zeta \gamma L}{AL} \gamma_{i_0}^2 \gamma_{j_0}^2 a_j^+ a_j^+.$$  

(3.1)

Explicitly, we have

$$r_{KK} = r_{K'K'} = \frac{\zeta}{2g_0},$$

$$r_{K'K} = \frac{\zeta e^{-i\phi_j}}{2g_0}, \quad r_{KK'} = \frac{\zeta e^{i\phi_j}}{2g_0},$$

$$t_{KK} = t_{K'K'} = 1 - \frac{\zeta}{2g_0},$$

$$t_{K'K} = \frac{\zeta e^{-i\phi_j}}{2g_0}, \quad t_{KK'} = \frac{\zeta e^{i\phi_j}}{2g_0}.$$  

(3.2)

Equation (2.77) shows that $\zeta / g_0 = 1$ when $g_0^0(\varepsilon) = -1/2\bar{u}$. In this case we have $t_{KK} = t_{K'K'} = 1/2$ and $|t_{KK'}| = |t_{K'K}| = 1/2$, which leads to the conductance given by $G = e^2/\pi h$, i.e., a half of the ideal value $2e^2/\pi h$. This means that for any impurity there exists an energy at which $G = e^2/\pi h$. In the limit $\bar{u} \to \infty$, in particular, this occurs at $\varepsilon = 0$, showing that the conductance is quantized into $G = e^2/\pi h$ in the case of a vacancy consisting of a single A or B site.

Fig. 3 Schematic illustration of vacancies in an armchair nanotube. The closed and open circles denote A and B lattice points, respectively. (a) A, (b) AB, (c) A3B, and (d) A3.

Next, we shall consider impurities located at two different A sites denoted as 1 and 2. The equation for $t^{AA}$ is given by

$$(1-\zeta+\zeta A)t^{AA} = 1.$$  

(3.3)

with

$$A = (a_1 a_2)^+ (a_1 a_2).$$  

(3.4)

Introduce an orthogonal matrix $U = (u_1 u_2)$ such that

$$U^+ AU = \begin{pmatrix} p_1 & 0 \\ 0 & p_2 \end{pmatrix},$$  

(3.5)

i.e.,

$$Au_j = p_j u_j, \quad (j = 1, 2).$$  

(3.6)

We choose the ordering of eigenvalues such that $p_1 \geq p_2 \geq \ldots$
we have \( u \to \infty \) or \( \zeta \to 1 \) gives
\[
T_S^{AA} = \frac{1}{AL\gamma_0} \frac{\gamma L}{2} 2a_1^+ \bar{a}_1^+.
\] (3.20)

This result is completely same as that for a single impurity and leads to the conclusion that the conductance is quantized into a half of the ideal value, i.e., \( G = e^2/\pi h \).

Next, we consider the case of \( N (N \geq 3) \) impurities located at \( A \) sublattices. The equations for \( T \) matrices are same as eq. (3.3) except that \( A \) is now given by eq. (2.84). Introduce an orthogonal matrix \( U = (u_1 u_2 \cdots u_N) \) such that
\[
A u_j = p_j u_j.
\] (3.21)

We choose the ordering of eigenvalues such that \( p_1 \geq p_2 \geq \cdots \geq p_N \geq 0 \). Then, the equation for \( t^{AA} \) can be solved as
\[
t^{AA} = U t'^{AA} U^+, \tag{3.22}
\]
with
\[
t'_{ij} = \frac{\delta_{ij}}{1-\zeta + \zeta p_j}.
\] (3.23)

Introduce two-component vectors
\[
a'_j = (a_1 a_2 \cdots a_N) u_j.
\] (3.24)

Then we have
\[
T_S^{AA} = \frac{1}{AL\gamma_0} \zeta \sum_{i,j} t_{ij}^{AA} 2a_i a_j^+ = \frac{1}{AL\gamma_0} \sum_j 2a'_j a_j^+. \tag{3.25}
\]

Unless all \( a'_j \)'s are same, eq. (2.84) shows rank \( A = 2 \). Therefore, we have \( p_j = 0 \) and \( a'_j = 0 \) for \( j = 3, \ldots, N \). Introducing two vectors using eq. (3.12), we can show immediately that the \( T \) matrix is exactly same as that in the case of two impurities given by eqs. (3.15) and (3.16).

When \( a'_j \)'s are all equal, the rank of \( A \) is reduced further, i.e., rank \( A = 1 \), and consequently \( p_2 = 0 \) and \( a'_2 = 0 \). Thus, the \( T \) matrix is exactly same as that in the case of a single impurity.

### 3.2 Pair of impurities: \( AB \)

We shall consider the case of a pair of an impurity at an \( A \) site \( r_1 \) and an impurity at a \( B \) site \( r_2 \) closely spaced with each other. We have
\[
t^{AA} = 1 - \zeta \gamma_0^{-1} g_{ij} a_i^+ b_i t^{BA},
\]
\[
t^{BA} = -\zeta \gamma_0^{-1} g_{ij} a_i^+ b_i t^{AB},
\]
\[
t^{BB} = 1 - \zeta \gamma_0^{-1} g_{ij} a_i^+ b_i t^{BB}.
\] (3.26)

Therefore, we have
\[
t^{AA} = t^{BB} = \frac{1}{1 + (\zeta \gamma_0^{-1} g_{ij} a_i^+ b_i)^2},
\]
\[
t^{BA} = -t^{AB} = \frac{\zeta \gamma_0^{-1} g_{ij} a_i^+ b_i}{1 + (\zeta \gamma_0^{-1} g_{ij} a_i^+ b_i)^2}.
\] (3.27)

where use has been made of \( \bar{g}_{ij}^{AA} = -\bar{g}_{ij}^{BA} \).

First, we consider the case that the energy is away from the band edge of the bands \( n = \pm 1 \), i.e., \( \pm 2\pi\gamma/L \).
In this case, we can safely assume that $|g_0| \sim 1$ and $|g_0^{-1} q_1| \propto L/a \gg 1$.

In the case of a sufficiently weak potential $|\tilde{u}| \ll 1$, for which $\xi \approx 2l_0 g_0$, we have $t^{AB} = t^{BB} \sim 1$ and $t^{BA} = -t^{AB} = 0$, i.e., $T^{BA} \approx T^{AB} \approx 0$ and

$$T^{AA} = \frac{1}{4L} u \Phi_i^A, \quad T^{BB} = \frac{1}{4L} u \Phi_i^B.$$  \hspace{1cm} (3.28)

This is equivalent to the lowest Born result and shows that the A and B impurities can be described by an effective potential at some lattice point $r_j \approx r_i$.

The lowest Born approximation becomes invalid when $|\xi g_0^{-1} \tilde{t}_i^A \tilde{t}_j^B| \sim 1$. The off-diagonal Green’s function is extremely large for impurities located at the distance of the order of the lattice constant and therefore the critical $\xi$ is well approximated by $\xi = 2l_0 g_0$. Define $\tilde{u}_e$ by

$$\frac{1}{2\varepsilon_0} = \tilde{g}^{ii}_A \tilde{t}_i^B r_j \tilde{t}_j^A = -\tilde{g}^{ii}_A \tilde{t}_i^B r_j \tilde{t}_j^A.$$  \hspace{1cm} (3.29)

Then, the above condition is achieved if $|\tilde{u}| \sim |\tilde{u}_e|$. We have $g_1(x, y) \approx (L/\pi)(x+iy)^{-1} = (L/\pi d_{AB}) \exp(-i\theta_{AB})$, where $d_{AB}$ is the distance between the impurities and $\theta_{AB}$ is the direction angle from an impurity at a B site to that at an A site. Then, we have from eq. (3.62)

$$\tilde{g}^{ii}_A \approx \frac{L}{\pi d_{AB}} \cos(\theta_{AB} + (\phi_i^A - \phi_j^B)/2) / \cos((\phi_i^A - \phi_j^B)/2),$$  \hspace{1cm} (3.30)

which gives

$$\tilde{u}_e = \frac{\pi d_{AB}}{2L} \cos(\theta_{AB} + (\phi_i^A - \phi_j^B)/2).$$  \hspace{1cm} (3.31)

Let $V$ be a local site energy at an impurity and $\gamma_0$ be the transfer integral in the nearest-neighbor tight-binding model. Then, we have

$$u = \frac{\sqrt{3}}{2} \varepsilon_0 a^2 V, \quad \gamma = \frac{\sqrt{3}}{2} \gamma_0 a, \quad \tilde{u} = \frac{1}{2} a V / L \gamma_0.$$  \hspace{1cm} (3.32)

Therefore, in terms of the local site energy, the critical value is given by

$$|V| = \frac{\pi d_{AB}}{\gamma_0} \frac{1}{\cos(\theta_{AB} + (\phi_i^A - \phi_j^B)/2)},$$  \hspace{1cm} (3.33)

which is of the order of unity for impurities with $d_{AB} \sim a$.

For small $\tilde{u}$, we have $\xi \approx 2l_0 g_0 (1 - 2l_0 g_0)$ and therefore

$$t^{AA} = t^{BB} \approx 1 - (\tilde{u}/\tilde{u}_e)^2 + 4l_0 g_0 (\tilde{u}/\tilde{u}_e)^2,$$

$$t^{BA} = -t^{AB} \approx 1 - (\tilde{u}/\tilde{u}_e)^2 + 4l_0 g_0 (\tilde{u}/\tilde{u}_e)^2.$$  \hspace{1cm} (3.34)

This shows that $t^{AA}$, etc. exhibit a resonance behavior at $\tilde{u} = \pm \tilde{u}_e$. The width of the resonance is given by $\Delta \tilde{u} = 2u^2 \propto (a/L)^2$ at $\varepsilon = 0$ and is quite narrow. At the resonance we have $|t^{AA}| \approx |t^{BB}| \approx |t^{BA}| \sim 1$. The resonance is in agreement with the results obtained in numerical tight-binding calculations.\textsuperscript{38,34,35}

In order to see the resonance behavior at $\tilde{u} = \pm \tilde{u}_e$ more explicitly, we shall consider the AB impurities in an armchair nanotube shown in Fig. 3(b). In this case we have $\theta_{AB} = \pi$ and $\phi_i^A - \phi_j^B = 0$ ($\eta = -\pi/2$), which give identically

$$r_{KK} = r_{KK'} = t_{KK'} = r_{KK''} = 0,$$  \hspace{1cm} (3.35)

according to eq. (2.88) and (2.89). This is a consequence of the mirror symmetry with respect to a plane containing the axis.\textsuperscript{26,34} The other coefficients are

$$r_{KK'} = -2i\tilde{u}[1 - (\tilde{u}/\tilde{u}_e)^2] \exp[i\pi/2],$$

$$r_{KK''} = -2i\tilde{u} [1 - (\tilde{u}/\tilde{u}_e)^2] \exp[-i\pi/2].$$

They show that for $\tilde{u} \sim |\tilde{u}_e| = \tilde{u}_c$, for example, the resonance appears only in $r_{KK'}$ and $r_{KK''}$ due to cancelation among different contributions and $|r_{KK'}| \sim 1$ and further $|r_{KK'}| \sim 0$ at the resonance. The conductance at the resonance is given by $G = e^2/\pi h$. These results explain the numerical results presented in §4 quite well.

Next, consider the case $|\tilde{u}| \gg |\tilde{u}_e|$. In this case, $t^{AA} = t^{BB} \ll |t^{BA}| = |t^{AB}|$ and

$$t^{BA} = -t^{AB} \approx \frac{2\tilde{u}_c g_0}{\xi}.$$  \hspace{1cm} (3.37)

Therefore, we have

$$r_{KK} = r_{KK'} = 2\tilde{u}_c \sin(\phi_i^A - \phi_j^B)/2,$$

$$r_{KK''} = r_{KK''} = -2\tilde{u}_c \exp(-i\phi_i^A - \phi_j^B)/2.$$  \hspace{1cm} (3.38)

Therefore, the conductance becomes

$$G = \frac{2e^2}{\pi h} \left[1 - 4\tilde{u}_c^2 (1 + \sin^2(\phi_i^A - \phi_j^B)/2)\right].$$  \hspace{1cm} (3.39)

This shows that the deviation from the ideal conductance $2e^2/\pi h$ is proportional to $(a/L)^2$ and vanishes in sufficiently thick nanotubes.

Consider the case that $\varepsilon \sim 2\pi\gamma/L$ for a strong scattering $|\tilde{u}| \gg 1$. In this case, eqs. (2.77) shows $\xi g_0 \approx g_0(\varepsilon) \sim 1$ because $g_0(\varepsilon) \rightarrow -\infty$. Therefore, $t^{AA} = t^{BB}$ and $t^{BA} = -t^{AB}$ given by eq. (3.9) show a resonance behavior at $g_0^\prime(\varepsilon) = \tilde{g}^{ii}_A \tilde{t}_i^B \tilde{t}_j^A$. The features of the resonance are same as those at $\tilde{u} = \pm \tilde{u}_e$ discussed above and consequently the conductance is reduced to $G = e^2/\pi h$ at the resonance. Because $|\tilde{g}^{ii}_A \tilde{t}_i^B \tilde{t}_j^A|$ is extremely large in the case $L/a \gg 1$, the resonance occurs at an energy very close to $2\pi\gamma/L$ as will be demonstrated by numerical results shown in §4.

Consider a pair of AB impurities located along a circumference direction with arbitrary distance $d_{AB}$ in an armchair nanotube. In this case, we cannot use eqs. (3.26) or (3.27) because they are valid only in the case $d_{AB}/L \ll 1$ and we have to start with eqs. (2.78) and (2.79). When $\varepsilon = 0$ and $|\tilde{u}| \gg 1$, with the use of $g_1(x, y)$ given by eq. (2.63), the conductance is shown to be given by the simple analytical formula $G = [e^2/\pi h][1 + \cos(2\pi d_{AB}/L)]$ in agreement with numerical results obtained previously in a tight-binding model.\textsuperscript{40} Analytic formula can be obtained for AB pairs
with a more general configuration but will not be presented here.

3.3 Impurities: $A_{N_A}B_{N_B}$

Let us consider the case of $N_A$ impurities at A sublattice sites and $N_B$ impurities at B sublattice sites. For simplicity, we assume that they are closely spaced from each other (within a distance of the order of $a$) and further consider the case of sufficiently thick nanotubes, i.e., $a/L \rightarrow 0$, in the energy range $|e| \ll 2\pi\gamma/L$. Equation (2.83) can be rewritten as

\[ (1-\zeta+\zeta A)t_{AA}^{AB} = 1 + \zeta^2 g_0^2 \Gamma_{BA}t_{BA}^{AA}, \]
\[ (1-\zeta+\zeta B)t_{BB}^{AB} = 1 + \zeta^2 g_0^2 \Gamma_{BA}t_{BA}^{BB}, \]
\[ (1-\zeta+\zeta A)t_{BA}^{AB} = -\zeta g_0^2 \Gamma_{BA}t_{BA}^{AA}, \]
\[ (1-\zeta+\zeta B)t_{BB}^{AB} = -\zeta g_0^2 \Gamma_{BA}t_{BA}^{BB}. \]

Equation (2.30) can be rewritten as

\[ (1-\zeta+\zeta A)t_{AA}^{AB} = 1 + \zeta^2 g_0^2 \Gamma_{BA}t_{BA}^{AA}, \]
\[ (1-\zeta+\zeta B)t_{BB}^{AB} = 1 + \zeta^2 g_0^2 \Gamma_{BA}t_{BA}^{BB}, \]
\[ (1-\zeta+\zeta A)t_{BA}^{AB} = -\zeta g_0^2 \Gamma_{BA}t_{BA}^{AA}, \]
\[ (1-\zeta+\zeta B)t_{BB}^{AB} = -\zeta g_0^2 \Gamma_{BA}t_{BA}^{BB}. \]

First, we consider the case $N_A = N_B$. In this case, we have usually det $\Gamma_{AB} \neq 0$ and det $\Gamma_{BA} \neq 0$. Therefore, we have

\[ t_{AA}^{AB} \approx -\zeta^2 g_0^2 (\Gamma_{BA})^{-1}(1-\zeta+\zeta B)(\Gamma_{BA})^{-1}, \]
\[ t_{BA}^{AB} \approx +\zeta g_0^2 (\Gamma_{BA})^{-1}, \]
\[ t_{BB}^{AB} \approx -\zeta^2 g_0^2 (\Gamma_{BA})^{-1}(1-\zeta+\zeta A)(\Gamma_{BA})^{-1}, \]
\[ t_{AB}^{AB} \approx +\zeta g_0^2 (\Gamma_{BA})^{-1}. \]

These become extremely small when $a/L \ll 1$ and lead to the ideal conductance $G \approx 2e^2/\pi h$.

Next, we consider the case $N_A > N_B$. In this case, the $(N_B, N_B)$ matrix $\Gamma_{BA}^{-1}(1-\zeta+\zeta A)\Gamma_{BA}$ is usually not singular. Therefore, we have

\[ t_{AB}^{BB} \approx -\zeta^2 g_0^2 (\Gamma_{BA})^{-1}(1-\zeta+\zeta A)(\Gamma_{BA})^{-1}, \]
\[ t_{AB}^{AB} \approx +\zeta g_0^2 (\Gamma_{BA})^{-1}. \]

These become extremely small in the limit of small $a/L$ and can be neglected. On the other hand, the $(N_A, N_A)$ matrix $\Gamma_{BA}^{-1}(1-\zeta+\zeta B)\Gamma_{BA}$ is always singular and its rank is usually $N_B (< N_A)$ which is the rank of $\Gamma_{AB}$ and $\Gamma_{BA}$.

We introduce a set of orthogonal vectors with $N_A$ components, $u_j$ ($j = 1, 2, \ldots, N_A$), such that

\[ \Gamma_{BA}u_j = 0, \quad (1 \leq j \leq N_A - N_B), \]
\[ \Gamma_{BA}u_j \neq 0, \quad (N_A - N_B < j \leq N_A) \]
and make an orthogonal transformation

\[ t_{AA}^{AB} = U \tilde{U} U^+, \quad A = U A U^+, \]
where

\[ U = (u_1, u_2, \ldots, u_{N_A}). \]

Define two component vectors $a_j'$ through

\[ a'_j = (a_1, a_2, \ldots, a_{N_A})u_j. \]

Then, we have

\[ A' = (a'_1, a'_2, \ldots, a'_{N_A})^T. \]

We have

\[ (1-\zeta+\zeta A)t_{AA}^{AB} = 1 + \zeta^2 g_0^2 Q t', \]
with

\[ Q = U^+ \Gamma_{BA}^{-1}(1-\zeta+\zeta B) \Gamma_{BA} U. \]

We separate the matrices as follows

\[ t' = \left( \begin{array}{c} t'_0 \\ t'_1 \\ t'_2 \\ t'_3 \end{array} \right), \quad A' = \left( \begin{array}{c} A'_0 \\ A'_1 \\ A'_2 \\ A'_3 \end{array} \right), \quad Q = \left( \begin{array}{cc} Q_0 & Q_1 \\ Q_2 & Q_3 \end{array} \right). \]

where $t'_0$, $A'_0$, and $Q_0$ are $(N_A-N_B, N_A-N_B)$ matrices, etc. We have

\[ Q_0 = 0, \quad Q_1 = 0, \quad Q_2 = 0, \quad Q_3 = 1, \]
and $Q_3$ is a matrix which is usually not singular. Then, we have

\[ \left( \begin{array}{c} 1 & \zeta A'_0 \\ \zeta A'_1 & 1 - \zeta + \zeta A'_2 \end{array} \right) \left( \begin{array}{c} t'_0 \\ t'_1 \\ t'_2 \\ t'_3 \end{array} \right) = \left( \begin{array}{c} 1 \cr 0 \cr 0 \cr 1 \end{array} \right) + \zeta^2 g_0^2 \left( \begin{array}{c} 0 \\ 0 \\ Q_3 \end{array} \right) \left( \begin{array}{c} t'_0 \\ t'_1 \\ t'_2 \end{array} \right). \]

In the limit $a/L \rightarrow 0$, matrix elements and therefore eigenvalues of $Q_3$ become infinitely large, i.e., $Q_3 \rightarrow \infty$, we then have

\[ (1-\zeta+\zeta A'_0)t'_0 = 1, \quad t'_1 = 0, \quad t'_2 = 0, \quad t'_3 = 0. \]

In the case $N_A - N_B > 2$, we have usually rank $A'_0 = 2$ and $A'_0$ has only two nonzero eigenvalues. Let $u'_j$ be eigenvectors of $A'_0$, i.e.,

\[ A'_0 u'_j = p_j u'_j. \]

Then, we can arrange them such that $p_1 \geq p_2 > 0$ and $p_3 = 0$ for $3 \leq j \leq N_A - N_B$. Define

\[ a_{1j} = (a_1, \ldots, a_{N_A-N_B})u'_j. \]

Then, we have $a_{1j}^2 = \delta_{1j}a_{1j}^2$, $a_{2j} = \delta_{1j}a_{2j}$, and $|a_{1j}| = |a_{2j}| = 1$. By making another orthogonal transformation

\[ t'_0 = U't'U'^+, \]
with $U' = (u'_1, u'_2, \ldots, u'_{N_A-N_B})$, we have

\[ t'_0 = \frac{1}{1 - \zeta + \zeta p_1} \delta_{1j}. \]

Therefore, we have

\[ t'_{ij} = \sum_{k=1}^{N_A-N_B} \sum_{m=1}^{N_A-N_B} \sum_{n=1}^{N_A-N_B} \frac{a_{im}u'_iu'_k u'_m v_{nk}}{1 - \zeta + \zeta p_k}, \]
and

\[ t'_{ij} = \frac{a_{im}u'_iu'_k u'_m v_{nk}}{1 - \zeta + \zeta p_k}. \]

Therefore, the T matrix is

\[ T'_{ij} = \sum_{i,j=1}^{N_A-N_B} \sum_{l=1}^{N_A-N_B} \sum_{m=1}^{N_A-N_B} \sum_{n=1}^{N_A-N_B} \frac{a_{im}u'_iu'_k u'_m v_{nk} a_{nj}}{1 - \zeta + \zeta p_k} \]
\[ = \frac{2p_1 a_{1j} a_{1j}^*}{1 - \zeta + \zeta p_1} + \frac{2p_2 a_{2j} a_{2j}^*}{1 - \zeta + \zeta p_2}. \]

This is formally the same expression as that of two
impurities at A sublattice points. Using eqs. (3.43) and (3.60), we have $t^{BA} = 0$ and consequently $T^{BA} = 0$. When the potential is sufficiently strong and $\zeta \approx 1$, the results become completely same as in the case of two strong impurities at A sublattice points.

When $N_A - N_B = 2$, $t'_0$ becomes a $(2, 2)$ matrix and therefore the T matrix becomes same as that of two impurities at A sublattice sites and is given by the above equation. When $N_A - N_B = 1$, $t'_0$ is reduced to $(1, 1)$ matrix and the T matrix becomes same as that of a single impurity at an A site. Therefore, we can conclude that in the limit $a/L \rightarrow 0$ the conductance vanishes, i.e., $G = 0$, for $N_A - N_B \geq 2$, $G = e^2/\pi h$ for $N_A - N_B = 1$, and $G = 2e^2/\pi h$ for $N_A - N_B = 0$. This explains results of recent elaborate numerical study.\(^{39}\)

§4. Numerical Results

As a first example, we consider a pair of nearest-neighbor A and B impurities, AB, located along the circumference direction in armchair nanotubes shown in Fig. 3(b). In this case, $t_{KK}$, $t_{KK'}$, $t_{K'K}$, and $t_{K'K'}$ are nonzero and other elements vanish identically as mentioned already. Figures 4 and 5 show numerical results of reflection and transmission coefficients as a function of the potential strength $\tilde{u}$ for $n_c = 20$ and 50, respectively, at $\epsilon = 0$. The lattice constant is chosen as $a = L/n_c$. For small $\tilde{u}$ both $|r_{KK'}|$ and $|t_{KK'}|$ increase with $\tilde{u}$ in proportion to $\tilde{u}$ in agreement with the lowest Born result given by a dotted line. At $\tilde{u} = |\tilde{u}| = n\pi a/2\sqrt{3}L$ both $r_{KK'}$ and $t_{K'K}$ exhibit a resonance behavior discussed in §3. For a sufficiently large value of $\tilde{u}$, both $|r_{KK'}|$ and $|r_{K'K}|$ approach a small value proportional to $(a/L)^2$. These results are in agreement with those of the analytical treatment discussed in the previous section.

Figure 6 shows results for three A impurities surrounding a single impurity located at a B site, A$_3$B, illustrated in Fig. 3(c) for $\epsilon = 0$. A resonance appears at a certain critical value of $\tilde{u}$, which is much more complicated than that of the AB pair. For $\tilde{u}$ smaller than the critical value all the reflection coefficients are essentially same as those of the lowest Born approximation. Above the critical value, $|r_{KK'}| (= |r_{K'K}|)$ rapidly decreases with the increase of $\tilde{u}$, while $|r_{KK}| (= |r_{K'K'}|)$ increases and approaches unity. Actually, $|r_{KK}|$ is almost the same as the dashed line corresponding to $|r_{KK}|$ for three impurities located at A sites surrounding the single B site, i.e. A$_3$ shown in Fig. 3(d).

![Fig. 4](image1.png)  
**Fig. 4** Calculated reflection and transmission coefficients as a function of the potential strength $\tilde{u} = u/2\gamma L$ in the presence of a pair of nearest-neighbor AB impurities located along a circumference direction in armchair nanotubes. $n_c = 20$ and $a/L = n_c^{-1}$.

![Fig. 5](image2.png)  
**Fig. 5** Calculated reflection and transmission coefficients as a function of the potential strength $\tilde{u} = u/2\gamma L$ in the presence of a pair of nearest-neighbor AB impurities located along a circumference direction in armchair nanotubes. $n_c = 50$ and $a/L = n_c^{-1}$.

![Fig. 7](image3.png)  
**Fig. 7** Calculated reflection and transmission coefficients as a function of the potential strength $\tilde{u} =$
The origin of this behavior can easily be understood by looking at the structure of the lattice. In fact, when the local site energy at three A sites is sufficiently large, the B site surrounded by the three A sites is separated from the system and therefore the result should be independent of the energy at the B site. It is quite interesting that this is reproduced well even in the effective-mass scheme which takes into account the lattice structure only in the form of the matrix Schrödinger equation.

Figure 8 shows the conductance in the presence of a pair of A and B impurities along the circumference direction in an armchair nanotube as a function of their distance $d_{AB}$. $n_c = 50$.

Figure 9 shows the conductance in the presence of a pair of A and B impurities along the axis direction in a zigzag nanotube as a function of their distance $d_{AB}$. $n_c = 50$.

Figure 10 shows the conductance as a function of the Fermi energy in the presence of a strong impurity at an A site in an armchair nanotube illustrated in Fig. 3(a).

Figure 11 shows the conductance for an AB vacancy located in the circumference direction illustrated in
Fig. 12 Calculated conductance for an A3B vacancy illustrated in Fig. 3(c).

At \( d_{AB} = 0 \) the off-diagonal Green’s function vanishes and eq. (3.27) gives immediately \( t^{AA} = t^{BB} = 1 \) and \( t^{AB} = t^{BA} = 0 \), which leads to the complete reflection or the vanishing conductance. When \( d_{AB} \) is comparable to or larger than the cutoff distance \( a \sim L/n_c \), on the other hand, the off-diagonal Green’s function becomes extremely large and the scattering is suppressed considerably, leading to the ideal conductance \( G = 2e^2/\pi h \). Therefore, the conductance exhibits a singular behavior in the vicinity of \( d_{AB} = 0 \). Actural lattices do not exhibit such a singular behavior because \( d_{AB} \) cannot be smaller than the cutoff distance \( \sim L/n_c \).

Figure 9 shows the conductance in the presence of a pair of A and B impurities along the axis direction in a metallic zigzag nanotube as a function of their distance \( d_{AB} \). The conductance is given by a value close to \( G = 2e^2/\pi h \) for small \( d_{AB} \), decreases with the increase of \( d_{AB} \), and approaches a quantized value \( G = e^2/\pi h \) for a sufficiently large \( d_{AB} \), i.e., \( d_{AB}/L \sim 1 \). This can be understood by the fact that \( g_1(0, y) \approx -i\text{sgn}(y) \) for \( |y| \gg L/\pi \).

Figure 10 shows the conductance as a function of the Fermi energy in the presence of a strong impurity at an A site in an armchair nanotube illustrated in Fig. 3(a). The conductance becomes half of the ideal value \( G = e^2/\pi h \) at \( \varepsilon = 0 \), increases gradually with the increase of \( \varepsilon \), and reaches the ideal value \( G = 2e^2/\pi h \) at \( \varepsilon(2\pi\gamma/L)^{-1} = 1 \). These results are in agreement with those obtained in a tight-binding model\(^{37}\) including the dependence on \( n_c \sim L/a \).

Figure 11 shows the corresponding result for a pair of strong impurities located in the circumference direction illustrated in Fig. 3(b). The conductance is slightly smaller than the ideal value \( G = 2e^2/\pi h \) and approaches it with the increase of \( n_c \sim L/a \) except in the vicinity of \( \varepsilon = 2\pi\gamma/L \). Near \( \varepsilon = 2\pi\gamma/L \) the conductance exhibits a dip with \( G = e^2/\pi h \), which moves to the higher energy side with the increase of \( n_c \sim L/a \). At \( \varepsilon = 2\pi\gamma/L \) the conductance recovers the ideal value \( G = 2e^2/\pi h \). Figure 12 shows the result for the A3B vacancy illustrated in Fig. 3(c). The conductance vanishes at \( \varepsilon = 0 \) and reaches the ideal value \( G = 2e^2/\pi h \) at \( \varepsilon(2\pi\gamma/L)^{-1} = 1 \). These behaviors are again in agreement with those in a tight-binding model\(^{37}\).

§5. Discussion

We have shown analytically that in the limit of \( a/L \rightarrow 0 \) and a strong scatterer the conductance at \( \varepsilon = 0 \) vanishes, i.e., \( G = 0 \), for \( |N_A - N_B| \geq 2 \), \( G = e^2/\pi h \) for \( |N_A - N_B| = 1 \), and \( G = 2e^2/\pi h \) for \( N_A - N_B = 0 \), where \( N_A \) and \( N_B \) are the number of impurities at A and B lattice sites, respectively. This may intuitively be understood in terms of a reduction of the scattering potential by multiple scattering from a pair of A and B scatterers. In fact, multiple scattering between an A impurity at \( r_i \) and a B impurity at \( r_j \) reduces their effective potential by the factor \( \sim (\varepsilon g_0^{-1} \delta_{AB} a_i^0 b_j)^{-2} \). By eliminating AB pairs successively, some A or B impurities remain. The conductance is determined essentially by the number of these unpaired impurities.

Unfortunately, such a direct procedure is not rigorous mathematically. The reason is that there are many different ways in the elimination of AB pairs. Further, multiple scattering between unpaired and eliminated impurities cannot be neglected completely because of large off-diagonal Green’s functions. The correct mathematical procedure given in §3.3 shows that a proper combination of A and B impurities lead to vanishing scattering potential and the residual potential is determined by another combination of remaining A or B impurities. This does not modify the fact that the conductance is determined by the number of remaining impurities, however.

Consider a pair of impurities at an A site \( r_A = (x_A, y_A) \) and a B site \( r_B = (x_B, y_B) \) closely spaced with each other and having a delta potential with strength \( u \). For \( \varepsilon = 0 \), the Schrödinger equation is given by

\[
\begin{align*}
&u_{A}(r) e^{i\phi_A} u_A(r) \gamma(k_x - i\varepsilon k_y) 0 \quad e^{-i\phi_A} u_A(r) u_A(r) 0 \quad \gamma(k_x + i\varepsilon k_y) 0 \quad u_B(r) e^{i\phi_B} u_B(r) \\
&\gamma(k_x + i\varepsilon k_y) 0 \quad u_B(r) 0 \quad \gamma(k_x - i\varepsilon k_y) e^{-i\phi_B} u_B(r) u_B(r)
\end{align*}
\]

(5.1)

with \( u_A(r) = u\varepsilon(r - r_A) \) and \( u_B(r) = u\varepsilon(r - r_B) \). First, we should note that

\[
\left( \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} \right) z = \left( \frac{\partial}{\partial x} - i\frac{\partial}{\partial y} \right) z = -2\pi i\varepsilon(r),
\]

(5.2)

where \( z = x + iy \) and \( z = x - iy \). For a wave corresponding to the K point incident from the left hand side the above equation can be solved approximately by putting

\[
\begin{align*}
F^{KA} &= \frac{1}{\sqrt{2\pi L}} \left( 1 + f_{A} \frac{z_{AB}}{z - z_{B}} \right), \\
F^{KB} &= \frac{i}{\sqrt{2\pi L}} \left( 1 + f_{B} \frac{z_{AB}}{z - z_{A}} \right), \\
F^{K'} &= \frac{1}{\sqrt{2\pi L}} \left( 1 + f_{A} \frac{z_{AB}}{z - z_{A}} \right), \\
F^{K''} &= \frac{i}{\sqrt{2\pi L}} \left( 1 + f_{B} \frac{z_{AB}}{z - z_{B}} \right)
\end{align*}
\]

(5.3)

where \( z_A = x_A + iy_A \), \( z_B = x_B + iy_B \), and \( z_{AB} = z_A - z_B \).
As long as $f_A$, $f'_A$, $f_B$, and $f'_B$ are of the order of unity and $|z_{AB}| \sim a$, the correction terms proportional to $(z-z_A)^{-1}$, etc. are small except in the close vicinity of $r_A$ or $r_B$ and the above wave functions satisfy the periodic boundary conditions approximately in nanotubes with a large circumference $L/a \gg 1$. We have

\[
\begin{pmatrix}
  u & u^{\phi_A} 2\pi\gamma z_{AB}^{\phi_A} 0 \\
  u & u^{\phi_A} 0 2\pi\gamma z_{AB}^{\phi_A} \\
  2\pi\gamma z_{AB}^{\phi_A} 0 & u \\
  0 & 2\pi\gamma z_{AB}^{\phi_A} u
\end{pmatrix}
\begin{pmatrix}
  f_A \\
  f'_A \\
  f_B \\
  f'_B
\end{pmatrix}
= u
\begin{pmatrix}
  1 \\
  1 \\
  -1 \\
  1
\end{pmatrix}.
\]

This gives in the case $\bar{u}=u/2\gamma L \gg 1$, in particular,

\[
f_A = e^{i\phi_A} z_{AB}^{\phi_A} f'_A = \frac{z_{AB}^{\phi_A} + z_{AB}^{\phi_A^*}}{z_{AB}^{\phi_A} + z_{AB}^{\phi_A^*}},
\]

\[
f_B = e^{i\phi_A} z_{AB}^{\phi_A} f'_B = \frac{z_{AB}^{\phi_A} + z_{AB}^{\phi_A^*}}{z_{AB}^{\phi_A} + z_{AB}^{\phi_A^*}},
\]

which are independent of $\bar{u}$ and are of the order of unity. It shows that the wave is transmitted without any reflection and effects of two strong impurities give only a small correction to the wave function except in the extreme vicinity of their positions.

For a given energy $\varepsilon$ satisfying the condition (2.44), there are evanescent modes associated with bands with $n \neq 0$. Define the corresponding decay or growth rate $\pm k_n$ by

\[
k_n = \sqrt{\kappa(n)^2 - (\varepsilon/\gamma)^2}.
\]

Then, evanescent modes are given by

\[
F_{n+}^{K}(r) = \frac{1}{\sqrt{LA}} \left( \begin{array}{c} 1 + k_n/s(n) \\ 1 - k_n/s(n) \end{array} \right) \exp[-k_n y + i(n)x],
\]

\[
F_{n-}^{K}(r) = \frac{1}{\sqrt{LA}} \left( \begin{array}{c} 1 + k_n/s(n) \\ 1 - k_n/s(n) \end{array} \right) \exp[+k_n y + i(n)x],
\]

where $+$ denotes modes decaying in the positive $y$ direction and $-$ in the negative $y$ direction. This shows that when the energy approaches the bottom $2\pi\gamma/L$ of the first excited bands with $n=\pm 1$, the decay rate $k_{\pm 1}$ vanishes and the amplitude for $A$ and $B$ components becomes equal to each other. Therefore, the continuity of the wave function at $y = y_0$ is satisfied by including a single traveling mode

\[
F_{0+}^{K}(r) = \frac{1}{\sqrt{LA}} \left( \begin{array}{c} 1 \\ i \end{array} \right) \exp(i ky),
\]

with $k = \varepsilon/\gamma$, and the evanescent modes $F_{1+}^{K}$ and $F_{1-}^{K}$ or $F_{-1+}^{K}$ and $F_{-1-}^{K}$, only. Further, by choosing the phase of the evanescent modes appropriately, the $A$ or $B$ component of the total wave function can be made vanish at an arbitrary value $x_0$ of the $x$ coordinate. It means that such a wave is not affected by a short-range impurity located at $(x_0, y_0)$ and is transmitted with probability one. The same is applicable to the wave function associated with the K' point. This is presumably the reason that the transmission coefficient always becomes unity at $\varepsilon = 2\pi\gamma/L$ in the examples of the numerical results shown in §4.

Consider the case that $n$ impurities $V_j$ ($j=1, \ldots, n$) are located at $A$ sites within the distance much smaller than $L$. In this case, only the diagonal Green’s function $g_0$ appears in the perturbation series for the $T$ matrix. Because $g_0$ does not vary with the distance so much, it can be replaced by that for $x = y = 0$. Then, the $T$ matrix is calculated as

\[
(\alpha|T|\beta) = f_{\alpha}^{-1} \left[ 1 - \sum_j \frac{1}{AL} V_j G \right]^{-1} \sum_j \frac{1}{AL} V_j f_{\beta} \times \exp[-i(\kappa_\alpha - \kappa_{\beta})x_0 - i(k_\alpha - k_{\beta})y_0],
\]

where $(x_0, y_0)$ is the center-of-mass of impurities. This result shows that the effective potential is given by the sum of the potential of each impurity. The same is true of the case of impurities at B sites. It is possible therefore to derive the results obtained in §3 for vacancies consisting of same sublattice points using eq. (5.9).

It would be expected, intuitively, that for a pair of nearest-neighbor A and B impurities, their positions may be regarded as same because the distance is much smaller than the typical electron wavelength which is actually infinite at $\varepsilon = 0$. Because of the singularity of the off-diagonal Green’s function, such an approximate procedure becomes completely invalid when impurities at A and B sites coexist, except in the case that the potential is weak and the lowest Born approximation is appropriate.

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