Chiral Anomaly in Toroidal Carbon Nanotubes

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It is pointed out that the chiral anomaly in 1+1 dimensions should be observed in toroidal carbon nanotubes on a planar geometry with varying magnetic field. We show that the chiral anomaly is closely connected with the persistent current in a one-dimensional metallic ring.

Recently carbon nanotubes(CNTs) [1] have attracted much attention from various points of view. Especially their unique mechanical and electrical properties have stimulated many people's interest in the analysis of CNTs [2, 3]. They have exceptional strength and stability, and they exhibit either metallic or semiconducting behavior depending on the diameter and helicity [4, 5]. Because of their small size, properties of CNTs should be governed by the law of quantum mechanics. Therefore it is quite important to understand the quantum behavior of electrons on CNTs. The bulk electric properties of (single-wall)CNTs are relatively simple, but the behavior of electrons at a metal-CNT junction is complicated and its understanding is necessary for building actual electrical devices. On the other hands, toroidal carbon nanotubes (Fullerence 'Crop Circles' [6], hereafter we use 'torus' or 'nanotorus' instead of 'toroidal carbon nanotube' for simplicity) are clearly simple because of their no-boundary shape and they would also exhibit either metallic or semiconducting properties. Even in the torus case, quite important effect: 'chiral anomaly' [7], which is of essentially quantum nature, might occur.

Low energy excitations in CNTs at half filling move along the tubule axis because the circumference degree of freedom(an excitation in the compactified direction) is frozen by a wide energy gap. Hence this system can be described as a 1+1 dimensional system. Furthermore in the case of metallic CNTs, the system describing small fluctuations around the Fermi point is equivalent to two components "massless" fermions in 1+1 dimensions. This situation can be modeled by the quantum field theory of massless fermion which couples to the gauge field through minimal coupling. This model realizes the chiral anomaly phenomenon [8, 9, 10].

The chiral anomaly is one of the most interesting phenomena in quantum field theory and has had an appreciable influence on the modern development of high energy physics [11] and of condensed matter physics [12]. The effect of the chiral anomaly on the electrons in a nanotorus appears directly as a current flow. On the other hand, it is known in solid state physics that a one-dimensional metallic ring shows the persistent current [13, 14] in an appropriate experimental setting. The current originating from the chiral anomaly shows the same magnetic field dependence to the persistent current. Therefore, the chiral anomaly in 1+1 dimensions is closely connected with the persistent current.

In this letter, we examine the anomaly effect on toroidal carbon nanotubes and discuss how such an effect



FIG. 1: Lattice structure of a two-dimensional graphite sheet $(u_1 = ae_y, \ u_2 = -\frac{\sqrt{3}}{2}ae_x - \frac{1}{2}ae_y, \ u_3 = \frac{\sqrt{3}}{2}ae_x - \frac{1}{2}ae_y)$

can be observed experimentally.

A CNT can be thought of as a layer of graphite sheet folded-up into a cylinder. A graphite sheet consists of many hexagons whose vertices are occupied by carbon atoms and each carbon supplies one conducting electron which determines the electric properties of the graphite sheet. The lattice structure of a two-dimensional graphite sheet is shown in Fig.1. There are two symmetry translation vectors on this planar honeycomb lattice, $T_1 = \sqrt{3}ae_x, T_2 = \frac{\sqrt{3}}{2}ae_x + \frac{3}{2}ae_y$. Here a denotes the length of the nearest carbon vertex, e_x and e_y are unit vectors which are orthogonal to each other $(e_x \cdot e_y = 0)$. If we neglect the spin degrees of freedom, because of these translation symmetries, the Hilbert space is spanned by the following two Bloch basis vectors,

$$|\Psi^{k}_{\bullet}\rangle = \sum_{i\in\bullet} e^{ikr_{i}}a^{\dagger}_{i}|0\rangle, \quad |\Psi^{k}_{\circ}\rangle = \sum_{i\in\circ} e^{ikr_{i}}a^{\dagger}_{i}|0\rangle, \qquad (1)$$

where the black(•) and blank(•) indices are indicated in Fig.1. r_i labels the vector pointing each site i, and a_i, a_j^{\dagger} are canonically annihilation-creation operators of the electrons of site i and j that satisfy $\{a_i, a_j^{\dagger}\} = \delta_{ij}$.

We construct a state vector which is an eigenvector of these symmetry translations as follows:

$$|\Psi^k\rangle = C^k_{\bullet}|\Psi^k_{\bullet}\rangle + C^k_{\circ}|\Psi^k_{\circ}\rangle. \tag{2}$$

In order to define the unit cell of wave vector k, we act the symmetry translation operators on the state vector and obtain the Brillouin zone

$$-\frac{\pi}{\sqrt{3}} \le ak_x < \frac{\pi}{\sqrt{3}}, \ -\pi \le \frac{\sqrt{3}}{2}ak_x + \frac{3}{2}ak_y < \pi, \quad (3)$$

where $k_x = k \cdot e_x$ and $k_y = k \cdot e_y$. Now we compactify the sheet into a torus by imposing a boundary condition to the state vector. For example, we may consider a zigzag type torus which has the following boundary conditions

$$\hat{G}(NT_1)|\Psi^k\rangle = |\Psi^k\rangle,$$

$$\hat{G}(M(2T_2 - T_1))|\Psi^k\rangle = |\Psi^k\rangle.$$
(4)

 \hat{G} denotes a symmetry translation operator. It is clear that there are many possibilities for the shape of the torus and each shape has its own boundary condition. So, some of them might have different properties from the above. Especially we can image a torus in which some twist exists along the tubule axis direction [15]. This system has the following boundary condition in general,

$$\hat{G}(M(2T_2 - T_1))|\Psi^k\rangle = \hat{G}(\tilde{N}T_1)|\Psi^k\rangle, \qquad (5)$$

where \tilde{N} is determined by the twist at the junction of CNT ends. Let us focus on the simple untwisted case given by Eq.(4). The periodic condition yields the discrete wave vectors

$$ak_x = \frac{2\pi}{\sqrt{3}} \frac{n}{N}, \quad ak_y = \frac{2\pi}{3} \frac{m}{M}.$$
 (6)

where n and m take an integer value.

Next we consider the Hamiltonian of this system [16]. Each carbon atom has an electron which makes π -orbital. The electron transfers from any site to the nearest three sites through the quantum mechanical tunneling or thermal hopping in finite temperature. Therefore there is some probability amplitude for this process. In this case, the tight-binding Hamiltonian is most suitable.

$$\mathcal{H} = E_0 \sum_i a_i^{\dagger} a_i + \gamma \sum_{\langle i,j \rangle} a_i^{\dagger} a_j, \qquad (7)$$

where the sum $\langle i, j \rangle$ is over pairs of nearest-neighbors carbon atoms i, j on the lattice. γ is the transition amplitude from one site to the nearest sites and E_0 is the one from a site to the same site. The parameter E_0 only fixes the origin of the energy and therefore is irrelevant. Hereafter we set $E_0 = 0$.

It is an easy task to find the energy eigenstates and eigenvalues of this Hamiltonian. In the matrix representation, the energy eigenvalue equation reads

$$\begin{pmatrix} 0 & \gamma \sum_{i} e^{iku_{i}} \\ \gamma \sum_{i} e^{-iku_{i}} & 0 \end{pmatrix} \begin{pmatrix} C_{\bullet}^{k} \\ C_{\circ}^{k} \end{pmatrix} = E_{k} \begin{pmatrix} C_{\bullet}^{k} \\ C_{\circ}^{k} \end{pmatrix}, \quad (8)$$

where $|\Psi_{\bullet}^{k}\rangle = (1,0)^{t}$, $|\Psi_{\circ}^{k}\rangle = (0,1)^{t}$, and the vector u_{i} is a triad of vectors pointing respectively in the direction of the nearest neighbors of a black(\bullet) cite shown in Fig.1. The energy eigenvalues and eigenvectors are as follows

$$E_k = \pm \Delta(k),\tag{9}$$

$$\begin{pmatrix} C^{\bullet}_{\bullet} \\ C^{k}_{\circ} \end{pmatrix} = \frac{1}{\sqrt{2}\Delta(k)} \begin{pmatrix} \gamma \sum_{i} e^{iku_{i}} \\ \pm \Delta(k) \end{pmatrix}, \quad (10)$$

where

$$\Delta(k) = \gamma \sqrt{1 + 4\cos\frac{\sqrt{3}}{2}ak_x\cos\frac{3}{2}ak_y + 4\cos^2\frac{\sqrt{3}}{2}ak_x.}$$
(11)

The structure of this energy band has striking properties when considered at half filling. This is the situation which is physically interesting. Since each level of the band may accommodate two states due to the spin degeneracy, the Fermi level turns out to be at midpoint of the band $(E_k = 0)$. Fermi points in the first Brillouin zone are located at $\tilde{k}_{1,2} = (ak_x, ak_y) = (\pm \frac{2\pi}{3\sqrt{3}}, \mp \frac{2\pi}{3})$. Hence, if N in Eq.(6) is a multiple of 3 then the torus shows metallic properties.

In order to understand the electric properties, we should take into account a small perturbation around the Fermi point. So we take $k = \tilde{k}_1 + \delta k$ as a small fluctuation. Perturbation around the point \tilde{k}_2 is same as around the point $k = \tilde{k}_1$. So we may only consider one of the pairs. In this case the effective Hamiltonian which describes the system is given by $\mathcal{H}_{pert} = v_F(\sigma \cdot p)$ [17] where $v_F(\equiv \frac{3\gamma a}{2\hbar})$ is the Fermi velocity, p is the momentum operator $(p = -i\hbar\nabla)$ and σ_i are the Pauli matrices. Hence the Schrödinger equation becomes

$$i\hbar\frac{\partial}{\partial t}\psi = v_F\left(\sigma\cdot p\right)\psi. \tag{12}$$

We conclude that the low energy excitations of a metallic torus at half filling are described by an effective theory of two components spinor obeying the Weyl equation.

It should be noted that the characteristic properties of metallic CNTs are all reproduced quite well by analyzing this equation with external fields such as a magnetic and electronic field [18]. In the following, we consider metallic tori that have small N and large M values $(M/N \sim 10^3)$. In this case, transitions between different k_x are rarely happen because of their costed energy $(\sim \gamma/N)$ as compared to that of $k_y:(\sim \gamma/M)$. Hence, the only surviving degree is a motion in the y-direction, i.e. this system is 1+1 dimensional effectively.

One can obtain the quantum field theory by promoting the wave function(ψ) to the field operator(Ψ) satisfying the canonical anticommutation relations. Because the Schrödinger equation is the Weyl equation it is appropriate to adopt the following Lagrangian density:

where $\overline{\Psi} = \Psi^{\dagger} \gamma^{0}$ and \mathcal{D} is the Feynman notation defined as $\mathcal{D} = \sum_{\mu=0,1} \left(i\hbar\partial_{\mu} - \frac{e}{c}A_{\mu}\right)\gamma^{\mu}$. Here $A_{\mu} = (A_{0}, A_{1}) \equiv (A_{t}, v_{F}A_{y})$ are the gauge fields and we adopt the following relativistic notation: $x^{\mu} = (x^{0}, x^{1}) \equiv (t, y/v_{F}), \partial_{\mu} = (\partial_{0}, \partial_{1}) \equiv \partial/\partial x^{\mu}, \gamma^{0} = \sigma_{x}, \gamma^{1} = i\sigma_{y}, \gamma^{5} = -\gamma^{0}\gamma^{1} = \sigma_{z}$. The Dirac matrices γ^{μ} obey $\{\gamma^{\mu}, \gamma^{\nu}\} = 2g^{\mu\nu}$ and $\gamma^{\mu}\gamma^{5} = \epsilon^{\mu\nu}\gamma_{\nu}$ with the metric $g^{\mu\nu} = \text{diag}(1, -1)$ and the antisymmetric tensor $\epsilon^{\mu\nu}, \epsilon^{01} = \epsilon_{01} = 1$. The electro-magnetic interaction is introduced according to the minimal coupling. The gauge fields propagate in four dimensional



FIG. 2: A toroidal carbon nanotube on a planar geometry with a magnetic field

space-time so that the Coulomb potential is given by the standard long-range interaction. As a gauge fixing, we take the Weyl gauge $A_0 = 0$; in this case, the Hamiltonian of the fermion becomes

$$\mathcal{H}_F = \Psi^{\dagger} h_F \Psi = \Psi^{\dagger} \begin{pmatrix} i\hbar\partial_1 - \frac{e}{c}A_1 & 0\\ 0 & -(i\hbar\partial_1 - \frac{e}{c}A_1) \end{pmatrix} \Psi.$$
(14)

We neglect the one-dimensional long-range Coulomb interaction [19] and regard the gauge field as a classical field here. Even in this case, it does not lose the nature of anomaly. We list some main results of the Hamiltonian; a detailed description of this system can be found in References [9, 10]. The energy eigenvectors are given by (Hereafter let us use x instead of y as a label of the coordinate of a tubule axis direction)

$$h_F \psi_n \begin{pmatrix} 1\\0 \end{pmatrix} = \epsilon_n \psi_n \begin{pmatrix} 1\\0 \end{pmatrix}, \ h_F \psi_n \begin{pmatrix} 0\\1 \end{pmatrix} = -\epsilon_n \psi_n \begin{pmatrix} 0\\1 \end{pmatrix},$$
$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{-i\frac{\epsilon}{\hbar c} \int_0^x A_1(x') dx' - i\frac{\epsilon_n}{\hbar v_F} x}, \tag{15}$$

where L is the circumferential length of a torus L = 3aMand ϵ_n are the energy eigenvalues. Because we take the periodic boundary condition, the following energy spectrum appears

$$\epsilon_n = \frac{2\pi\hbar v_F}{L} \left[n - \frac{e}{2\pi\hbar c} \oint A_1 dx \right]. \tag{16}$$

The gauge field in the spectrum can be controlled externally by the following experimental setup. On the planar geometry we put a nanotorus and penetrate some magnetic field inside the torus perpendicular to the plane as is shown in Fig.2. In this case the gauge field that expresses this magnetic field is given by, in the vector notation, $A = \frac{N_{\Phi}\phi_D}{2\pi}\nabla\theta$. Therefore we get a component, $A_1 = \frac{N_{\Phi}\phi_D}{L}$, where $\phi_D = \frac{2\pi\hbar c}{e}$ is the flux quanta. This vector potential expresses N_{Φ} flux inside the torus and by tuning the magnetic field, N_{Φ} can be taken as a real number.

We expand the fermion field using the energy eigenvectors as

$$\Psi = \sum_{n \in \mathbb{Z}} \left[a_n \psi_n(x) e^{-i\frac{\epsilon_n}{\hbar}t} \begin{pmatrix} 1\\ 0 \end{pmatrix} + b_n \psi_n(x) e^{+i\frac{\epsilon_n}{\hbar}t} \begin{pmatrix} 0\\ 1 \end{pmatrix} \right],$$
(17)

where a_n, b_n are independent fermionic annihilation operators satisfying the anti-commutators

$$\{a_n, a_m^{\dagger}\} = \{b_n, b_m^{\dagger}\} = \delta_{nm}.$$
 (18)

All the other anticommutators vanish. The dynamics of this field is governed by the Lagrangian density (13), which has two conserved currents that are electric current J^{μ} and chiral current J_{5}^{μ} ,

$$J^{\mu}(x) = \bar{\Psi}(x)\gamma^{\mu}\Psi(x), \qquad (19)$$

$$J_5^{\mu}(x) = \bar{\Psi}(x)\gamma^{\mu}\gamma^5\Psi(x) = \epsilon^{\mu\nu}J_{\nu}(x).$$
(20)

Therefore, the following two charges conserve in the time evolution of the system,

$$Q = \oint J^0(x) dx, \quad Q_5 = \oint J^0_5(x) dx.$$
 (21)

Conservation of the electric current $\partial_{\mu}J^{\mu} = 0$ ($\partial_{0} = \partial_{t}, \partial_{1} = v_{F}\partial_{x}$) is due to the gauge symmetry and the chiral current conservation $\partial_{\mu}J_{5}^{\mu} = 0$ is due to the global chiral symmetry $\Psi \rightarrow e^{i\gamma^{5}\alpha}\Psi$. For unquantized fermion field the chiral invariance ensures conservation of the unquantized chiral current. However after the second quantization the chiral current ceases to be conserved even though the interaction appears to be chirally invariant. Because, different from classical mechanics, in the world of quantum mechanics, the chiral symmetry is broken [7] by the vacuum. So the chiral anomaly is similar to the spontaneous symmetry breaking in the sense that in both phenomena physical asymmetry is attributed to the vacuum state and not to the dynamics.

In order to find what is happening, we need to analyze the vacuum structure $|vac; N_L, N_R\rangle = |vac; N_L\rangle \otimes |vac; N_R\rangle$, where

$$|vac; N_L\rangle = \prod_{n=-\infty}^{N_L-1} a_n^{\dagger} |0\rangle, \quad |vac; N_R\rangle = \prod_{N_R}^{n=\infty} b_n^{\dagger} |0\rangle. \quad (22)$$

We define $|vac; N_L\rangle(|vac; N_R\rangle)$ such that the levels with energy lower than $\epsilon_{N_L}(-\epsilon_{N_R-1})$ are filled and the others are empty. On this vacuum, the expectation values of the charges and the energy become [9, 10]

$$\langle Q \rangle = N_L - N_R, \tag{23}$$

$$\langle Q_5 \rangle = N_L + N_R - 2N_\Phi - 1,$$
 (24)

$$\langle H_F \rangle = \frac{2\pi\hbar v_F}{L} \left(\frac{\langle Q \rangle^2 + \langle Q_5 \rangle^2}{4} - \frac{1}{12} \right). \quad (25)$$

To obtain the above results, we have regularized the divergent eigenvalues on the vacuum by ζ -function regularization. For example, the gauge charge is regularized as follows:

$$Q = \lim_{s \to 0} \left(\sum_{n \in \mathbb{Z}} a_n^{\dagger} a_n \frac{1}{|\lambda \epsilon_n|^s} + \sum_{n \in \mathbb{Z}} b_n^{\dagger} b_n \frac{1}{|-\lambda \epsilon_n|^s} \right), \quad (26)$$

where λ is an arbitrary constant with dimension of length which is necessary to make $\lambda \epsilon_n$ dimensionless. This regularization respects gauge invariance because the energy of each level is a gauge invariant quantity.

The gauge charge $\langle Q \rangle$ remains a constant if no electron flows into the system. We now have $N_L = N_R$ for an isolated nanotorus. From the above equation (24), it can be seen that if N_L and N_R are conserved, then, by varying the magnetic field N_{Φ} , the chiral charge also changes. Therefore it is not a conserved quantity. We thus see that the vacuum is responsible for non-conservation of chirality even though the dynamics is chirally invariant. From Eq.(20) we see that the chiral current J_5^0 is proportional to the electric current($ev_F J^1(x)$) in the tubule axis direction, then we have an average value of the electric current J as

$$J \equiv \frac{ev_F}{L} \oint J^1(x) dx = -\frac{ev_F}{L} \oint J_5^0(x) dx = -\frac{ev_F}{L} Q_5.$$
(27)

Hence, in order to observe the anomaly, we should observe the electrical current in the torus.

It is clear from the above equations that there are two origins of the usual current flow along the torus. One is the $N_L + N_R$ term which can be induced in thermal bath or by a sudden change of the magnetic field. On the other hand, the magnetic field can change the quantum vacuum structure and lead to the anomaly. In order to avoid the unexpected changes of $N_L(=N_R)$, the magnetic field must be changed adiabatically at low temperature($\langle \frac{2\pi\hbar v_F}{L} \rangle$). However, in an adiabatic process, when the strength of the magnetic field reaches the point that N_{Φ} is an integer, then $N_L(=N_R)$ also have to change. The reason is that, when increasing N_{Φ} starting from the point $N_{\Phi} = -\frac{1}{2}, N_L = 0$, the energy is going up as Eq(25). At $N_{\Phi} = 0$, the spectrum meets an another line of spectrum coming from the $N_{\Phi} = \frac{1}{2}, N_L = 1$ as is shown in Fig.3. Therefore the circular current in the ring

$$J = \frac{ev_F}{L} \left[2 \left(N_{\Phi} - N_L \right) + 1 \right]$$
 (28)

follows the line shown in Fig.4. We should remark that there are two spin degrees of freedom at each Fermi point. Therefore the actual current is four times the J, that is, the amplitude of this total current is $\frac{4ev_F}{L}$. A numerical value of this amplitude is about $0.5[\mu\text{A}]$ for a nanotorus with $L = 1[\mu\text{m}]$. This current for an untwisted torus shows the same magnetic field dependence to the persistent current in ref. [14]. Our results (28) are in agreement with the results of other papers.

Let us explain how to measure the current briefly. Some methods could be considered in order to detect the current in the torus. As an example, the current generates a magnetic field around torus, then one can observe the current via magnetic field which is generated by the current. However the current could not be observed by the standard electrical contact because the electrical perturbation can not affect the current flow.



FIG. 3: Flux dependence of the fermionic vacuum energy $\langle H_F \rangle$. The energy value is labeled in the unit of $\frac{2\pi\hbar v_F}{L}$.



FIG. 4: Magnetic field dependence of the induced current. We plot the current in the unit of $\frac{ev_F}{L}$.

This means that we can not measure the current by an electrical contact.

In conclusion, low energy excitations in metallic toroidal carbon nanotubes can be described by the two components "massless" fermion which couples to a gauge field through minimal coupling. The anomaly effect should be observed by an adiabatic change of the vector potential, since this induces peculiar electrical current along the torus through the chiral anomaly. The chiral anomaly provides a deeper understanding for the persistent current.

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