Weak-localization in metallic carbon nanotubes

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The weak-localization correction to the Boltzmann conductivity due to impurity scattering is calculated in metallic carbon nanotubes within the effective-mass approximation. The correction is positive for the impurity with interaction range larger than the lattice constant, while the impurity with shorter interaction range turns the correction into a negative value destroying the anti-localization. The crossover from anti-localization to weak localization is realized by controlling the coherence time.

KEYWORDS: carbon nanotube, impurity scattering, weak localization, anti-localization, dynamical conductivity

1. Introduction

An increasing number of studies have been carried out since the discovery of carbon nanotubes (CNs). In terms of transport properties, metallic CNs have turned out to be quite a good conductor, and there exist several experimental reports on the realization of the conductance quantization. From the theoretical viewpoint, there is an astonishing prediction that backward scattering is entirely suppressed for the impurities with potential range larger than the lattice constant. The purpose of this paper is to clarify quantum interference effects in electrical transport in metallic CNs.

The effective-mass approximation enables us to describe the electronic states in CNs by the Weyl equation which is originally introduced for massless neutrinos, and the two-component wavefunction is accompanied by what we call the Berry phase, which causes the $\pi$ phase shift, or gives the negative sign for the $2\pi$ spatial rotation. The suppression of the backward scattering is ascribed to the destructive interference by the Berry phase for any pairs of the two scattering paths which are related to each other by the time-reversal. Further, the existence of a perfectly conducting channel has been proved rigorously in the case of multi conducting channels, leading to a conductance larger than $2e^2/\pi h$.

Such exotic features of the transport in CNs remind us of the transport in the presence of a strong spin-orbit coupling. Actually, the graphene sheet constituting the CNs has been shown to belong to the same universality class as the system with the spin-orbit scattering does, that is, symplectic class. The presence of a perfectly conducting channel has been extended to similar models with odd channel numbers and symplectic symmetry.

In real situations, there exist several types of perturbations breaking the symplectic symmetry. Recent studies reveal the fact that the perfectly conducting channel is fragile in the presence of such perturbations in the multi-channel case although the suppression of the backward scattering is robust. The impurity potential causing inter-valley scattering, which we call the short-range potential hereafter, is one of the most typical perturbations. In this study, we carry out the perturbative calculations of the quantum correction to the conductivity to study how the short-range impurity changes the destructive interference which is essential to the perfectly conducting channel.

This paper is organized as follows: In §2, we introduce the effective-mass equations for CNs and the impurity potential. In §3, we discuss the Boltzmann conductivity calculated by the Kubo formula. We present the weak-localization correction in §4 and give discussions in §5. Finally, conclusions are given in §6.

2. Model

Electronic states around the two Fermi points of metallic CNs are described by the following $4 \times 4$ effective-mass equation,

$$\mathcal{H}_0 \mathbf{F}(r) = \varepsilon \mathbf{F}(r),$$  \hspace{1cm} (1)

with $r = (x, y)$. Retaining the lowest-order terms, we obtain the effective Hamiltonian,

$$\mathcal{H}_0 = \gamma \begin{pmatrix} 0 & \hat{k}_x - i\hat{k}_y & 0 & 0 \\ \hat{k}_x + i\hat{k}_y & 0 & 0 & 0 \\ 0 & 0 & \hat{k}_x + i\hat{k}_y & 0 \\ 0 & 0 & \hat{k}_x - i\hat{k}_y & 0 \end{pmatrix},$$ \hspace{1cm} (2)

where $\hat{k}_x$ and $\hat{k}_y$ are the wavenumber operators in the $x$ and $y$ direction, respectively, and $\gamma$ is a band parameter. Note that this Hamiltonian does not contain the chiral angle $\eta$. In this study, we choose the $x$ axis in the circumference direction and the $y$ axis in the tube-axis direction. The Fermi surface of metallic CNs consists of two discrete points, which are called $K$ and $K'$ points, and the unit cell contains two sublattices, which are called A and B sites. Therefore, four types of the envelope functions are necessary to describe the electronic states, and they define the four-component wavefunction,

$$\mathbf{F}(r) = \begin{pmatrix} F^K_A(r) \\ F^K_B(r) \\ F^{K'}_A(r) \\ F^{K'}_B(r) \end{pmatrix} = \begin{pmatrix} \mathbf{F}^K(r) \\ \mathbf{F}^{K'}(r) \end{pmatrix}. \hspace{1cm} (3)$$

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This equation decouples into two $2 \times 2$ matrix equations for each Fermi point, and the eigenfunction for the $K$ point is given by

$$ F^K_{sk}(r) = \frac{1}{\sqrt{2}} \left( \frac{1}{J_{sk}} \right) e^{i(k_x x + k_y y)}, \tag{4} $$

with

$$ J_{sk} = \frac{k_x + ik_y}{|k_x + ik_y|} \equiv se^{i\phi_k}, \tag{5} $$

where $s = +1$ for the conduction band and to $-1$ for the valence band, and $\phi_k$ is the direction angle of $k$. Now that we impose the periodic boundary condition in the circumference direction, $k_x$ is quantized as

$$ k_x = \frac{2\pi n}{L}, \tag{6} $$

where $L$ denotes the circumference length and $n$ is an integer number. The dispersion relation is given by

$$ \varepsilon_{sk} = s\gamma\sqrt{\left(\frac{2\pi n}{L}\right)^2 + k^2}, \tag{7} $$

with $k = k_y$.

Impurities cause the mixing of these levels. Here, we introduce two types of the effective potential for impurities and, as a matter of convenience, we call one the long-range potential and the other the short-range potential, respectively.\(^7\)\(^,\)\(^2\)\(^1\)

The long-range potential is defined as

$$ U_L(r) = \sum_{i=1}^{N_L} u_{Li}(r - R^L_i) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{8} $$

with $N_L$ the number of impurities, and $R^L_i$ the position of an impurity. Throughout calculations in the following sections, we replace $u_{Li}(r - R^L_i)$, representing the spatial dependence of the single-impurity potential, with the delta potential

$$ u_L(i) = u_{Li}(r - R_i^L), \tag{9} $$

where $u_L(i)$ shows the strength of the $i$th long-range impurity. This replacement is justified as far as the electron wavelength, typically of the order of $L$, is much smaller than the interaction range of the impurity potential.

In the standard scheme of the effective-mass approximation, the impurity generates a diagonal potential like this and there are no off-diagonal components or sublattice-dependent terms because we neglect rapidly oscillating contributions and maintain only slowly-varying envelope functions. However, this is not the case with point defects\(^8\)\(^,\)\(^2\)\(^1\) or extremely-short-range impurities. The cancellation for the integral of the rapidly oscillating functions does not work for the impurities with the interaction range smaller than the lattice constant. This is why we should take the possibility for another type of the impurity potential into consideration.

The short-range potential consists of two terms as follows,

$$ U_S(r) = U_S^A(r) + U_S^B(r), \tag{10} $$

The first term $U_S^A$ represents the potential for impurities localized around A sites only,

$$ U_S^A(r) = \sum_{i=1}^{N_{SA}} u_{SA}(i)\delta(r - R_i^A) \begin{pmatrix} 1 & 0 & e^{i\phi_i^A} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & e^{-i\phi_i^A} & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{11} $$

with

$$ \phi_i^A = (K' - K) \cdot R_i^A + \eta, \tag{12} $$

where $K$ and $K'$ are the wave vector of the $K$ and $K'$ points, respectively, and $\eta$ is the chiral angle.

In a similar manner, the second term $U_B$ for B sites is given by

$$ U_S^B(r) = \sum_{i=1}^{N_{SB}} u_{SB}(i)\delta(r - R_i^B) \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & e^{i\phi_i^B} \\ 0 & 0 & 0 & 0 \\ e^{-i\phi_i^B} & 0 & 1 \end{pmatrix}, \tag{13} $$

with

$$ \phi_i^B = (K' - K) \cdot R_i^B - \eta + \frac{\pi}{3}. \tag{14} $$

It should be noted that both types of the potentials cause intra-valley scattering, but the inter-valley scattering is induced only by the short-range potential.

## 3. Boltzmann conductivity

Based on the model above, we calculate the static conductivity by the Kubo formula. We take the ensemble average of randomly distributed impurities and obtain the Boltzmann conductivity

$$ \sigma_B = \frac{e^2 \hbar}{2\pi A} \sum_\alpha v_\alpha G_\alpha^+(\varepsilon_F)G_\alpha^-\eta(\varepsilon_F)v_\alpha, \tag{15} $$

with $A$ the tube length. In this expression, $G_\alpha^+(\varepsilon_F)$ is the impurity-averaged Green’s function of the eigenstate $|\alpha\rangle$ (+ retarded and $-$ advanced), $v_\alpha$ is the velocity, $\varepsilon_F$ is the Fermi energy, and $\eta(\varepsilon_F)$ is the vertex correction.\(^2\)\(^4\)\(^2\)\(^5\)

The impurity-averaged Green’s function is defined as

$$ G_\alpha^\pm(\varepsilon_F) = \frac{1}{\varepsilon_F - \varepsilon_\alpha - \Sigma^\pm(\varepsilon_F)}, \tag{16} $$

with $\Sigma^\pm(\varepsilon_F)$ being the self-energy. In this paper we do not count the spin degrees of freedom.

The index $\alpha$ contains the valley index $j$ (+1 for the $K$ point and $-1$ for the $K'$ point), the band index $s$, the subband index $n$, and the wavenumber $k$. We define further

$$ k_\alpha \equiv \left(\frac{2\pi n}{L}\right)k. \tag{17} $$

The velocity for the state $|\alpha\rangle$ is given by

$$ v_\alpha = sv_0 \frac{k}{\sqrt{(2\pi n/L)^2 + k^2}}, \tag{18} $$

where $v_0$ is the velocity of the band with linear dispersion relation given by

$$ v_0 = \frac{\gamma}{\hbar}. \tag{19} $$
For convenience, we define the velocity for each subband at the Fermi energy as

\[ v_n(\varepsilon_F) = v_0 \sqrt{\frac{\varepsilon_F^2 - (\varepsilon_L n)^2}{\varepsilon_F}}. \]  

with

\[ \varepsilon_L = \frac{2\pi\gamma}{L}. \]

We calculate the self-energy in the Born approximation

\[ \Sigma^\pm_\alpha(\varepsilon_F) = \sum_\beta \frac{\Gamma^0_{\alpha\beta\alpha}}{\varepsilon_F - \varepsilon_B \pm i\delta}. \]  

The bare vertex function, \( \Gamma^0_{\alpha\alpha'\beta\beta'} \), is defined by

\[ \Gamma^0_{\alpha\alpha'\beta\beta'} = \langle \langle \beta U | \alpha \rangle \langle \beta' U | \alpha' \rangle \rangle_{\text{imp}} \]  

where \( U = U_L + U_S \) and \( \langle \cdots \rangle_{\text{imp}} \) shows the ensemble average for impurity configurations.

Here, we introduce the diagrams representing these functions. Figure 1(a) shows the bare vertex function, and Fig. 1(b) does the self energy. Dyson’s equation for the self energy is given by Fig. 1(c). In these diagrams, broken lines represent the impurity potential, and thick and thin lines show the impurity-averaged Green’s functions and bare ones, respectively.

In the Boltzmann limit, we have only to take the imaginary part as

\[ \Sigma^\pm_\alpha(\varepsilon_F) = \mp i \frac{\hbar}{2\pi \tau(\varepsilon_F)}. \]  

and the relaxation time is given by

\[ \frac{1}{\tau(\varepsilon_F)} = \frac{4\pi v_0}{L} WF_1(\varepsilon_F), \]  

with

\[ F_1(\varepsilon_F) = \sum_{|n| \leq N_F} \frac{v_n(\varepsilon_F)}{v_0(\varepsilon_F)} = \sum_{|n| \leq N_F} \sqrt{\varepsilon_F^2 - (\varepsilon_L n)^2}. \]  

The upper limit of the summation, \( N_F \), is an integer part of \( \varepsilon_F/\varepsilon_L \), and the number of conducting channels is equal to \( 2(2N_F + 1) \). The factor two comes from the number of valleys. In this paper, we call the metallic CN with \( N_F = 0 \) the single-channel system and, otherwise, the multi-channel system.

The dimensionless parameter, \( W \), characterizing the strength of the impurity scattering is given by

\[ W = W_L + W_S, \]  

\[ W_S = W_{SA} + W_{SB}, \]  

\[ W_X = \frac{1}{4\pi\gamma^2LA} \sum_{i=1}^{N_X} u_X(i)^2 = \frac{n_X u_X^2}{4\pi\gamma^2}. \]  

\( (X = L, SA, SB) \),

where \( n_X \) and \( u_X^2 \) indicate the density of the impurity of type \( X \) and its averaged intensity, respectively, and we have assumed \( W_{SA} = W_{SB} = W_S/2 \) and \( \sum_i u_X(i) = 0 \) for all types of impurities.

Now, we can calculate the Boltzmann conductivity neglecting the velocity vertex corrections

\[ \sigma_B = \frac{e^2\gamma^2}{2\pi\hbar A} \sum_\alpha \frac{(\gamma_k)^2}{(\varepsilon_F - \varepsilon_\alpha)^2 + [\hbar/2\tau(\varepsilon_F)]^2}. \]  

which is diagrammatically shown in Fig. 2(a). We assume the weak-scattering limit for positive \( \varepsilon_F \)

\[ \frac{\hbar}{2\tau(\varepsilon_F)} = WF_1(\varepsilon_F) \ll 1. \]  

Then, we obtain

\[ \sigma_B = \frac{e^2}{2\pi\hbar W F_1(\varepsilon_F)}, \]  

with

\[ F_2(\varepsilon_F) = \sum_{|n| \leq N_F} \frac{v_n(\varepsilon_F)}{v_0} = \sum_{|n| \leq N_F} \frac{\sqrt{\varepsilon_F^2 - (\varepsilon_L n)^2}}{\varepsilon_F}. \]  

The potential range of the impurity consisting of the short-range potential is localized at a single site. Either \( A \) or \( B \) components in the wavefunction of initial and final states contribute to the scattering amplitude. That is to say, the scattering strength does not depend either on the wave vector of the initial state or on that of the final state because we assume the delta potential. As is the case with usual impurity-scattering treatment, the short-range potential generates only isotropic scattering and the vertex correction vanishes.

In contrast, there exists the wave vector dependence in the inner-product of the wavefunctions which contributes to the scattering due to the long-range potential. For example, the scattering amplitude between \( |jsk\rangle \) and \( |jsk'\rangle \) is proportional to

\[ \langle jsk' | U_L | jsk \rangle \propto \frac{1}{2}(1 + f_{sk} f_{sk'}) \propto \cos \left( \frac{\phi_k - \phi_{k'}}{2} \right), \]  

and this clearly shows that the scattering by long-range potential is anisotropic. This factor makes significant reduction of the probability for backward scattering and, in particular, the amplitude identically vanishes when \( k' = -k \). Therefore, we should not neglect what we call ladder diagrams shown in Figs. 2(b) and 2(c). Rather,
we collect the infinite series of them and Fig. 2(d) represents the Boltzmann conductivity with vertex corrections defined by eq. (15). The vertex correction is given by

\[ \Xi(\varepsilon_F) = \frac{1}{1 - (W_L/W)(F_2(\varepsilon_F)/F_1(\varepsilon_F))}, \]  

(35)
as a solution of an integral equation described by Fig. 2(e). This multiplicative factor is always positive and larger than unity, which enhances the conductivity as shown in eq. (15).

Finally, the Boltzmann conductivity with the vertex correction taken into account is given by

\[ \sigma_B = \frac{2e^2}{\pi h} \sum_{n | n \leq N_F} \Lambda_n(\varepsilon_F), \]  

(36)\[ \Lambda_n(\varepsilon_F) = \nu_n(\varepsilon_F)\tau_{tr}(\varepsilon_F), \]  

(37)where \( \Lambda_n(\varepsilon_F) \) denotes the mean free path for the band \( n \) and \( \tau_{tr}(\varepsilon_F) \) is the transport relaxation time defined by

\[ \tau_{tr}(\varepsilon_F) = \tau(\varepsilon_F)\Xi(\varepsilon_F). \]  

(38)It is necessary to multiply the conductivity by the factor two when we consider the spin degrees of freedom.

The Boltzmann conductivity derived here via Kubo formula completely agrees with the result derived from the Boltzmann transport equation.\(^{11,26,27}\) Clearly, the conductivity becomes infinite in the single-channel system \((F_1 = F_2 = 1 \text{ for } N_F = 0)\) without short-range potential \((W_S = 0)\) because the vertex correction becomes divergent. The infinite conductivity is a consequence of the absence of backward scattering\(^7\) leading to nonzero Drude weight.\(^{25}\) However, the conductivity has a finite value in the multi-channel case even if there is no short-range impurity. This disagrees with the conductance of finite-length CNs without short-range scatterers which is larger than the conductance quantum corresponding to the presence of a perfect conducting channel.\(^{11}\)

4. Weak-localization correction

Throughout calculations performed in the previous section, an electron is supposed to lose its phase coherence after every scattering event, and this is why the perfect channel has disappeared for the multi-channel case. This is an inevitable consequence due to the breakdown of the destructive interference effects.

In the weak-scattering regime, the first quantum correction is known to be the weak-localization correction, which is calculated by collecting what we call maximally crossed diagrams in terms of perturbative expansion with the impurity-averaged Green’s functions.\(^{28–30}\) In this section, we calculate such a correction to the Boltzmann conductivity for metallic CNs containing short-range impurities as well as long-range ones and try to grasp not only a sign of the perfect channel but also the role of the short-range potential as a perturbation to break the interference effect.

Figure 3(a) shows the diagram giving the quantum correction which is written as

\[ \delta\sigma_{WL} = \frac{e^2}{2\pi A} \sum_{\alpha\beta} \nu_\alpha \Xi^{\alpha\beta}_{\alpha\beta} \Gamma_{\alpha\beta\alpha\beta}^{0} G_{\alpha\beta}^{0} G_{\alpha\beta}^{0} \Xi_{\alpha\beta} \Xi_{\alpha\beta}. \]  

(39)The sum of maximally crossed diagrams up to the infinite order is represented by the vertex function, \( \Gamma_{\alpha\beta\alpha\beta}^{0} \), and the ladder corrections are taken into consideration for both velocity vertex parts.\(^{13}\) In this section, we suppress the expression with regards to the dependence on \( \varepsilon_F \).

In order to obtain the vertex function, we solve the Bethe-Salpeter equation

\[ \Gamma_{\alpha\beta\alpha\beta}^{0} = \Gamma_{\alpha\beta\alpha\beta}^{0} + \sum_{\mu\nu} \Gamma_{\alpha\mu\beta\nu} G_{\mu\nu} G_{\mu\nu} \Gamma_{\mu\nu\beta\nu}, \]  

(40)which is diagrammatically shown in Fig. 3(b). For the system with time-reversal symmetry, the vertex function contains a divergent term originating from the interference between a scattering path and its time-reversed one, giving the correction.

As we take the weak-scattering limit \( W_F(\varepsilon_F) \ll 1 \), the band index \( s \) is assumed to be the same value for any states since we have only to treat the conduction bands for \( \varepsilon_F > 0 \). Further, the momentum conservation gives the following constraints while we solve the equation above,

\[ j = j_\alpha + j_\beta = j_\beta + j_\beta', \]  

(41)\[ n = n_\alpha + n_\alpha' = n_\beta + n_\beta', \]  

(42)\[ q = q_\alpha + q_\alpha' = q_\beta + q_\beta', \]  

(43)and we represent the vertex function as \( \Gamma_{\alpha\beta}(q,j) = \Gamma_{\alpha\alpha'\beta\beta'}^{0} \) with \( q = (2\pi n/L, q) \). Then, it is divided into three sectors with \( j = \pm 2, 0, -2 \) and, from symmetry consideration, the equations for \( j = \pm 2 \) are identical to each other. Only intra-valley scattering takes place in the
sector with \( j = \pm 2 \), while the inter-valley scattering play an essential role in the \( j = 0 \) sector.

The time-reversal symmetry in metallic CNs is never broken either by the short-range potential or by the long-range one and, certainly, the vertex function in the sector with \( j = 0 \) has contributions which become divergent in the limit \( q \to (0, 0) \). Hereafter, we discuss the most strongly divergent contributions with \( n = 0 \) and replace the index \( q \) with \( q \) in the vertex function. The bare vertex in that sector is given by

\[
\Gamma_{\alpha\beta}(q, 0) = \frac{n_s u_{\alpha}^2}{4 L A} \left[ e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_\beta})} + e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_{\beta}})} \right] \delta_{\alpha j_\beta} + \frac{1}{2} \left[ e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_{\beta}})} + e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_{\beta}})} \right] (1 - \delta_{\alpha j_\beta}) + \frac{n_L u_{\gamma}^2}{4 L A} \left[ 1 + e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_{\beta}})} \right] \left[ 1 + e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_{\beta}})} \right] \delta_{\alpha j_\beta},
\]

and we solve the equation for small \( q \) on the condition \( |v_\alpha q \tau| \ll 1 \) to obtain the vertex function

\[
\Gamma_{\alpha\beta}(q, 0) = \frac{W \varepsilon_L \gamma}{2 A} j_{\alpha j_\beta} e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_{\beta}})} \times \left( \frac{1}{D_0 q^2 \tau + \tau/\tau_0} - \frac{1}{D_1 q^2 \tau + \tau/\tau_0 + W_S/W_L} \right),
\]

with

\[
D_0 = \frac{F_2}{F_1} \varepsilon_0^2 \tau_0 \quad \text{and} \quad D_1 = \frac{F_2}{F_1 - F_2} \varepsilon_0^2 \tau_0. \tag{46}
\]

In the denominator of the vertex function, we have introduced the effect of the finite phase-relaxation time \( \tau_0 \) satisfying \( \tau_0 \ll \tau_0. \tag{30} \) The phase-relaxation arises from inelastic scattering caused by interactions with phonons, electrons themselves, etc. Although there have been reported no theoretical calculation, \( \tau_0 \) is expected to decrease with temperature. In fact, in metallic CNs, electron-phonon scattering causes weak resistance in proportion to the temperature.\(^{31}\)

In the sectors with \( j = \pm 2 \), all scattering events in a single path take place within a valley and we can suppress the valley index here. Then, the bare vertex function is given by

\[
\Gamma_{\alpha\beta}(q, \pm 2) = \frac{n_s u_{\alpha}^2}{4 L A} \left[ 1 + e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_\beta})} \right] \delta_{\alpha j_\beta} + \frac{n_L u_{\gamma}^2}{4 L A} \left[ 1 + e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_{\beta}})} \right] \left[ 1 + e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_{\beta}})} \right], \tag{47}
\]

and, on the condition that \( W_S \) is much smaller than \( W_L \), we find the divergent solution

\[
\Gamma_{\alpha\beta}(q, \pm 2) = \frac{W \varepsilon_L \gamma}{A} e^{i(\phi_{\alpha k_{\alpha}} - \phi_{\alpha k_{\beta}})} \times \frac{1}{D_2 q^2 \tau + \tau/\tau_0 + W_S/W_L} \tag{48}
\]

with

\[
D_2 = \frac{W_L F_2}{W_L F_1 - (W_L + W_S/2) F_2} \varepsilon_0^2 \tau. \tag{49}
\]

We need a component with \( \alpha' = \beta \) and \( \beta' = \alpha \) of the vertex function \( \Gamma_{\alpha'\beta';\beta\gamma} \) to calculate the correction and this imposes the conditions, \( j_\beta = j - j_\alpha \) and \( k_\beta = -k_\alpha \). Then, the summation over \( \beta \) is replaced by that over \( q \) and \( j \), and the correction is given by

\[
\delta \sigma_{WL} = -\frac{e^2 \gamma}{2 \pi h A} \sum_{\alpha} \frac{(\tau_{k_{\alpha}})^2}{\tau_0} \left[ (\varepsilon_{\alpha} - \varepsilon_\alpha)^2 + (h/2 \tau)^2 \right]^2 \times \sum_q \left[ \Gamma_{\alpha\beta}(q, 0) + \Gamma_{\alpha\beta}(q, j_\alpha) \right]. \tag{50}
\]

Because we are retaining the leading-order terms with regard to \( W_S/W_L \), we can neglect \( W_S \) in the diffusion constants, \( D_0, D_1, \) and \( D_2 \). They become equal to one another and we represent them by \( D_1 \). In addition, the factor due to the vertex function is also simplified as

\[
\Xi = \frac{F_1}{F_1 - F_2}. \tag{51}
\]

It must be noted that \( \Xi \), as well as \( D_1 \), becomes divergent in the single-channel system.\(^{25}\) Therefore, we have to restrict the following results only to the multi-channel cases.

Collecting all the divergent contributions in the limit of \( q \to 0 \) and \( W_S/W_L \to 0 \), we get

\[
\delta \sigma_{WL} = \frac{e^2 \Xi D_1}{2 \pi h A} \sum_{q} \left[ \frac{3}{D_1 q^2 + \tau_0^2 + \tau_0^2} - \frac{1}{D_1 q^2 + \tau_0^2} \right], \tag{52}
\]

with

\[
\tau_S = \frac{W}{W_S}. \tag{53}
\]

We define the phase-coherence length \( L_\phi \) as

\[
L_\phi = \sqrt{D_1 \tau_0}. \tag{54}
\]

and the elastic scattering length due to the short-range
impurities as

\[ L_S = \sqrt{D_1 \tau_0}. \]  

We consider the nanotubes with length \( A \) much larger than the phase-coherence length and the elastic scattering length due to the short-range impurities, \( A \gg L_0^\phi \) and \( A \gg L_S \). Then, \( q \)-summation in eq. (50) is safely replaced by \( \phi \)-integration and we obtain

\[ \delta \sigma_{\text{WL}} = \frac{e^2}{2\pi \hbar} \Xi \left( 3 \left[ \frac{1}{L_0^\phi} \right] - L_0^\phi \right). \]  

The actual correction needs a factor two for the spin degrees of freedom.

First, we consider the case that scattering due to short-range impurities frequently takes place during the phase-relaxation time, that is to say, \( L_S \ll L_0^\phi \). The quantum correction becomes

\[ \delta \sigma_{\text{WL}} = -\frac{e^2}{2\pi \hbar} \Xi L_0^\phi. \]  

This negative quantum correction showing weak-localization agrees with that for one-dimensional systems with orthogonal symmetry except for the factor of the vertex correction due to the long-range potential.

The condition \( \tau_0 \gg \tau \) leads to \( L_0^\phi \gg v_0 \tau \), while the mean free path for each subband, \( \Lambda_n \), is comparable to \( v_0 \tau \). Consequently, the number of channels should be quite large so that the correction (eq. (57)) can really be a small correction to the Boltzmann conductivity (eq. (36)). Otherwise, the conductivity is strongly reduced by the quantum correction and it might be reasonable to regard a metallic CN as an insulating wire like other one-dimensional systems showing Anderson localization.

However, the situation drastically changes when the majority of impurities are long-ranged so that the short-range impurities hardly induce electron scattering during the phase-relaxation time. In fact, this assumption is expected to be reasonable for CNs without point defects as discussed in §2. Actually, in the opposite limit, \( L_S \gg L_0^\phi \), the correction becomes

\[ \delta \sigma_{\text{WL}} = -\frac{e^2}{\pi \hbar} \Xi L_0^\phi, \]  

where inter-valley scattering is ineffective. Without mixing between two valleys, the system is divided into two independent massless Dirac equations under diagonal disorders. The two-component spinor wavefunction contains the Berry phase shown by \( e^{i\phi_k} \) as a relative phase between two components of the vector wavefunction and the vertex function always has the total phase shift \( e^{i(\phi_k \alpha - \phi_k \beta)} \) which is equal to \(-1\), changing the sign of the correction into positive. This is what we call anti-localization. It is certain that the destructive interference reduces backward scattering although there is no perfectly conducting channel.

From the viewpoint of the universality class, we can think of this Hamiltonian as that of the system under spin-orbit scattering in the limit of the strong spin-orbit coupling, namely, the system of symplectic symmetry in which the spin-rotational symmetry is broken.\(^{12}\) This is consistent with the positive quantum correction to the classical conductivity showing anti-localization. Here, the two component pseudo-spin is composed of the envelope functions at two types of sublattices, and its rotational symmetry is destroyed by scattering due to the short-range impurities.

The short-range potential causes inter-valley mixing and breaks the rotational symmetry of another pseudo-spin related to the valley index. Then, the Hamiltonian belongs to the same universality class as the disordered integer-spin systems,\(^{13}\) that is, the orthogonal class. This is why the quantum correction becomes negative as is the case with the system without any special symmetry except the time-reversal symmetry, showing usual weak-localization property.

In the intermediate region, \( L_S \approx L_0^\phi \), the crossover takes place from anti-localization to localization, or from symplectic to orthogonal class. This behavior is identical to that in the two-dimensional graphite.\(^{13}\)

5. Discussion

We consider the Einstein relation between the conductivity and the diffusion constant,

\[ \sigma = e^2 D \epsilon_F, \]  

with \( D \) the diffusion constant. The density of states is defined by

\[ D(\epsilon_F) = \frac{1}{A} \sum_{\alpha} \delta(\epsilon_F - \epsilon_{\alpha}) = \frac{2}{\pi \gamma} F_1, \]  

where the valley degeneracy is counted but the spin degrees of freedom is not. Considering the diffusion constant \( D_1 \) and the Boltzmann conductivity \( \sigma_B \), we can see that the Einstein relation exactly holds for any parameter values of \( W_S \) and \( W_L \) as is the case with the graphene sheet.\(^{24}\)

The diffusion constant is usually given by

\[ D = \frac{1}{d} \frac{e^2}{\hbar^2} \pi r, \]

where \( d \) is the dimensionality of the space and \( r_F \) is the Fermi velocity. This is different from \( D_1 \) which is used for the Einstein relation, but it seems reasonable that we think of \( F_1/F_2 \) as the effective dimension, \( d_{\text{eff}} \). In fact, in the single-channel case, \( F_1 = F_2 = 1 \), or \( d_{\text{eff}} = 1 \), which corresponds to the fact that the system becomes purely one-dimensional. In the limit \( N_F \to \infty \),

\[ F_1 = N_F \int_{-1}^{1} \frac{dx}{\sqrt{1 - x^2}} = N_F \pi, \]

\[ F_2 = N_F \int_{-1}^{1} dx \sqrt{1 - x^2} = N_F \frac{\pi}{2}, \]

unless \( \epsilon_F \) is located above the subband edge when the perturbative calculations are not justified. Thus, we obtain

\[ d_{\text{eff}} = \lim_{N_F \to \infty} \frac{F_1}{F_2} = 2, \]

and \( D_1 \) is equal to the diffusion constant in the two-dimensional graphene sheet.\(^{24}\)

In the limit \( N_F \to \infty \), the Boltzmann conductivity \( \sigma_B \)
becomes
\[ \sigma_B \to \frac{e^2}{4\pi^2 \hbar W} L, \]  
(65)
showing that \( \sigma_B/L \) approaches that in the graphene sheet.\(^{13,24} \) On the other hand, the quantum correction \( \delta \sigma_{\text{WL}} \) is different from that in the graphene sheet, which depends on \( L_\phi \) logarithmically. The reason lies in the restriction to the term \( n = 0 \) in the summation over \( q \) in the evaluation of the correction. In fact, in the two-dimensional limit, the circumference exceeds the phase-coherence length and therefore nonzero \( n \) satisfying the condition \( D_1 (2\pi \ell/L)^2 \ll 1/\tau_\phi \) should also be included in the summation. If the summation over \( n \) is replaced by the integration in the limit \( L \to \infty \) with \( L_\phi \) fixed, the resulting weak-localization correction agrees with that in the graphene sheet.

Perturbative calculations have revealed that the quantum correction to the Boltzmann conductivity, can be positive for the multi-channel CNs in which the density of the short-range impurities is so small that inter-valley scattering is ineffective. Further, we can say that the short-range potential is a relevant perturbation which can easily reduce the conductivity of metallic CNs. This is consistent with the previous numerical results showing that the perfectly conducting channel in the multi-channel case is fragile in the presence of various perturbations like inelastic scattering,\(^{11} \) magnetic fields,\(^{17} \) short-range impurities,\(^{18} \) and effects of trigonal warping.\(^{19} \)

With no short-range impurities, we have obtained a positive conductivity on the assumption that \( A \gg L_\phi \), and the conductance is given by
\[ G = \frac{(\sigma_B + \delta \sigma_{\text{WL}})}{A} \]
\[ = \frac{e^2}{2\pi^2 \hbar} \left( \frac{F_2}{F_1} \frac{L}{2\pi W} + L_\phi \right) \times \frac{1}{A}. \]  
(66)
This is consistent with the numerical results for finite-length CNs on the same condition in that the conductance contains a term proportional to \( L_\phi/A \).\(^{11} \) Moreover, that term dominates the conductance and, even for the system with finite coherence time, the effect of the quantum interference turned out to be strong enough to invalidate the Boltzmann conductivity which is independent of the phase-coherence length.

It does not seem that preceding discussions about the weak-localization correction unveil the nature of the perfectly conducting channel. Actually, we can also obtain a positive correction for a CN without such a channel. Consider a metallic CN in the magnetic field parallel to the tube axis. What we call the Aharonov-Bohm flux gives a constant shift to the quantized momentum in the circumference direction.\(^{9} \) Generally, the magnetic flux breaks the time-reversal symmetry and the universality class of the CN changes into the unitary. However, when the flux piercing through the nanotube is equal to a half flux quantum, the time-reversal symmetry recovers, and we can realize the CN with symplectic symmetry containing an even number of conducting channels. In this case, there is no perfectly conducting channel and conductance shows exponential decrease in the limit of \( L_\phi \to \infty \) and \( A \to \infty \) where Anderson localization takes place even with no short-range impurity.\(^{33} \)

On the other hand, the weak-localization correction gives no distinction between a CN with no flux and that with a half flux quantum except the shift in the index of quantized momentum in the circumference direction as
\[ n \to n + \frac{1}{2}. \]
(67)
for the summation appearing in \( F_1 \) and \( F_2 \). The positive correction indicates nothing but the fact that the system belongs to the symplectic class. In other words, we need to evaluate higher-order quantum corrections beyond the weak-localization in order to clarify the origin of the perfectly conducting channel within this perturbative scheme.

In contrast, it is possible that the weak-localization correction can well describe the symmetry crossover independent of the number of channels. For the CN with the short-range impurities, a very rough information on the localization length, \( L_{\text{loc}} \), may be obtained from the phase-coherence length at which the sum of the Boltzmann conductivity and the quantum correction vanishes.

In the limit \( L_\phi \gg L_S \) and \( W_S/W \ll 1 \), we have
\[ \sigma_B + \delta \sigma_{\text{WL}} = \frac{e^2}{2\pi \hbar} \left( \frac{F_2}{F_1} \frac{L}{2\pi W} + L_\phi \right), \]  
(68)
and the localization length is estimated to be
\[ L_{\text{loc}} \sim \frac{F_2}{F_1} \frac{1}{\pi W} L + 3L_S. \]  
(69)
For large \( N_F \), this becomes
\[ L_{\text{loc}} \sim \frac{L}{2\pi W} \left( 1 + \frac{3}{2\pi N_F} \frac{W}{W_S} \right), \]  
(70)
and the following condition is necessary to justify this estimation,
\[ \frac{9}{4\pi N_F} \ll \frac{W_S}{W} \ll 1. \]  
(71)
With the circumference length, \( L \), being fixed, the localization length gradually becomes smaller as the number of conducting channels increases and it approaches a constant value in the limit \( N_F \to \infty \). To increase the density of short-range impurities, or \( W_S \), also reduces the localization length. What is more, the dependence on \( N_F \) is more striking when \( W_S \) is smaller. These properties are in agreement with very rough features of the results obtained previously.\(^{18} \) If we look at them more in detail, however, they are different even qualitatively. For example, the localization length obtained numerically decreases in proportion to \( W_S^{-1} \) with the increase of \( W_S \) quite in contrast to \( 1/\sqrt{W_S} \) dependence in eq. (70).

Finally, we discuss the dynamical conductivity. The Boltzmann part is written by\(^{25} \)
\[ \sigma_B(\omega) = \frac{\sigma_B(0)}{1 + \omega^2 \tau_{tr}^2}, \]  
(72)
where \( \sigma_B(0) \) is the static conductivity eq. (36). This represents the Drude conductivity with nonzero width pro-
portion to $1/\tau_{\phi}$. For the quantum correction, we have only to replace $1/\tau_{\phi}$ with $1/\tau_{\phi} + \omega$ and to take its real part as \[ \delta\sigma_{WL} = \frac{\omega^2}{2\pi\hbar} \Re \left[ \frac{D_1}{\omega + \frac{1}{\tau_{\phi}} + \frac{1}{\tau_{\phi}^*}} - \frac{D_1^*}{\omega + \frac{1}{\tau_{\phi}}^*} \right]. \]

for the multi-channel system with $W_L \gg W_S$. In this case, the positive correction can definitely be realized by controlling the frequency, $\omega$, even if $L_0 \gg L_S$. Figure 4 shows some examples of the frequency dependence of the weak localization correction.

In the derivation of the vertex function, we use the condition $\omega \tau \ll 1$, and can neglect the frequency dependence of the Boltzmann conductivity when we discuss the effect of the weak-localization correction in the dynamical conductivity. In the low frequency limit, $\omega \tau_{\phi} \ll 1$, the conductivity remains constant, giving the static value. The frequency displaces the phase relaxation time to control the phase coherence as it becomes larger and overwhelms $\tau_{\phi}^{-1}$. Therefore, we can repeat the same speculation on the sign of the correction. When $\omega \ll \tau_{\phi}^{-1}$, the second term in eq. (73) is dominant and $\delta\sigma_{WL}$ becomes negative, while we can neglect the scattering due to the short-range potential and $\delta\sigma_{WL}$ becomes positive in the limit $\omega \gg \tau_{\phi}^{-1}$. What should be stressed here is that it is possible to observe the crossover from weak localization to anti-localization, that is, the transition from orthogonal to symplectic class in the dynamical conductivity as a sharp dip structure around $\omega = 0$.

6. Summary and Conclusions

We have calculated the weak-localization correction to the Boltzmann conductivity in metallic carbon nanotubes. The correction becomes positive without scattering with short-range potential, which shows anti-localization in the system of symplectic symmetry. This fact is consistent with the presence of a perfectly conducting channel, but may not be regarded as a direct evidence of its presence because the essentially same result is obtained in the case of even channel numbers where no perfect channel is present. Short-range scatterers with potential range smaller than the lattice constant of the two-dimensional graphite constitute a relevant perturbation and make the correction negative no matter how small their density is. This is consistent with the fact that there is no special symmetry except the time-reversal invariance so that the system belongs to the orthogonal class from the viewpoint of the universality.

A finite phase-coherence length due to phase-relaxation time $\tau_{\phi}$ changes the situation. In fact, the anti-localization manifests itself when the phase-coherence length becomes smaller than the diffusion length due to short-range scatterers. The frequency, $\omega$, plays the same role of the decoherence as $\tau_{\phi}$ and, consequently, the crossover from localization to anti-localization takes place not only in the static conductivity but also in the dynamical conductivity.

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