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The full symmetry and irreducible representations of nanotori

Majid Arezoomand[a] and Bijan Taeri[b]*

[a]Islamic Azad University, Majlesi Branch, Isfahan, Iran, and [b]Department of Mathematical Sciences, Isfahan University of Technology, Isfahan 84156-83111, Iran. Correspondence e-mail: b.taeri@cc.iut.ac.ir

The full symmetry groups of carbon nanotori are investigated. It is shown that that the symmetry group of a chiral (n_1, n_2) nanotorus is isomorphic to $D_{2mq/n}$, where m and q are the number of lattice points on the torus circumference vector and the number of graphene hexagons in the nanotorus unit cell, respectively, and $n = \gcd(n_1, n_2)$. It is also shown that the symmetry group of zigzag and armchair (achiral) nanotori is $D_{4m} \times \mathbb{Z}_2$, where D_{2k} and $\mathbb{Z}_k$ are the dihedral group of order $2k$ and the cyclic group of order k, respectively. The irreducible representations and characters of these groups are discussed.

1. Introduction

Carbon nanotubes, which are multi-walled structures of pure carbon, were discovered in 1991 (Iijima, 1991). They show remarkable mechanical properties and extensive experimental and theoretical investigations have been carried out on them (Endo *et al.*, 1996; Wong *et al.*, 1997; Yakobson *et al.*, 1996). Their mechanical characteristics clearly predestinate them for advanced composites. A single-wall carbon nanotube is a cylindrical structure with a diameter of a few nanometres; it is periodic along its axis and can be visualized as a rolled-up honeycomb lattice. Nanotubes are attractive subjects for study in solid-state physics due to their potential applications in nanotechnology. Their symmetry is important in theoretical investigations and has been investigated by Damnjanović *et al.* (1999*a*, 2001, 1999*b*, 2002); Barros *et al.* (2006) and Dresselhaus *et al.* (1995). The high symmetry of carbon nanotubes has facilitated the theoretical investigation of the physical phenomena occurring in these materials. The spatial symmetries (translations, rotations and screw axes, mirror and glide planes *etc.*) leave the nanotube invariant. The role of the symmetry group is analogous to that of a crystallographic space group in solid-state physics. Some important properties of the band structure (electronic, phonon *etc.*) can be directly deduced from the symmetry group.

A nanotube is a graphene sheet wrapped to form a cylinder. A nanotorus is a nanotube whose ends are connected (see Fig. 1). The physical properties of nanotori have been studied, for example, by Zhanga *et al.* (2006) and Sasaki (2002). In this paper we study the symmetry groups of chiral and achiral carbon nanotori and the irreducible representations of their symmetry groups.

2. Full symmetry groups

A single carbon nanotorus may be described as a long rolled-up graphite sheet bent around to the form of torus as shown in Fig. 2. The vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are the unit vectors of a graphite sheet and the angle between them is $\pi/3$. The transverse vector $\mathbf{C} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$, which is called the chiral vector, and the longitudinal vector $\mathbf{T} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2$ correspond to the tube and torus circumferences, respectively.

Let $\mathbf{C}'$ and $\mathbf{T}'$ be the unit vectors of $\mathbf{C}$ and $\mathbf{T}$, respectively. The numbers of lattice points on the chiral vector $\mathbf{C}$ and on the torus circumference $\mathbf{T}$ are given by the greatest common divisors n of integers n_1, n_2 and m of integers m_1, m_2, respectively. We have $n\mathbf{C}' = \mathbf{C}$, $m\mathbf{T}' = \mathbf{T}$,

$$\mathbf{T}' = \frac{n_1 + 2n_2}{nR}\mathbf{a}_1 - \frac{2n_1 + n_2}{nR}\mathbf{a}_2, \qquad (1)$$

$|\mathbf{C}| = a_0(n_1^2 + n_2^2 + n_1n_2)^{1/2}$ and $|\mathbf{T}'| = a_0[3(n_1^2 + n_2^2 + n_1n_2)]^{1/2}/nR$, where $a_0 = |\mathbf{a}_1| = |\mathbf{a}_2| = 2.461$ Å, $R = 3$ if $n_1 \equiv n_2 \pmod{3n}$ and $R = 1$ otherwise. The direction of the chiral vector is measured by the chiral angle θ, which is defined as the angle between $\mathbf{a}_1$ and $\mathbf{C}$. The chiral angle θ can be calculated from $\theta = \arccos\{(2n_1 + n_2)/[2(n_1^2 + n_2^2 + n_1n_2)^{1/2}]\}$. As the tube cell is on a two-dimensional lattice, the rectangle over $\mathbf{C}'$ and $\mathbf{T}'$ contains two-dimensional lattice cells. Moreover, if q is the number of hexagons in the unit cell of the graphene, then $q = 2(n_1^2 + n_1n_2 + n_2^2)/nR$ and in the elementary cell of the tube there are q/n monomers, each of them containing n elementary honeycomb cells (see Damnjanović *et al.*, 1999*b*; Zhanga *et al.*, 2006).

The translations of the rolled-up lattice along the torus circumference vector become the rotations. The group of

Table 1
Character table of a chiral nanotorus.

$\varepsilon = \exp(2\pi i n/mq)$ and $1 \le r, j \le (mq/2n) - 1$.

	1	$W^{mq/2n}$	W^r	U	WU
μ_1	1	1	1	1	1
μ_2	1	1	1	-1	-1
μ_3	1	$(-1)^{mq/2n}$	$(-1)^r$	1	-1
μ_4	1	$(-1)^{mq/2n}$	$(-1)^r$	-1	1
χ_j	2	$2(-1)^j$	$\varepsilon^{jr} + \varepsilon^{-jr}$	0	0

these rotations is a cyclic group of order m, generated by $\mathbf{T}'$. Since the tubule length is much larger than its diameter [see for example §3 of Dresselhaus *et al.* (1995)], all two-dimensional lattice translations remain symmetries of the tube. The translations of the graphene sheet along the direction of combination of translations in $\mathbf{T}'$ and $\mathbf{C}$ inevitably yield helical (screw-axis) symmetry, as a consequence of the underlying hexagonal two-dimensional symmetry. Let $\mathbf{W}$ be such a translation, and let $\mathbf{W} = \alpha\mathbf{C} + \beta\mathbf{T}'$. Then since $\mathbf{W} = w_1\mathbf{a}_1 + w_2\mathbf{a}_2$, using equation (1) and the independence of $\mathbf{a}_1$ and $\mathbf{a}_2$ we can see that

$$\alpha = \frac{(2n_1 + n_2)w_1 + (n_1 + 2n_2)w_2}{2(n_1^2 + n_1 n_2 + n_2^2)}, \quad \beta = \frac{nR(n_1 w_2 - n_2 w_1)}{2(n_1^2 + n_1 n_2 + n_2^2)}$$

and thus $\mathbf{W} = (u/q)\mathbf{C} + (v/q)\mathbf{T}'$, where $u = [(2n_1 + n_2)w_1 + (n_1 + 2n_2)w_2]/nR$, $v = n_1 w_2 - n_2 w_1$ and $q = [2(n_1^2 + n_1 n_2 + n_2^2)]/nR$, which is the number of hexagons in the unit cell of the graphene. By choosing w_1 and w_2 such that $v = n$ and $\mathbf{W}$ has minimum length, we have $q\mathbf{W} = u\mathbf{C} + n\mathbf{T}'$. Thus the order of $\mathbf{W}$ is mq/n.

From the sixfold rotation of the hexagon about its midpoint, only the twofold rotation U remains a symmetry operation in a carbon nanotorus. Rotations by any other angle do not preserve the ring axis and therefore are not symmetry operations of the nanotorus. This rotational axis, which is present in both chiral and achiral nanotori, is perpendicular to the ring axis. Mirror planes perpendicular to the graphene sheet must either contain the ring axis or be perpendicular to it in order to transform the nanotorus into itself. Only in achiral nanotori are the vertical and horizontal mirror planes present (respectively σ_v and σ_h). They contain the midpoints of the graphene hexagons. In addition, in achiral nanotori the vertical and horizontal planes through the midpoints between two carbon atoms form vertical glide planes and horizontal rotoreflection planes. The generators of the symmetry group of chiral nanotori are the twofold rotation U and the screw axis W. Note that $\mathbf{W}^{q/n} = \mathbf{T}'$ [see p. 131 of Cotfas (2005), where $\mathbf{W} = g_w, g_b = \mathbf{T}'$ and $q' = q/n$]. Thus the symmetry group of a chiral nanotorus is

$$G = \langle U, W \mid U^2 = W^{mq/n} = (WU)^2 = 1\rangle.$$

It is easy to check that $G \cong D_{2mq/n}$, the dihedral group of order $2mq/n$. Note that by Lemma 1 of Damnjanović *et al.* (1999*b*) we have $q/n \equiv 2 \pmod{12}$.

Let G' be the symmetry group of an achiral nanotorus. The set of generators of G' is the set of generators of G and σ_v. Note that $\sigma_h = U\sigma_v$. In the achiral case we have $q = 2n$ [see for example Damnjanović *et al.* (1999*b*), p. 3]. So it is clear that $G' \cong D_{4m} \times \mathbb{Z}_2$, where $\mathbb{Z}_2$ is a cyclic group of order 2.

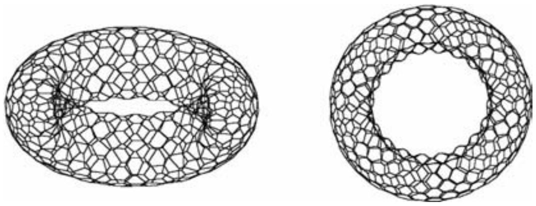

Figure 1
A nanotorus with $\mathbf{C} = 10\mathbf{a}_1 + 10\mathbf{a}_2$, $\mathbf{T}' = \mathbf{a}_1 - \mathbf{a}_2$, $\mathbf{T} = 20\mathbf{T}'$. The side view is shown on the left and the top view is shown on the right. Reproduced with permission from Diudea *et al.* (2001).

3. Conjugacy classes, irreducible representations and characters

In this section we discuss the irreducible representations and characters of the symmetry groups of chiral and achiral nanotori. Irreducible representations and characters of dihedral groups and direct products of groups are well known, but we make a few brief comments here for completeness. Let us recall some facts from representation theory [for details see James & Liebeck (1993)]. Let $D_{2p} = \langle a, b \mid a^p = b^2 = (ab)^2 = 1\rangle$ be the dihedral group of order $2p$. First we determine two-dimensional irreducible representations of D_{2p}. Write $\xi = \exp(2\pi i/p)$. For each integer j with $1 \le j < p/2$, define

$$\mathbf{A}_j = \begin{bmatrix} \xi^j & 0 \\ 0 & \xi^{-j} \end{bmatrix}, \quad \mathbf{B}_j = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{2}$$

It is easy to see that $\mathbf{A}_j^p = \mathbf{B}^2 = \mathbf{I}$ and $\mathbf{B}_j^{-1}\mathbf{A}_j\mathbf{B}_j = \mathbf{A}_j^{-1}$. Thus $\mathbf{A}_j$ and $\mathbf{B}_j$ define a matrix representation of the group D_{2p}. It is

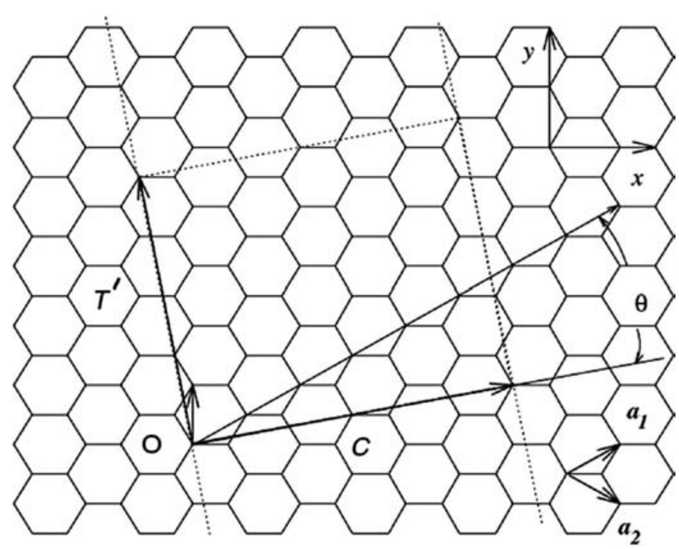

Figure 2
The unrolled honeycomb lattice of a graphite sheet [after Barros *et al.* (2006)]. Here $\mathbf{C} = 4\mathbf{a}_1 + 2\mathbf{a}_2$, $\mathbf{T}' = 4\mathbf{a}_1 - 5\mathbf{a}_2$ and $\theta = \arccos\{5/[2(7)^{1/2}]\}$.

Table 2
Character table of an achiral nanotorus.

$\varepsilon = \exp(\pi i/m)$ and $1 \le r, j \le m-1$.

	1	W^m	W^r	U	WU	σ_v	$W^m\sigma_v$	$W^r\sigma_v$	$U\sigma_v$	$WU\sigma_v$
μ_1	1	1	1	1	1	1	1	1	1	1
μ_2	1	1	1	−1	−1	1	1	1	−1	−1
μ_3	1	$(-1)^m$	$(-1)^r$	1	−1	1	$(-1)^m$	$(-1)^r$	1	−1
μ_4	1	$(-1)^m$	$(-1)^r$	−1	1	1	$(-1)^m$	$(-1)^r$	−1	1
χ_j	2	$2(-1)^j$	$\varepsilon^{jr}+\varepsilon^{-jr}$	0	0	2	$2(-1)^j$	$\varepsilon^{jr}+\varepsilon^{-jr}$	0	0
μ'_1	1	1	1	1	1	−1	−1	−1	−1	−1
μ'_2	1	1	1	−1	−1	−1	−1	−1	1	1
μ'_3	1	$(-1)^m$	$(-1)^r$	1	−1	−1	$-(-1)^m$	$-(-1)^r$	−1	1
μ'_4	1	$(-1)^m$	$(-1)^r$	−1	1	−1	$-(-1)^m$	$-(-1)^r$	1	−1
χ'_j	2	$2(-1)^j$	$\varepsilon^{jr}+\varepsilon^{-jr}$	0	0	−2	$-2(-1)^j$	$-\varepsilon^{jr}-\varepsilon^{-jr}$	0	0

well known from representation theory that if $\boldsymbol{\rho}$ is a complex representation of dimension 2 of a finite group G, such that the matrices $g\boldsymbol{\rho}$ and $h\boldsymbol{\rho}$ for some elements g, h in G do not commute, then $\boldsymbol{\rho}$ is irreducible. Clearly $\mathbf{A}_j$ and $\mathbf{B}_j$ do not commute. Therefore the above representations are irreducible. If i and j are distinct integers with $1 \le i < p/2$ and $1 \le j < p/2$, then $\xi^i \ne \xi^j$ and $\xi^i \ne \xi^{-j}$, so $\mathbf{A}_i$ and $\mathbf{A}_j$ have different eigenvalues. Therefore there is no matrix $\mathbf{T}$ with $\mathbf{A}_i = \mathbf{T}^{-1}\mathbf{A}_j\mathbf{T}$, and so the above representations are not equivalent. Let χ_j be the character of the representation defined by $\mathbf{A}_j$ and $\mathbf{B}_j$.

Now suppose that p is even. It is a well known fact that D_{2p} has exactly $(p/2) + 3$ conjugacy classes

$$\{1\}, \{a^{p/2}\}, \{a, a^{-1}\}, \ldots, \{a^{(p/2)-1}, a^{-(p/2)+1}\},$$
$$\{a^{2j}b \mid 0 \le j \le (p/2)-1\}, \{a^{2j+1}b \mid 0 \le j \le (p/2)-1\}.$$

Using this fact we can find all conjugacy classes of the symmetry groups of chiral and achiral nanotori.

Since D_{2p} has $(p/2) + 3$ conjugacy classes, it has $(p/2) + 3$ irreducible characters. There are $(p/2) - 1$ characters of degree 2, namely $\chi_1, \chi_2, \ldots, \chi_{(p/2)-1}$, and four linear characters, μ_1 [the trivial character, $\mu_1(g) = 1$ for all g], μ_2, μ_3 and μ_4 where

$$\mu_2(g) = \begin{cases} 1 & \text{if } g = a^j \text{ for some } j \\ -1 & \text{if } g = a^j b \text{ for some } j \end{cases}$$

$$\mu_3(g) = \begin{cases} 1 & \text{if } g = 1 \\ (-1)^{p/2} & \text{if } g = a^{p/2} \\ (-1)^j & \text{if } g = a^j \text{ for } 1 \le j \le (p/2)-1 \\ 1 & \text{if } g = a^{2j}b \text{ for some } j \\ -1 & \text{if } g = a^{2j+1}b \text{ for some } j \end{cases}$$

$$\mu_4(g) = \begin{cases} 1 & \text{if } g = 1 \\ (-1)^{p/2} & \text{if } g = a^{p/2} \\ (-1)^j & \text{if } g = a^j \text{ for } 1 \le j \le (p/2)-1 \\ -1 & \text{if } g = a^{2j}b \text{ for some } j \\ 1 & \text{if } g = a^{2j+1}b \text{ for some } j. \end{cases}$$

Now, by Lemma 1 of Damnjanović *et al.* (1999*b*), we can write $q/n = 2k$, where k is an odd integer, and so $mq/n = 2km$, *i.e.* mq/n is an even number. Therefore, by the above observations with $a = W$, $b = U$ and $p = mq/n$, we can find the conjugacy classes, irreducible representations and character tables of the symmetry group of a chiral nanotorus. The character table of the symmetry group of a chiral nanotorus is given in Table 1.

Now if G is a cyclic group of order n generated by g, then the number of its conjugacy classes is n and it has n one-dimensional irreducible representations ρ_{w^j}, $0 \le j \le n-1$, where $\rho_{w^j}(g^k) = w^{jk}$, $0 \le k \le n-1$ and $w = \exp(2\pi i/n)$. Let $G = H \times K$ be a decomposition of the group G. Then every conjugate of an element (h, k) [note that we can write $hk = (h, k)$] is of the form (a, b), where a is a conjugate of h and b is a conjugate of k. Therefore the number of conjugacy classes of G is the product of the number of conjugacy classes of H and the number of conjugacy classes of K. It is also known that every irreducible character of $G = H \times K$ is of the form $\chi \times \mu$, where χ is an irreducible character of H. μ is an irreducible character of K and $(\chi \times \mu)(h, k) = \chi(h)\mu(k)$ for all h in H and k in K.

From the explanations above we can find the conjugacy classes, irreducible representations and character tables of the symmetry group of an achiral nanotorus. The character table of the symmetry group of an achiral nanotorus is given in Table 2.

4. Concluding remarks

A nanotube is a graphene sheet wrapped to form a cylinder. A nanotorus is a nanotube whose ends are connected. Thus, a nanotorus can be classified according to its chiral and translational vectors. Many physical properties of a system can be determined by its symmetry. Since nanotubes can be viewed as quasi-one-dimensional systems, the line-group symmetry approach is suited to the description of the properties of nanotubes (Damnjanović *et al.*, 1999*a*). Line-group symmetry allows two different types of quantum numbers: linear and helical. Both types have been used in the literature (Damnjanović *et al.*, 2002; Barros *et al.*, 2006) for carbon nanotubes. The symmetry and electro-optical properties of nanotubes have been studied before (Damnjanović *et al.*, 2002; Barros *et al.*, 2006). The symmetry properties and the character tables of chiral and achiral single-walled carbon nanotubes were reported by Barros *et al.* (2006). In this paper we have discussed the symmetry groups of chiral and achiral carbon nanotori and the irreducible representations of the groups. The structure of these groups, and hence the irreducible representations *etc.*, is similar to that obtained using the line-group formalism for carbon nanotubes (Damnjanović *et al.*, 1999*a*, 2001, 1999*b*, 2002). This suggests that the group theory developed here could, in principle, be obtained directly from the line group of the nanotubes and *vice versa*. The connection between the two formalisms is evidence that this group-theory analysis is correct.

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