Aharonov-Bohm effect in higher genus materials

K. Sasaki and Y. Kawazoe
Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

R. Saito
Department of Physics, Tohoku University and CREST, JST, Sendai 980-8578, Japan

(Dated: January 7, 2022)

Flux periodicity of conducting electrons on a closed surface with genus two \( g = 2 \) (double torus) are investigated theoretically. We examine flux periodicity of the ground-state energy and of the wave functions as a function of applied magnetic field. A fundamental flux period of the ground-state energy is twice a fundamental unit of magnetic flux for uniformly applied magnetic field, which is shown to be valid for a simple ladder geometry and carbon double torus. Flux periodicity of the wave functions in a double torus is complicated compared with a simple torus \((g = 1)\), and an adiabatic addition of magnetic fluxes does not provide a good quantum number for the energy eigenstates. The results are extended to higher genus materials and the implications of the results are discussed.

Geometrical structure of materials and behavior of the conducting electrons are closely connected with each other. Carbon nanotube is a typical example where the electric properties are directly related to its unique structure \( \text{a} \). It is known that global geometry (topology) of materials, which consist of a closed surface, can be classified mathematically by the number of genus \((g)\). The genus number is the number of “holes” of a closed orientable surface. For example, as for carbon based materials, \( \text{C}_{60} \) \( \text{b} \), nanotubes \( \text{c} \), and tori \( \text{d} \) were found in nature, and they are classified by \( g = 0 \) or \( g = 1 \). However, they are only a part of materials from the topological point of view. In the present letter, we examine characteristics of quantum mechanical states of the conducting electrons in a closed surface of genus two \((g = 2, \text{ double torus})\). As electronic and magnetic properties of materials are affected by their geometry, one may expect that, when considers different global structures, one could find a novel phenomenon originated in the topology. We consider two problems associated with the topological nature of the materials: (1) What is a characteristic phenomenon of higher genus \((g \geq 2)\) materials that can not be expected in a lower genus \((g = 0 \text{ or } g = 1)\) material? (2) What kind of physical quantity can be used to characterize the energy eigenstates of the conducting electrons?

The former question is to find a phenomenon which is closely related to the global geometry of a material. Aharonov-Bohm (AB) effect is an example of such a phenomenon and is one of the most important consequence of quantum mechanics \( \text{e} \). Ring geometries are common to investigate the AB effect where the wave functions of electrons interfere to one another \( \text{f} \). Also as for \( g = 2 \) materials, one may expect the AB effect and the physics should be described as a function of two independent magnetic fields penetrating through the two holes. There may be a general consequence of how the electrons response to the magnetic field in higher genus materials. The latter problem relates to taking a convenient choice of basis vectors in the Hilbert space. The basis vectors in ordinary materials (or bulk) are labeled by the wave vectors. For periodic lattice systems, one can adopt the Bloch basis vectors or plane waves because of the lattice translational symmetry and the wave vectors are a good quantum number. However, as for a double torus (or higher genus materials), because of its nontrivial topology, it seems to be difficult to define a good quantum number. In this letter, we examine the above two questions by analyzing the ground-state energy, wave functions, and their periodicity as a function of magnetic fluxes penetrating through the holes.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{(a) A simple ladder consists of six sites (Each site is indicated by \( \bullet \)). (b) An example of a double torus made of only carbon atoms. We attach two elongated toroidal carbon nanotubes \( \text{g} \), both of which consist of 240 carbon atoms, by cutting some part of them. A resultant carbon double torus possesses 460 carbon atoms. The topological structure of (b) reduces to (a) in a limit of very thin tube structure.}
\end{figure}

Although we consider general problems associated with the topological nature of materials, we use two models for
A double torus made of carbon atoms depicted in Fig. 1(b). Hereafter we will use the units: $\hbar = c = 1$.

First of all, we define flux lines which are necessary to analyze the AB effect in those systems. We define four external flux lines (or gauge fields) for a double torus geometry: $A = \alpha_1 A_1 + \alpha_2 A_2 + \beta_1 B_1 + \beta_2 B_2$ where the vector potential $A_1(A_2)$ corresponds to a fundamental unit of magnetic flux $\Phi_0 = 2\pi/e$ ($-e$ is the electron charge) penetrating through the left(right) hole. $B_1(B_2)$ is the gauge field that is assigned by a magnetic flux circling inside the surface of the left(right) ring. The coefficients $(\alpha_1, \alpha_2, \beta_1, \beta_2)$ measure the number of a unit flux of each component and can be a real number. We depict these flux lines in Fig. 2.

We examine the ground-state energy of the conducting electrons in a double torus and its period as a function of applied magnetic field expressed by $(\alpha_1, \alpha_2)$. The other types of flux $(\beta_1, \beta_2)$ are fixed at zero. This is because a phenomenon peculiar to the number of genus seems to be insensitive to the perturbation driven by $(\beta_1, \beta_2)$. Suppose we obtain the energy eigenvalues of the Hamiltonian as $\epsilon_i(\alpha_1, \alpha_2)$ ($i \in \{1, \cdots, N\}$ where $N$ is the number of lattice site). The ground state of the Hamiltonian is defined as the lowest energy state at any external gauge field. The spectra of the Hamiltonian and the ground-state energy are invariant with respect to the addition of a unit flux. Let us define the ground-state energy as $E(\alpha_1, \alpha_2)$ and then it has the following periodicity:

$$E(\alpha_1, \alpha_2) = E(\alpha_1 + 1, \alpha_2) = E(\alpha_1, \alpha_2 + 1).$$

(1)

The ground-state energy can be rewritten as a function of $\alpha_1 + \alpha_2$ and $\alpha_1 - \alpha_2$, so that for a uniform magnetic field $\alpha_1 = \alpha_2 = \alpha$, it becomes a function of only $\alpha_1 + \alpha_2$, and has the following periodicity:

$$E(\alpha_1 + \alpha_2) = E(\alpha_1 + \alpha_2 + 2).$$

(2)

To check this periodicity (hereafter we call this “period doubling”), we have performed numerical estimation of the ground-state energy of the carbon double torus and the ladder system (Fig. 3), assuming that the Hamiltonian of the conducting electrons is given by the following nearest-neighbor tight-binding Hamiltonian with an external gauge field $A$:

$$\mathcal{H}(A) = V_\pi \sum_{(i,j)} \alpha_j^\dagger e^{-ie} \int_{r_i} A ds a_i,$$

(3)

where $V_\pi$ is the hopping integral and the sum $(i, j)$ is over pairs of nearest neighbor sites $i, j$. The vector $r_i$ labels the vector pointing each site $i$, $a_i$ and $a_j^\dagger$ are canonical annihilation-creation operators of the electrons of site $i$ and $j$ that satisfy a standard anti-commutation relation $\{a_i, a_j^\dagger\} = \delta_{ij}$, and $ds$ is the differential line element.

We have numerically checked that the period doubling effect is valid in both samples (see Fig. 3). In Fig. 3(a) and (b), numerical estimation of the ground-state energy of each sample is given. Two curves are plotted for each sample, one is for a flux penetrating only through the left hole(solid line) and the other is for a uniform magnetic field(dashed line). The periodicity of dashed lines corresponds to Eq. (3), which is a straightforward consequence of Eq. (1).

We consider a possibility that the ground-state energy has the periodicity of a unit flux with respect of a uniform magnetic field, that is $E(\alpha_1 + \alpha_2) = E(\alpha_1 + \alpha_2 + 1)$. Suppose there is no hopping interaction between site A and B in the ladder system (see the right inset of Fig. 3(b)), then the geometry of the ladder reduces to a torus ($g = 1$) and the period should become a unit flux. Hence, the period doubling effect may be a phenomenon which reflects the topological nature of materials.

The period doubling effect can be easily extended to higher genus materials ($g$) under a uniform magnetic field, in which a fundamental period of the ground-state energy can be thought of as $g$ times a flux unit: $\Phi_{\text{unit}} = g\Phi_0$. We have checked for this extension using two different ladder systems shown in the right insets of
consider an adiabatic process in which we are adding a unit magnetic flux by changing the number of $\alpha$ and $\beta$ gradually. We denote these operations as $G_1$ and $G_2$, $G_1 : \alpha \rightarrow \alpha + 1$, $G_2 : \beta \rightarrow \beta + 1$. The difference between the Hamiltonian before and after these operations may be thought of as the large gauge transformation and the spectra of the Hamiltonian must be periodic in the unit of flux quanta. During the adiabatic process, the eigenstates change and when we finish adding just one unit flux, a state have to go to one of the eigenstates in the spectra of the original Hamiltonian. The resultant state is generally different from the original state. Here we define the state vectors that are obtained from an eigenstate by the adiabatic addition of magnetic fluxes as

$$|k_1 - aeA_1, k_2 - beA_2\rangle = (G_1^a(G_2^b)|k_1, k_2\rangle, \quad (4)$$

where $a$ and $b$ are integers. The periodicity of the wave functions depends on the lattice structure of a torus (or the congruent vectors, $K_i$) because $k_i$ and $k_i + K_i$ express the same state so that the periodicity of the wave functions can be derived as $a_i$ from the following equations: $a_i eA_i = K_i$. Therefore, the periodicity of the wave functions depends on its lattice structure, and the wave vectors (or the number of magnetic fluxes) work as good quantum numbers. The flow of energy spectra as a function of an applied magnetic field can be used to examine if the resultant state is different from the original state and the periodicity of the wave functions.

Let us return to the double torus. We have examined the periodicity of the wave functions by analyzing the spectral flow of the energy eigenvalues of the two systems shown in Fig. 4. We first show a numerical result of the ladder system in Fig. 5. We observe that

FIG. 4: (a) Numerical results of ground-state energy of ladders (whose geometrical configuration is shown in the right inset) as a function of total number of magnetic flux ($\alpha_1 + \alpha_2 + \alpha_3$). (b) The case of another ladder system. We have assumed half-filling in both calculations.

We proceed to examine flux periodicity of wave functions of the conducting electrons. It is first noted that the flux periodicity of wave functions does not need to be the same as that of the ground-state energy and it relates to the detail of the geometry (or the lattice structure). To make this point clear, let us mention the kinematics of the conducting electrons in a torus ($g = 1$) and explain periodicity of the wave functions. A torus can be mapped to a parallelogram with two side vectors $T_1$ and $T_2$ for around and along the tubule axis respectively. Because of the periodic boundary conditions along these vectors, the wave vectors of the conducting electrons ($k$) have to satisfy the following constraints: $T_1 \cdot k_1 = 2\pi n$, $T_1 \cdot k_2 = 0$, $T_2 \cdot k_1 = 0$, $T_2 \cdot k_2 = 2\pi m$, where we set $k = k_1 + k_2$ and both $n$ and $m$ are integers. The wave vectors are of great use to characterize a quantum state and a full set of them forms a complete basis in the Hilbert space. When the Hamiltonian possesses lattice translational symmetries along those vectors, $k$ can be used as labels for the energy eigenstates. Here we denote the Bloch basis vectors as $|k_1, k_2\rangle$.

We define two flux lines for a torus geometry: $A = \alpha A_1 + \beta A_2$, where the vector $A_1$ is a gauge field corresponding to a fundamental unit of magnetic flux penetrating through the center of a ring and $A_2$ a unit flux circling inside the surface of a torus. The coefficients $\alpha$ and $\beta$ are defined as the number of a unit flux for $A_1$ and $A_2$ respectively, and can be a real number. Let us
the addition of the $\alpha_+$ magnetic flux does not result in a connection between different states, which means that the wave function's periodicity is the same as that of the ground-state energy. On the other hand, $\alpha_-$ flux gives the transition from the lowest(highest) energy eigenstate to a state nearest to the Fermi level. Next we analyze the carbon double torus (see Fig. 6). In Fig. 6, we see that the transition from the lowest(highest) energy eigenstate is governed as a function of magnetic field denoted in the vertical axis indicates the energy eigenvalue in unit of the ground-state energy and wave functions of the conducting electrons in double torus systems under a magnetic field. We have numerically checked the periodicities expressed by Eq. (1) and its consequence: Eq. (2) for the hopping integral. We have also checked that different flux configurations such as $\alpha_1 \pm \beta_1$ and $\alpha_1 \pm \beta_2$, and could not find the transition between different states near the Fermi level.

any of the adiabatic processes does not provide a transition from one energy eigenstate to a different eigenstate. Thus, for this carbon double torus, it is difficult to assign a quantum number by the number of magnetic flux and it suggests that it is better to use site basis vectors to express the energy eigenstate near the Fermi level.

Here let us refer to some possible extensions of our results. The ground-state energy is closely related to the persistent currents [9] and the differential susceptibility, for example, the periodicity of the ground-state energy is preserved in them. Therefore, it could be possible to extract a kind of topological information, e.g., whether the conducting electrons are hopping through the line lying between two holes (hopping between site A and B in the ladder system) or the line is cut (broken), by studying the periodicity of persistent currents or differential susceptibility. Because, if the hopping is not active, the period would recover a standard periodicity of a unit flux.

Next, we comment on the periodicity of the fluxes corresponding to $\left(\beta_1, \beta_2\right)$. The ground-state energy is also a function of these parameters and is periodic in the unit of flux quanta, hence we have $E(\beta_1, \beta_2) = E(\beta_1 + 1, \beta_2) = E(\beta_1 , \beta_2 + 1)$. In case of $\beta_1 = \pm \beta_2$, different from the $\left(\alpha_1, \alpha_2\right)$ magnetic field, the periodicity can not be regarded as doubling because their flux lines can be connected to form one flux line, i.e., $\beta_1 = 1$ corresponds to one flux line (see Fig. 6).

Finally, let us comment on an existing material which can be thought of as a limiting shape of higher genus materials. A line of 16 GaAs/GaAlAs connected mesoscopic rings have already manipulated and persistent currents in the rings were examined by Rabaud et al. [10]. In their setting, each ring is order of $\mu m^2$, which requires a magnetic field $B \sim 40$[gauss] as a flux quanta because of $\Phi_0 = 4 \times 10^{-7}$[gauss · cm$^2$].

In summary, we have examined periodicity of the ground-state energy and wave functions of the conducting electrons in double torus systems under a magnetic field. We have numerically checked the periodicities expressed by Eq. (1) and its consequence: Eq. (2) for the ladder and carbon double torus. It is expected that, for higher genus materials ($g$), fundamental periodicity under a uniform magnetic field is $g\Phi_0$. It has been shown that the periodicity of the energy eigenstate near the Fermi level is the same as that of the ground-state energy, which indicates that it is difficult to assign a quantum number by the number of magnetic flux.

Acknowledgments

K. S. wishes to thank Dr. T. Tani for fruitful discussion. He is supported by a fellowship of 21st century COE program of international center of research and education for materials of Tohoku university. R. S. acknowledges a Grant-in-Aid (No. 13440091) from the Ministry of Education, Japan.

[1] R. Saito, G. Dresselhaus, and M.S. Dresselhaus, Physical Properties of Carbon Nanotubes, Imperial College Press, London (1998).
[2] H.W. Kroto, J.R. Heath, S.C. O’Brien, R.F. Curl, and R.E. Smalley, Nature 318, 162 (1985).
[3] S. Iijima, Nature 354, 56 (1991).
[4] J. Liu, H. Dai, J.H. Hafner, D.T. Colbert, R.E. Smalley, S.J. Tans, and C. Dekker, Nature 385, 780 (1997).
[5] Y. Aharonov and D. Bohm, Phys. Rev. 115, 485 (1959).
[6] R.A. Webb, S. Washburn, C.P. Umbach, and R.B. Laibowitz, Phys. Rev. Lett. 54, 2696 (1985).
[7] S. Itoh and S. Iihara, Phys. Rev. B 48, 8323 (1993).
[8] R. Rajaraman, Solitons and Instantons, North-Holland Personal Library (1982).
[9] M. Büttiker, Y. Imry, and R. Landauer, Phys. Lett. A 96, 365 (1983).
[10] W. Rabaud, L. Saminadayar, D. Mailly, K. Hasselbach, A. Benoit, and B. Etienne, Phys. Rev. Lett. 86, 3124 (2001).