Conductance through the disclination dipole defect in metallic carbon nanotubes

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Abstract. The electronic transport properties of a metallic carbon nanotube with the five-seven disclination pair characterized by a lattice distortion vector are investigated. The influence of the disclination dipole includes induced curvature and mixing of two sublattices. Both these factors are taken into account via a self-consistent perturbation approach. The conductance and the Fano factor are calculated within the transfer-matrix technique.

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1. Introduction
Transport properties of variously shaped carbon nanostructures and graphene are of great practical and theoretical interest. In particular, the conductivity of carbon nanotubes is currently the subject of wide investigations. It is known that disclination topological defects (fivefolds) can convert planar graphene surface into the conical one with a marked modification of the electronic states \cite{1}. In the nanotubes, however, the presence of an isolated pentagonal ring is not allowed and the simplest topological defect is the 5-7 disclination dipole (DD). The simple model for the junction between two metallic tubes was investigated in \cite{2}.

In this paper, we study the electronic transport properties of a metallic nanotube containing closely spaced 5-7 disclination dipole (i.e., the junction composed of two semi-infinite metallic nanotubes).

2. Geometry
A metallic or semiconducting character of the tube is governed by the translational vector $\mathbf{T}_0(n,m)$, where $(n,m)$ are the numbers of steps along two unit cell vectors in the honeycomb lattice. The boundary conditions for the tube with a translational vector $\mathbf{T}$ transforms to the angular vector field $a_\varphi$ which dependis on chirality as $(n+m) \mod 3$. This field, along with the angular momentum, subsequently generates the mass-type term in the effective Dirac equation (see \cite{3} for detail).

As for the fivefold-sevenfold pair in the nanotube, it appears to be the source of translational-type holonomy \cite{4}, therefore it should produce additional gauge vortex field. However, in this paper we restrict our consideration to a special case when the condition $(n+m) \mod 3 = 0$ is fulfilled at both sides. Additionally, at low energies below the first gap value ($|E| \ll hV_F/R_0$, where $V_F$ is the Fermi velocity and $R$ is the tube radius) one can take into account for the
estimation of first-order perturbation only the main conducting channel corresponding to the lowest angular momentum.

As is known, the dislocation-type defect touches both the chirality and the radius of the carbon nanotube. In the general case, the tube with DD can be characterized by the distortion vector \( \vec{b} \): for the translational vector \( \vec{T} \) one can find, that it has the value \( \vec{T}_0 \), \( T_0 = 2\pi R_0 \) on the one side and \( \vec{T}_0 + \vec{b} \) on the other. Trying to describe a shape of the nanotube, it is useful to perform a development of the junction region onto a 2D plane.

Let us associate the development with the xy-plane and choose the axis along the tube on the left side as the x-axis. In this case, one has \( \vec{T}_0(0, T_0, 0) \) and \( \vec{T}(\xi) = \vec{T}(T_x, T_y, 0) \). It is convenient to introduce the new frame with the vector \( \vec{n} = (\vec{T} \times \vec{e}_z)/T \) (\( \vec{e}_i (i = x, y, z) \) are the orthogonal basis vectors) which follows the tube axis (see Fig. 1).

The orthogonal to \( \vec{n} \) vectors are \( \vec{\tau}_1 = -\vec{e}_z \) and \( \vec{\tau}_2 = \vec{\tau}_1 \times \vec{n} = \vec{T} / T \). To take into account the disclination dipole, which is situated at the top of the cylinder, one needs to describe the skewed conical surface between \( Q \) and \( P \) points. Actually, the DD has two effects: it changes the radius and shifts the surface of the tube in the direction normal to the tube axis. Since the radius \( R(\xi) = T(\xi)/(2\pi) \) changes its value on \( \Delta R \), the ring will be shifted in the direction of \( \vec{\tau}_2 \) by \( \Delta R \), so that we must add the shift \( \vec{\tau}_2 T /(2\pi) \).

Finally, the surface is parametrized as following:

\[
\vec{r} = \vec{n} \xi + \vec{\tau}_2 \frac{T}{2\pi} + \vec{\tau}_1 \frac{T}{2\pi} \cos \varphi + \vec{\tau}_2 \frac{T}{2\pi} \sin \varphi, \tag{1}
\]

where \( -\infty < \xi < \infty \) and \( 0 \leq \varphi < 2\pi \) are the normal and the transversal coordinates, respectively.

The form of the tube with 5-7 rings is supposed to be

\[
\vec{r}(\xi) = \vec{T}(\xi) + \frac{\vec{b}}{2} \left( \tanh \frac{\xi}{\xi_0} + 1 \right) \tag{2}
\]

where we assume

\[
\vec{T}(\xi) = \vec{T}_0 + \frac{\vec{b}}{2} \left( \tanh \frac{\xi}{\xi_0} + 1 \right) \tag{3}
\]

to be the tube translation vector, depending on the coordinate \( \xi \), the distortion vector \( \vec{b} \) and an effective parameter \( \xi_0 \), which corresponds to the half-width of the surface region curved by the DD.

Figure 1. A schematic picture of the nanotube surface. The fivefold is located at the point Q, and the sevenfold - at the point P. The thick tube axis BB’ coincides with the x-axis. The thin tube axis CC’ is shifted due to the disclination dipole QP.
3. Conductance

From (2, 3) one can find metrical tensor, metrics connection coefficients $\Gamma^{\nu}_{\mu\lambda}$, tetradic coefficients $e^i_j$, which are determined as $g_{\mu\nu} = e^i_\mu e^j_\nu \delta_{ik}$, and the spin connection coefficients which are determined as $(\omega^a)_{\mu\nu} = e^a_\mu \Omega^b_{\mu\nu}$, where $\Omega_{\mu\nu} := \partial_{\mu} + \Gamma_{\mu\nu}$. From now on we set $E_F = 0$, $V_F = h = 1$. The effective Dirac equation on the curved surface is defined as

$$-i\sigma_j e^j_\mu (\nabla_\mu - iA_\mu)\psi = E\psi,$$

with $\sigma_i$ being the Pauli matrices ($i = 1, 2$), $\psi$ is a 2-component spinor wavefunction, and $A_\mu (\mu = \xi, \varphi)$ being the DD field. The derivative includes a spin connection term $\Omega_\mu$ and it is written as $\nabla_\mu = \partial_\mu + \Omega_\mu$, $\Omega_\mu = \frac{1}{2} \omega^{ab}_\mu [\sigma_a, \sigma_b]$. In the linear in $\tilde{b}$ approximation and for the momentum equal to zero, the unperturbed Dirac operator has the form $-i\sigma_1 \partial_\xi$, and the perturbation has the form

$$\hat{\nu} = i\sigma_1 \frac{(\tilde{b} \times \tilde{T}_0)_z}{8\pi^2 R_0 \xi_0 \cosh^2(\xi/\xi_0)} \partial_\xi - \sigma_1 < A_\xi >_\varphi - \sigma_1 \frac{\tilde{b} \cdot \tilde{T}_0}{16\pi^2 R_0^2 \xi_0 \cosh^2(\xi/\xi_0)} - \frac{\sigma_2}{R_0} < A_\varphi >_\varphi. \quad (5)$$

Here $< >_\varphi$ denotes the averaging over $\varphi$ and $(\tilde{b} \times \tilde{T}_0)_z = b_z T_{0y} - T_{0x} b_y$. Now the perturbation (5) is localized near $\xi = 0$ with a half-width $\xi_0$. In order to remove the differentiation in (5) one can multiply the operator $\hat{D}_0 + \hat{\nu}$ by $\left(1 + \frac{(\tilde{b} \times \tilde{T}_0)_z}{8\pi^2 R_0^2 \xi_0 \cosh^2(\xi/\xi_0)}\right)$. In this case, the additional potential $ IE(\tilde{b} \times \tilde{T}_0)_z/(8\pi^2 R_0^2 \xi_0 \cosh^2(\xi/\xi_0))$ appears, where $I$ is a unit matrix.

The field $\tilde{A}$ describes the DD-induced valley mixing. It may be written as $A_j = \mu \epsilon_{jk} \partial_k G$ where $j, k = \xi, \varphi$, $\mu$ is an effective ”charge” of each disclination, $G$ is a dipole potential, which satisfies the equation

$$\nabla^2 G(\xi, \varphi) = \frac{2\pi}{R} [d_\xi \delta'(\xi) \delta(\varphi) + d_\varphi \delta(\xi) \delta'(\varphi) / R_0], \quad (6)$$

$\nabla^2 = \partial^2_\xi + \partial^2_\varphi / R_0^2$, $\epsilon_{jk}$ is a unit antisymmetric tensor, $\delta(x)$ and $\delta'(x)$ are the Dirac delta function and its derivative, and $\tilde{T}$ is a vector connecting five- and sevenfold (it has the same order as $\tilde{b}$ [5]). One can find $G$ with the Fourier expansion $G = \sum_n e^{in\varphi} G_n(\xi)$. For the zero momentum $n = 0$, the field $\tilde{A}$ has the form

$$A_\xi = 0, A_\varphi = \frac{4\pi^2 \mu b_\xi}{R_0} \delta(\xi), \quad (7)$$

where $\delta(\xi)$ is a Dirac delta function. Finally, the perturbation operator looks as follows:

$$\hat{\nu} = -I \frac{(\tilde{b} \times \tilde{T}_0)_z E}{8\pi^2 R_0 \xi_0 \cosh^2(\xi/\xi_0)} - \sigma_1 \frac{\tilde{b} \cdot \tilde{T}_0}{16\pi^2 R_0^2 \xi_0 \cosh^2(\xi/\xi_0)} - \frac{\sigma_2}{R_0^2} \delta(\xi). \quad (8)$$

Notice that the last term in (8) corresponds to the $\xi$-dependent mass term $\sigma_2 m_\xi(\xi)$ in the Dirac equation. Let us calculate the transfer matrix and the conductance according to the method described in [6] and [7]. To transform the initial Dirac equation to the diagonal form, the unitary rotation is performed: $\psi \rightarrow L \psi$, $\tilde{\nu} \rightarrow \tilde{L} \tilde{L} \tilde{\nu} L^\dagger$, $\sigma_1 \rightarrow L \sigma_1 L^\dagger$, $\tilde{L} = (\sigma_1 + \sigma_3)/\sqrt{2}$. For zero angular momentum, the equation for the transfer matrix is

$$T(\frac{L}{2}, -\frac{L}{2}) = T^{(0)}(\frac{L}{2}, -\frac{L}{2}) - i \int_{-\frac{L}{2}}^{\frac{L}{2}} dx T^{(0)}(\frac{L}{2}, x) \sigma_3 \tilde{\nu}(x) T(x, -\frac{L}{2}), \quad (9)$$
where $T^{(0)}(x_2, x_1) = \exp(i\sigma_3 E(x_2 - x_1))$ and $L$ is the length of the tube.

Taking into account $\mu = \tau_2/4$, one can find the transfer matrix in the form

$$T = \exp(i\sigma_3 E L) + i\left[\vec{b} \cdot \vec{T}_0 + \sigma_3 \frac{(\vec{b} \times \vec{T}_0)_z E}{4\pi^2 R_0} \right] \exp(i\sigma_3 E L) + \mu d_\epsilon \sigma_1 \tau_2 \frac{4\pi^2}{R_0}.$$  \hspace{1cm} (10)

The scattering matrix $(t^\dagger)^{-1}$ is defined by the upper-left element of the transfer matrix, so that the last term in (10) is neglected. The conductance is defined as $G = (4e^2/h)Tr[t^\dagger t]$, where the trace is taken over the channel space. It takes the form

$$G = \frac{4e^2}{h} \left[ 1 - \left( \frac{\vec{b} \cdot \vec{T}_0}{2T^2_0} + \frac{(\vec{b} \times \vec{T}_0)_z \epsilon}{T^2_0} \right)^2 \right],$$ \hspace{1cm} (11)

where $\epsilon = ER_0$ is a dimensionless energy (in the absolute units of $hV_F/R_0$). Correspondingly, the Fano factor $F = 1 - Tr[(t^\dagger t)^2]/Tr[t^\dagger t]$ reads

$$F = \left( \frac{\vec{b} \cdot \vec{T}_0}{2T^2_0} + \frac{(\vec{b} \times \vec{T}_0)_z \epsilon}{T^2_0} \right)^2.$$ \hspace{1cm} (12)

4. Conclusion

In this paper, we have investigated the electronic transport properties of metallic nanotubes with the disclination dipole defect. The case of disclination dipoles preserving the chirality (metallic character of the tube) was considered. This assumption simplifies the problem under consideration and allows us to construct a self-consistent expansion scheme for the effective Dirac equation. The perturbation includes both the curvature term, which appear as the Gaussian-like smooth localized potential, and the DD-induced term. The standard transfer-matrix approach is used to calculate the conductance and the Fano factor of the structure. As the marked effect of the curvature, the energy-dependent term in both the conductance and the Fano factor appears, depending on the angle between vectors $\vec{b}$ and $\vec{T}_0$. For the angle less than $\pi/2$ the conductance was found to decrease with energy, and vice versa.

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[1] Lammert P and Crespi V. 2004 Phys. Rev. B 69 035406
[2] Tamura R and Tsukada M. 2000 Phys. Rev. B 61 8548
[3] Kane C L and Mele E J. 1997 Phys. Rev. Lett 78 1932
[4] Vozmediano M A H, Katzenelson M I, and Guinea F. 2010 Preprint arXiv:1003.5179
[5] For the planar case, $|\vec{d}| = |\vec{b}|$; see Yazyev O V and Louie S G. 2010 Preprint arXiv:1004.203
[6] Titov M. 2007 Europhys. Lett 79 17004
[7] Schuessler A et al. 2009 Phys. Rev. B 79 075405