Dynamical Conductivity and Zero-Mode Anomaly in Honeycomb Lattices

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A topological anomaly present at zero energy is shown to give rise to a peculiar and singular behavior of the dynamic and static conductivity in two-dimensional honeycomb lattices. A calculation in a self-consistent Born approximation reveals that this singular dependence prevails although being somewhat smoothed out even if level broadening effects are taken into account.

KEYWORDS: graphite, carbon nanotube, effective-mass theory, Berry’s phase, topological singularity
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1. Introduction

Since the discovery of carbon nanotubes,1) transport properties of the carbon network of the nanometer scale have attracted much attention. There have been a lot of experimental works focusing on the transport measurement in various nanotube structures and theoretical calculation of the conductance of carbon nanotubes.2) A carbon nanotube consists of coaxially rolled two-dimensional graphite sheets characterized by a honeycomb lattice. Therefore, the theoretical investigation on transport properties of honeycomb lattices is instructive for the comprehensive understanding of the transport property of nanotubes. Further, a honeycomb lattice can be realized at semiconductor heterostructures with hexagonal antidot arrays. In a previous work,3,4) the density of states and the static magnetoconductivity were calculated by the quantum transport theory, in which short- and long-range scatterers were taken into account. It was found that the quantum theory provides conductivity exhibiting almost singular behavior in the vicinity of vanishing Fermi energy. In this paper, this behavior is shown to be a manifestation of zero-mode anomalies due to a topological singularity through the study of the dynamical conductivity.

In §2 an effective-mass scheme is reviewed briefly. In §3 the dynamical conductivity is calculated in a simplest relaxation-time approximation and it is shown that its frequency dependence is scaled by the Fermi energy and therefore becomes singular for the vanishing Fermi energy. In §4 effects of level broadening are included in a self-consistent Born approximation. It is shown that singularities prevail even in the presence of level broadening in the case of weak scattering. A summary and conclusions are given in §5.

2. Effective-Mass Description

In a honeycomb lattice such as a two-dimensional graphite, a unit cell contains two atoms denoted as A and B as shown in Fig. 1. Two bands having approximately a linear dispersion cross the Fermi level at K and K' points of the first Brillouin zone, whose wave vectors are given by $K = (2\pi/\alpha)(1/3, 1/\sqrt{3})$ and $K' = (2\pi/\alpha)(2/3, 0)$ with \(\alpha\) being the lattice constant. Under the half-filled condition, electronic properties are governed by states in the vicinity of

![Fig. 1. The structure of a honeycomb lattice and its first Brillouin zone. A unit cell contains two atoms denoted as A and B (small circles). The corner points of the Brillouin zone are denoted as K and K'. A honeycomb lattice can be realized at a semiconductor heterostructure by fabrication of a short-period hexagonal antidot array (shadowed big circles).](image-url)
K and K’ points. The Schrödinger equation for such states is
given by\(^5\)
\[ \mathcal{H}_0 F = \varepsilon F, \]  
(2.1)
with
\[ \mathcal{H}_0 = \begin{pmatrix} 0 & \gamma(k_x - i k_y) & 0 & 0 \\ \gamma(k_x + i k_y) & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma(k_z) \\ 0 & 0 & \gamma(k_z - i k_y) & 0 \end{pmatrix}, \]
(2.2)
where \( \gamma \) is a band parameter, \( \vec{k} = \text{e}^{-i \vec{V}} \) is the wave vector operator, and \( F \) is a four-component wave function.

The eigenfunction of \( \mathcal{H}_0 \) is given by
\[ F\kappa(r) = \frac{1}{\sqrt{2L}} \exp(\imath \vec{k} \cdot \vec{r}) \begin{pmatrix} s \\ 0 \\ 0 \end{pmatrix}, \]
(2.3)
and
\[ F\kappa'(r) = \frac{1}{\sqrt{2L}} \exp(\imath \vec{k} \cdot \vec{r}) \begin{pmatrix} 0 \\ 0 \\ s \end{pmatrix}, \]
(2.4)
where \( L^2 \) is the area of the system, \( \varphi(k) \) is the angle of the wave vector \( \vec{k} \), and \( s \) denotes the bands (\( s = +1 \) for the conduction band and \( s = -1 \) for the valence band). The corresponding energy is given by
\[ \varepsilon_{sk} = s \gamma k, \]
(2.5)
with \( k = |\vec{k}| \).

The first two components of the wave function \( F \) describe the amplitudes at a site A and B associated with the K point, and the next two those associated with the K’ point. The (4, 4) Hamiltonian \( \mathcal{H}_0 \) is completely separable into (2, 2) components for the K and K’ points in the absence of scatterers. The (2, 2) Hamiltonian for the K point is written as \( \gamma (\sigma \cdot \vec{k}) \) in terms of Pauli’s spin matrices \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \).

We consider two different kinds of scatterers. First, the range of the scattering potential is smaller than the lattice constant of the two-dimensional graphite. When such a short-range scatterer is present at an A site \( r_A^s \), the effective Hamiltonian has been calculated as\(^6\)
\[ U_s^A(r) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \gamma(r - r_A^s), \]
(2.6)
with \( \phi_A^s = (K’ - K) \cdot r_A^s \) and \( U_s^A \) being the strength. Similarly, for a scatterer located at a B site \( r_B^s \),
\[ U_s^B(r) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \gamma(r - r_B^s), \]
(2.7)
where \( \phi_B^s = (K’ - K) \cdot r_B^s \).

Next, the range is larger than the lattice constant but much smaller than the typical electron wavelength (which is infinite at \( \varepsilon = 0 \)). In this case matrix elements between K and K’ points can be neglected and the potential is given by a diagonal matrix, i.e.,
\[ U_s(r) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \gamma(r - r_i), \]
(2.8)
where \( r_i \) is the impurity position. This type of scatterers is called long-range, although the potential is given by a \( \delta \) function.

3. Dynamical Conductivity

The current operator is given by
\[ j = -e \gamma \sigma, \]
(3.1)
for the K point. The corresponding matrix elements are calculated as
\[ \langle s \vec{k}|j_i|s’ k’\rangle = -\frac{e \gamma}{\hbar} \frac{1}{2} (\varphi e^{\imath \vec{k} \cdot \vec{r}} + \varphi e^{-\imath \vec{k} \cdot \vec{r}}), \]
(3.2)
for the K point. The dynamical conductivity is isotropic and given by
\[ \sigma(\omega) = \frac{1}{L^2} \frac{e^2}{\hbar} \frac{m^*}{\pi} \frac{f(\varepsilon_{k}) - f(\varepsilon_{k + \hbar \omega + i \delta})}{\hbar (\omega + i \delta)} \]
(3.3)

The relaxation time in the absence of a magnetic field is defined as
\[ \tau_0 = \frac{2 \pi}{\varepsilon_F} \sum_{s} |\langle j \vec{s}|U|j’ \vec{s}' \rangle|^2 \delta(\varepsilon_{s k} - \varepsilon_{s k’}), \]
(3.5)
where \( U \) is the effective Hamiltonian for scatterers. In the case of short-range scatterers it is given by
\[ \frac{1}{\tau_0} = \frac{1}{2} \left[ n_s^0 \langle \varphi_s^0 \rangle^2 + n_s^1 \langle \varphi_s^1 \rangle^2 \right] |\varepsilon| \frac{1}{\hbar \gamma^2}, \]
(3.6)
where \( n_s^0 \) and \( n_s^1 \) are the concentration of scatterers in a unit area and \( \langle \ldots \rangle \) means the average. The relaxation time for long-range scatterers is given by
\[ \frac{1}{\tau_0} = n_l \langle \varphi_l \rangle \frac{|\varepsilon|}{2 \hbar \gamma^2}, \]
(3.7)
When we assume $\nu^2 = \langle \nu^2 \rangle = \langle \nu' \rangle^2 = \langle \nu'' \rangle^2$ and $n_i = n_i^0 + n_i^R$ and $n_i^0 = n_i^R$, the relaxation time becomes same between short- and long-range cases and

$$\frac{1}{\tau_0} = \frac{2\pi |e|}{\hbar A},$$

(3.8)

where we have introduced a dimensionless parameter to characterize the scattering strength given by

$$A = \frac{4\pi \nu^2}{n_i \mu}.$$  

(3.9)

With the use of the Boltzmann transport equation, the transport relaxation time is given by

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} \sum_{j<k} \sum_{j'k'} |\langle j | U | j' k' \rangle|^2 (1 - \cos \theta) \delta (\varepsilon_{j'k} - \varepsilon_{j'k'}).$$

(3.10)

where $\cos \theta = k \cdot k' / k^2$. We have

$$\tau(\varepsilon) = \tau_0(\varepsilon) \alpha^{-1},$$

(3.11)

with $\alpha = 1$ in the case of short-range scatterers and $\alpha = 1/2$ in the case of long-range scatterers.

In order to include effects of level broadening due to scatterers, we shall replace $\delta$ by $\hbar / \tau$, where $\tau$ is a relaxation time. Because of the energy dependence of the relaxation time, we shall assume $\tau(\varepsilon)$ with $\varepsilon = \varepsilon F$ in the first term in the right hand side of eq. (3.4) and $\varepsilon = h\omega / 2$ in the second term, corresponding to the energy of the states giving a major contribution to the transition. Then, the dynamical conductivity is calculated as

$$\sigma(\omega) \equiv \frac{e^2}{\hbar} \left[ \frac{4}{\pi} \hbar \omega_0 + i \hbar |\omega| / \tau(\omega) \right] + 1 + i \hbar \omega_0 - i \hbar |\omega| / \tau(\omega) + 2 e F,$$

(3.12)

Because $\hbar / \tau(\omega) \propto |\omega|$, the frequency dependence of the dynamical conductivity is scaled by $\omega_0 / e F$. Figure 2 shows $\sigma(\omega)$ as a function of $\omega_0 / e F$ for several values of $A$.

The scaling of the dynamical conductivity $\sigma(\omega_0 / e F)$ shows that $\sigma(\omega)$ exhibits a singular behavior at the point $(\omega, \omega_0) = (0, 0)$. In fact, when we set $\omega = 0$ first, the static conductivity is given by

$$\sigma(0) = \sigma_0 = \frac{e^2}{\hbar} \frac{A}{\pi^2 h 4e^2},$$

(3.13)

independent of the Fermi energy $e F$ in agreement with the Boltzmann result. When we set $\omega_0 = 0$ first with nonzero $\omega$, on the other hand, the static conductivity at $\omega \to 0$ becomes $e^2 / 8h \omega$ which is much smaller than $\sigma_0$ in the Boltzmann limit $A \gg 1$. The correct way is to let $\omega \to 0$ at each $\varepsilon F$, leading to a singular jump of the static conductivity at $\varepsilon F = 0$. The calculation in a self-consistent Born approximation shows that this anomaly manifests itself as a near singular dependence of $\sigma$ on $\varepsilon F$ even if level broadening effects are included and that the conductivity at $\varepsilon F = 0$ is given by a universal conductivity quantum $e^2 / \pi^2 h$ as will be discussed in the following.

4. Self-Consistent Born Approximation

4.1 Green’s function

In the following we shall use Green’s function technique to evaluate the dynamical conductivity. This technique allows us to consider broadening effects self-consistently and is widely used. The Green’s function (resolvent) is defined by

$$G(\varepsilon) = \frac{1}{\varepsilon - H}.$$  

(4.1)

The matrix elements of unperturbed Green’s function are diagonal:

$$G^{(0)}_{\mu\nu}(\varepsilon) = \left( \frac{1}{\varepsilon - H_0} \right)_{\mu\nu} = \delta_{\mu\nu} G^{(0)}_{\mu}(\varepsilon),$$

(4.2)

where $\mu = (j, s, k)$ with $j = K$ or $K'$ and $s = \pm 1$. For evaluating physical quantities, we need $(G_{\mu\nu}(\varepsilon))$, which is the average of the matrix element of $G(\varepsilon)$ over all possible configuration of random distributions of impurities. The averaged Green’s function is connected to the proper self-energy $\Sigma_{\mu\nu}(\varepsilon)$ by Dyson’s equation:

$$(G_{\mu\nu}(\varepsilon)) = \delta_{\mu\nu} G^{(0)}_{\mu}(\varepsilon) + G^{(0)}_{\mu}(\varepsilon) \sum_{\nu'} \Sigma_{\mu\nu'}(\varepsilon) (G_{\nu\nu'}(\varepsilon)).$$

(4.3)

Figure 3 shows a diagramatic representation of the self-consistent Born approximation. The self-energy is given by

$$\Sigma_{\mu\nu}(\varepsilon) = \sum_{\mu' \mu''} (U_{\mu\mu', \mu''}) (G_{\mu\mu'}(\varepsilon)), $$

(4.4)

where terms lowest-order in $U$ are neglected because they can be absorbed into a shift in the energy origin. For the choice of the scattering parameters discussed in the previous section, the self-energy and Green’s function become independent of short- and long-range scatterers. We have

$$\Sigma_{\mu\nu}(\varepsilon) = \delta_{\mu\nu} \Sigma(\varepsilon),$$

(4.5)

$$\langle G_{\mu\nu}(\varepsilon) \rangle = \delta_{\mu\nu} G_{\mu}(\varepsilon),$$

with

$$G_{\mu}(\varepsilon) = \frac{1}{\varepsilon - \Sigma(\varepsilon)}.$$
Then, the self-consistency equation is rewritten as
\[ \sigma_{xx}(\omega) = \frac{1}{\pi \varepsilon_0} \int \frac{d\varepsilon}{\varepsilon - \varepsilon_i - \Sigma(\varepsilon)} \]
and
\[ G_\mu(\varepsilon) = \frac{1}{\varepsilon - \varepsilon_\mu - \Sigma(\varepsilon)} \]
Explicitly, we have
\[ \Sigma(\varepsilon) = \frac{n_i u^2}{4\pi} \int_0^\infty \frac{k dk}{\varepsilon - \Sigma(\varepsilon)} - \gamma^2 k^2 \]
where \( k_c \) is a cutoff wave number. Define
\[ X(\varepsilon) = \varepsilon - \Sigma(\varepsilon) \]
Then, the self-consistency equation is rewritten as
\[ \varepsilon = X(\varepsilon) + \frac{X(\varepsilon)}{A} \left( \ln X(\varepsilon)^2 - \ln[X(\varepsilon)^2 - \varepsilon_c^2] \right) \]
where
\[ \varepsilon_c = \gamma k_c \]
The cutoff \( k_c \) is given by \( k_c \approx 2\pi/a \) where \( a \) is the lattice constant and the corresponding \( \varepsilon_c \) is of the order of the band width.\(^9,10\)
The Boltzmann result for scattering rate can be obtained by taking the limit \( X(\varepsilon) = X_0(\varepsilon) = \varepsilon + i0 \) in the second term of the right hand side of eq. (4.10) as
\[ X''(\varepsilon + i0) \equiv X_0''(\varepsilon + i0) = \frac{\pi}{A} |\varepsilon| = \frac{\hbar}{2\varepsilon_0(\varepsilon)} \]
with \( X'(\varepsilon + i0) = \text{Re} X(\varepsilon + i0) \) and \( X''(\varepsilon + i0) = \text{Im} X(\varepsilon + i0) \). This lowest order result is valid in the case of weak scattering \( A \gg 1 \) and \( \varepsilon \neq 0 \).
The density of states is given by
\[ D(\varepsilon) = -\frac{1}{\pi L^2} \sum_\mu \text{Im}(G_{\mu\mu}(\varepsilon + i0)) = \frac{4}{\pi n_i u^2} \frac{\text{Im} X(\varepsilon + i0)}{X''(\varepsilon + i0)} \]
which gives that in the absence of impurities upon substitution of \( X_0(\varepsilon + i0) = X_0''(\varepsilon + i0) + iX_0'(\varepsilon + i0) \),
\[ D_0(\varepsilon) = \frac{|\varepsilon|}{\pi \gamma^2} \]
\[ (4.14) \]
\[ 4.2 \text{ Dynamical conductivity} \]
The conductivity is written as
\[ \sigma_{xx}(\omega) = -\frac{2\hbar}{4\pi L^2} \int d\varepsilon \frac{f(\varepsilon) - f(\varepsilon + \hbar \omega)}{\hbar \omega} \sum_\pm \sum_\pm \sum_{srk}(\varepsilon + \hbar \omega \pm i0)G_{srk}(\varepsilon \pm i0) \]
\[ \times J_{srk}(\varepsilon + \hbar \omega \pm i0, \varepsilon \pm i0) \]
(4.15)
where \( J_{srk}(\varepsilon + \hbar \omega \pm i0, \varepsilon \pm i0) \) is the current vertex part as shown in Fig. 3 and the factor two is due to the presence of the \( K \) and \( K' \) points. In the case of short-range scatterers, vertex corrections vanish identically and we have
\[ J_{srk} = (sk|j_s|k) \]
In the case of long-range scatterers, we have
\[ J_{srk}(\varepsilon, \varepsilon') = (sk|j_s|k) \left[ 1 - A^{-1} \phi(\varepsilon, \varepsilon') \right]^{-1} \]
(4.17)
with
\[ \phi(\varepsilon, \varepsilon') = \frac{\pi \gamma^2}{L^2} \sum_{srk} G_{sr}(\varepsilon)G_{srk}(\varepsilon') \]
(4.18)
Explicitly, we have
\[ \phi(\varepsilon, \varepsilon') = \frac{X(\varepsilon)X(\varepsilon')}{X(\varepsilon)^2 - X(\varepsilon')^2} \left( \ln X(\varepsilon)^2 - \ln X(\varepsilon')^2 \right) \]
\[ - \frac{\ln[X(\varepsilon')^2 - \varepsilon_c^2] + \ln[X(\varepsilon')^2 - \varepsilon_c^2]} \]
(4.19)
When \( \varepsilon' = \varepsilon \) we have
\[ \phi(\varepsilon + i0, \varepsilon + i0) = -1 \]
\[ \phi(\varepsilon + i0, \varepsilon - i0) = S(\varepsilon) \]
(4.20)
with
\[ S(\varepsilon) = \frac{|X(\varepsilon + i0)|^2}{X'(\varepsilon + i0)X''(\varepsilon + i0)} \tan^{-1} \frac{X'(\varepsilon + i0)}{X''(\varepsilon + i0)} \]
(4.21)
Therefore, the dynamical conductivity is given by
\[ \sigma(\omega) = -\frac{\varepsilon^2}{4\pi^2 \hbar} \int d\varepsilon \frac{f(\varepsilon) - f(\varepsilon + \hbar \omega)}{\hbar \omega} \sum_\pm \sum_\pm \sum_{srk} \phi(\varepsilon + \hbar \omega \pm i0, \varepsilon \pm i0)G(\varepsilon + \hbar \omega \pm i0, \varepsilon \pm i0) \]
(4.22)
with
\[ G(\varepsilon + \hbar \omega \pm i0, \varepsilon \pm i0) = \left[ 1 - A^{-1} \phi(\varepsilon + \hbar \omega \pm i0, \varepsilon \pm i0) \right]^{-1} \]
(4.23)
for short-range scatterers and
\[ G(\varepsilon + \hbar \omega \pm i0, \varepsilon \pm i0) = \left[ 1 - A^{-1} \phi(\varepsilon + \hbar \omega \pm i0, \varepsilon \pm i0) \right]^{-1} \]
(4.24)
for long-range scatterers.
The above results give the static conductivity calculated previously\(^3\) in the limit \( \omega \to 0 \). In fact, in the case of short-range scatterers, the static conductivity becomes
\[ \sigma = \frac{1}{2} \frac{e^2}{\pi \hbar} \left[ S(\varepsilon_F) + 1 \right] \]
(4.25)
at zero temperature. In the Boltzmann limit \( A \gg 1 \), we have
\[ |\epsilon| X'(\epsilon + i0) \gg 1 \] and therefore \( \sigma = \sigma_0 \) given by eq. (3.13) with \( \alpha = 1 \). In the particular case \( \epsilon = 0 \), the real part of the self-energy vanishes at \( \epsilon = 0 \) because of the symmetry between \( \epsilon > 0 \) and \( \epsilon < 0 \) and eq. (4.10) gives immediately \( X(t+i0) = i\epsilon \exp(-A/2) \). The conductivity at \( \epsilon_F = 0 \) is also calculated analytically and becomes
\[
\sigma = \frac{e^2}{\pi^2 \hbar}.
\] (4.26)

This conductivity is given only by natural constants and independent of the scattering strength and the band parameter. Further, it is much smaller than the Boltzmann conductivity \( \sigma_0 \) in the case of weak scattering \( A \gg 1 \).

In the case of long-range scatterers, on the other hand, we have
\[
\sigma = \frac{e^2}{\pi^2 \hbar} \frac{S(\epsilon_F) + 1}{1 + A^{-1}[1 - A^{-1}S(\epsilon_F)]}.
\] (4.27)

In the Boltzmann limit, we have \( S(\epsilon_F) = A/2 \) and \( \sigma = \sigma_0 \) with \( \alpha = 1/2 \). Further, at \( \epsilon_F = 0 \), we have \( S(\epsilon_F) = 1 \) and therefore
\[
\sigma = \frac{e^2}{\pi^2 \hbar} \frac{1}{1 - A^{-1}} \approx \frac{e^2}{\pi^2 \hbar}.
\] (4.28)

This value is slightly larger than \( e^2/\pi^2 \hbar \) and dependent on the scattering parameter. This dependence is extremely small in the case of weak scattering \( A \gg 1 \).

5. Numerical Results

The important energy scale in the present problem is the cutoff energy \( \epsilon_c \) which is of the order of the band width. However, in this paper, following ref. 3, we shall introduce an arbitrary energy scale \( \epsilon_0 \) which is assumed to have the same order of magnitude as other relevant energies such as \( \epsilon \) and \( X(\epsilon + i0) \) and choose the cutoff energy as \( \epsilon_c/\epsilon_0 = 50 \).

Figure 4 shows some examples of calculated \( \sigma(\omega) \) for different values of \( \epsilon_F \) and for \( A = 50 \) and 20 in the case of short-range scatterers. The frequency dependence is scaled by \( \hbar \omega/\epsilon_F \) as long as \( \epsilon_F \neq 0 \) for weaker scattering \( A = 50 \). When \( \epsilon_F \) is very close to 0, however, the conductivity at \( \omega = 0 \) becomes small and the discrete jump present in the Boltzmann conductivity is removed as is more clear in the case of stronger scattering \( A = 20 \). The energy scale causing this crossover behavior becomes smaller with \( A \) leading to a singular behavior of the dynamical conductivity in the weak scattering limit.

Figure 5 shows some examples in the case of long-range scatterers. The behavior is essentially same as in the case of short-range scatterers except that effects of scattering are reduced. This reduction corresponds to the increase of the transport relaxation time due to the absence of backward scattering.3,6,11)

6. Discussion

The anomalous behaviors of the static and dynamic conductivities at \( \epsilon_F = 0 \) are closely related to the zero-mode anomaly due to a topological singularity at \( k = 0 \) present in Weyl’s equation describing the electronic states near the K and K’ points. In fact, when \( k \) is rotated once in the anticlockwise direction adiabatically as a function of time \( t \) for a time interval \( 0 < t < T \) with \( k(T) = k(0) \), the wavefunction \( F_{sk} \) is changed into \( F_{sk} \exp(-i\varphi) \), where \( \varphi \) is Berry’s phase given by11,12)
\[
\varphi = -i \int_0^T dt \left( \frac{d}{dt} \right) F_k(t) = -\pi. \tag{6.1}
\]

It should be noted that \( \varphi = -\pi \) when the closed contour encircles the origin \( k = 0 \) but \( \varphi = 0 \) when the contour does not contain \( k = 0 \). Further, the wavefunction at \( k = 0 \) depends on the direction of \( k \) and is undefined at \( k = 0 \). These facts show the presence of a topological singularity at \( k = 0 \).

This nontrivial Berry’s phase leads to the unique property of a metallic carbon nanotube that there exists no backward scattering and the tube is a perfect conductor even in the
The presence of scatterers as long as their potential range is larger than the lattice constant.\textsuperscript{6,11) This Berry’s phase is closely related to the helicity of a neutrino and the signature change of a wave function under a spin rotation. In fact, the Schrödinger equation near the $K$ point is written as
\begin{equation}
\gamma(\sigma \cdot \hat{k}) \mathbf{P}_k = \varepsilon \mathbf{P}_k,
\end{equation}
using the spin matrix $\sigma$. This shows clearly that the spin is quantized into the direction of $\hat{k}$ and the wave function is given by a spinor with its spin in the $\hat{k}$ direction. The spin function changes its signature when the spin is rotated by $2\pi$.

This well-known signature change under the spin rotation corresponds to the above Berry’s phase.

A singularity at $\varepsilon = 0$ manifests itself in magnetic fields even in classical mechanics. The equation of motion is given by
\begin{equation}
\frac{dk}{dt} = -\frac{e}{c} \mathbf{v} \times \mathbf{B},
\end{equation}
This gives the cyclotron frequency $\omega_c = eBv^2/\hbar$, where $v$ is the electron velocity given by $v = |v| = \gamma/\hbar$. The cyclotron frequency $\omega_c$ diverges and changes its signature at $\varepsilon = 0$.\textsuperscript{4)}

In quantum mechanics $\hat{k}_x$ and $\hat{k}_y$ satisfy the commutation relation $[\hat{k}_x, \hat{k}_y] = -i/\hbar$, where $l$ is the magnetic length given by $l = \sqrt{\hbar/eB}$. Semiclassically, the Landau levels can be obtained by the condition
\begin{equation}
f k_x dk_y = \frac{2\pi}{l^2} (n + \delta),
\end{equation}
with integer $n$ and an appropriate small correction $\delta$. This gives $\varepsilon_n = \pm \sqrt{n + \delta (2\gamma/l)}$. Because of the uncertainty relation $\Delta k_x \Delta k_y \sim l^{-2}$, $k^2 = 0$ is not allowed and there is no Landau level at $\varepsilon = 0$. However, a full quantum mechanical treatment of a magnetic field leads immediately to the formation of Landau levels at $\varepsilon_n = \text{sgn}(n)(\sqrt{2}\gamma/l)^{1/2}$ with $n = 0, \pm 1, \pm 2, …$. A peculiar and intriguing feature is the presence of a Landau level at $\varepsilon = 0$. This is presumably related also to the anomaly present at $\varepsilon = 0$.

In the Boltzmann transport theory the conductivity tensor $\sigma_{\mu\nu}$ with $\mu = x, y$ and $\nu = x, y$ is given by
\begin{eqnarray}
\sigma_{xx} &=& \sigma_{yy} = \frac{\sigma_0}{1 + (\omega_c \tau)^2}, \\
\sigma_{xy} &=& -\sigma_{yx} = -\frac{\sigma_0 \alpha \gamma}{1 + (\alpha \tau)^2},
\end{eqnarray}
where $\sigma_0$ is defined in eq. (3.13). Using the explicit expressions for $\omega_c$ and $\tau$, we have
\begin{eqnarray}
\sigma_{xx} &=& \sigma_0 \frac{\xi^4}{1 + \xi^4}, \\
\sigma_{xy} &=& -\sigma_0 \frac{\xi^2}{1 + \xi^4},
\end{eqnarray}
with
\begin{equation}
\xi = \sqrt{\frac{2\pi \alpha \varepsilon_F}{A \varepsilon_B}}.
\end{equation}
where $\varepsilon_B$ is the magnetic energy defined by $\varepsilon_B = \gamma/l$. Because the dependence on the Fermi energy is fully scaled by $\varepsilon_B$, the conductivities exhibit a singular behavior at $\varepsilon_F = 0$ in the limit of the vanishing magnetic field $\varepsilon_B \to 0$.

This singularity at $\varepsilon_F = 0$ disappears in the quantum theory based on the self-consistent Born approximation. Figure 6 compares classical and quantum $\sigma_{xx}$ and $\sigma_{xy}$ as a function of $\xi$ for $A = 50$ in the case of short-range scatterers and Fig. 7 shows corresponding comparison in the case of long-range scatterers. In contrast to the Boltzmann result the quantum results depend on $\varepsilon_B/\varepsilon_0$ and $\sigma_{xx}$ depends on the Fermi energy in the limit $\varepsilon_B/\varepsilon_0 \to 0$, in consistent with previous results.\textsuperscript{3,4)
7. Summary

In summary, we have discussed anomalies appearing in the static and dynamic conductivity associated with the topological singularity at $k = 0$. In the Boltzmann transport theory, the frequency dependence of the dynamical conductivity is determined by $\hbar\omega/\epsilon_F$ leading to a singular jump at $\omega = 0$ and $\epsilon_F = 0$. Therefore, the static conductivity has a singularity at $(\omega, \epsilon_F) = (0, 0)$ and depends critically on which of $\omega$ and $\epsilon_F$ is set equal to zero first. In a self-consistent Born approximation in which level broadening effects are properly taken into account, this singular dependence is somewhat smoothed out but the corresponding energy scale is determined by the broadening at $\epsilon_F \approx 0$ and is extremely small in the case of weak scattering.

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1) S. Iijima: Nature (London) 354 (1991) 56.
2) See, for example, T. Ando: Semicond. Sci. Technol. 15 (2000) R13 and references cited therein.
3) N. H. Shon and T. Ando: J. Phys. Soc. Jpn. 67 (1998) 2421.
4) Y. Zheng and T. Ando: submitted to Phys. Rev. B.
5) J. C. Slonczewski and P. R. Weiss: Phys. Rev. 109 (1958) 272.
6) T. Ando and T. Nakanishi: J. Phys. Soc. Jpn. 67 (1998) 1704.
7) T. Ando and Y. Uemura: J. Phys. Soc. Jpn. 36 (1974) 959.
8) T. Ando: J. Phys. Soc. Jpn. 36 (1974) 1521; ibid. 37 (1974) 622; ibid. 37 (1974) 1233.
9) T. Ando, T. Nakanishi and M. Igami: J. Phys. Soc. Jpn. 68 (1999) 3994.
10) H. Matsumura and T. Ando: J. Phys. Soc. Jpn. 70 (2001) 2657.
11) T. Ando, T. Nakanishi and R. Saito: J. Phys. Soc. Jpn. 67 (1998) 2857.
12) M. V. Berry: Proc. R. Soc. London A 392 (1984) 45.