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Phys. Rev. B **84**, 085444 — Published 29 August 2011

DOI: [10.1103/PhysRevB.84.085444](https://doi.org/10.1103/PhysRevB.84.085444)

Isospectral But Physically Distinct: Modular Symmetries and their Implications for Carbon Nanotori

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Recently there has been considerable interest in the properties of carbon nanotori. Such nanotori can be parametrized according to their radii, their chiralities, and the twists that occur upon joining opposite ends of the nanotubes from which they are derived. In this paper, however, we demonstrate that many physically distinct nanotori with wildly different parameters nevertheless share identical band structures, energy spectra, and electrical conductivities. This occurs as a result of certain geometric symmetries known as modular symmetries which are direct consequences of the properties of the compactified graphene sheet. Using these symmetries, we show that there is a dramatic reduction in the number of spectrally distinct carbon nanotori compared with the number of physically distinct carbon nanotori. The existence of these modular symmetries also allows us to demonstrate that many statements in the literature concerning the electronic properties of nanotori are incomplete because they fail to respect the spectral equivalences that follow from these symmetries. We also find that as a result of these modular symmetries, the fraction of spectrally distinct nanotori which are metallic is approximately three times greater than would naively be expected on the basis of standard results in the literature. Finally, we demonstrate that these modular symmetries also extend to cases in which our carbon nanotori enclose non-zero magnetic fluxes.

PACS numbers:

I. INTRODUCTION

Soon after the experimental discovery¹ of carbon nanotubes, it was suggested² that there might also exist carbon *nanotori* — *i.e.*, carbon nanotubes in which the ends of the tube are identified and sewn together. Within a few years, experimental evidence for such structures emerged^{3,4}, and since then they have attracted a great deal of experimental^{5,6} and theoretical^{7–20} attention. There are a variety of reasons for this intense interest. For example, certain species of carbon nanotori exhibit unusual magnetic properties^{7–10}, including persistent magnetic moments at nearly zero flux⁸ and colossal paramagnetic moments⁹. These objects can also display a diverse variety of electric properties: some nanotori are inherently metallic, while others are semiconducting and still others are insulators.

As we shall discuss, the most general nanotorus can be parametrized by four integers (m, n, p, q) . Together and in various combinations, these describe the radius of the underlying nanotube, the chirality of the underlying nanotube, the length of the underlying nanotube, and the relative twist^{11,12} that might occur upon sewing opposite ends of the tube together to form the torus. The important point, however, is that nanotori with different (m, n, p, q) are fundamentally physically distinct: they have different sizes, different shapes, and different twisted “honeycomb” patterns of carbon atoms laid out

on their surfaces. Of course, there are certain symmetries of the underlying graphene sheet which lead to trivial equivalences amongst these nanotori. For example, 60° rotations of the underlying graphene sheet will produce identical nanotori. Such nanotori are therefore not physically distinct.

In this paper, however, we shall demonstrate that there are additional symmetries that relate *physically distinct* nanotori to each other, forcing such nanotori to exhibit identical energy spectra and electrical properties. These so-called “modular” symmetries therefore transcend the traditional hexagonal lattice symmetries of the graphene sheet, and arise solely in the process of compactifying the graphene sheet in order to form the nanotorus. In some sense, the appearance of these modular symmetries is entirely expected, for they result directly from the geometry of the compactification. However, to the best of our knowledge, the significance and consequences of these symmetries have not been fully appreciated thus far in the nanotorus literature.

As we shall demonstrate, these symmetries have a number of profound effects. First, we shall see that use of these symmetries allows us to partition the set of carbon nanotori into distinct equivalence classes as far as their spectral properties are concerned, and leads to a dramatic reduction in the numbers of *spectrally distinct* carbon nanotori as compared with the numbers of *physically distinct* nanotori. Moreover, as we shall show, many of the standard rules of thumb advanced in the literature in order to describe the conductivity properties of these nanotori actually fail to respect these symmetries. Such rules of thumb are therefore incomplete as descriptions of the physics of these nanotori, and must be replaced

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by statements which respect the full symmetry structure of the compactified graphene sheet. Finally, we demonstrate that these symmetries even extend to situations in which the carbon nanotori enclose different types of magnetic flux. They thus should have applicability for many of the fascinating magnetic properties of carbon nanotori, including the possibility of persistent currents.

II. PRELIMINARIES: THE GRAPHENE SHEET, THE CARBON NANOTUBE, AND THE CARBON NANOTORUS

In order to explain the origins of these spectral symmetries, we begin with a brief review which will also serve to highlight our notation and conventions.

In general, the graphene sheet is nothing but a set of carbon atoms arranged on an extended, two-dimensional hexagonal lattice generated by two basis vectors \vec{a}_1 and \vec{a}_2 . We shall choose a Euclidean coordinate system such that $\vec{a}_1 = (1, 0)$ and $\vec{a}_2 = (\frac{1}{2}, -\frac{1}{2}\sqrt{3})$ in units of $\sqrt{3}R_{cc}$, where R_{cc} is the fundamental carbon-carbon bond length. As always, the band structure associated with a given lattice can be described in terms of a dispersion relation $E(\vec{k})$ which relates an electron wavevector \vec{k} to its energy E . For the graphene sheet, and in the tight-binding (or Hückel) approximation in which the only significant overlap integrals are those between the $2p_z$ orbitals associated with nearest-neighbor carbon atoms, this dispersion relation is given by¹³⁻¹⁵

$$E(\vec{k}) = \pm\gamma_0 \left[3 + 2 \cos[\vec{k} \cdot (\vec{a}_1 - \vec{a}_2)] + 2 \cos(\vec{k} \cdot \vec{a}_2) + 2 \cos(\vec{k} \cdot \vec{a}_1) \right]^{1/2}. \quad (1)$$

Here $\gamma_0 \approx 0.266$ eV is the energy-transfer resonance integral between two neighboring $2p_z$ orbitals. A contour plot of this dispersion relation, clearly indicating the band structure within the first Brillouin zone, is shown in Fig. 1.

For the uncompactified graphene sheet, all electron wavevectors \vec{k} are allowed. However, this situation changes when we “roll up” one dimension of the graphene sheet to produce a single-walled carbon nanotube, or equivalently when we identify any two carbon atoms on the graphene sheet whose positions differ by an arbitrary lattice vector $\vec{V}_1 = m\vec{a}_1 + n\vec{a}_2 = (m + \frac{1}{2}n, -\frac{1}{2}\sqrt{3}n)$ with $(m, n) \in \mathbb{Z}$. Imposing the Bloch condition on the electron wavefunctions $\psi(\vec{r})$ in addition to the new periodicity condition $\psi(\vec{r}) = \psi(\vec{r} + \vec{V}_1)$ then restricts $\vec{k} = (k_x, k_y)$ to the set of wavevectors satisfying the condition

$$k_x L_1 \cos \beta + k_y L_1 \sin \beta = 2\pi\ell_1, \quad \ell_1 \in \mathbb{Z}, \quad (2)$$

where $L_1^2 \equiv |\vec{V}_1|^2 = m^2 + mn + n^2$ and $\cos \beta \equiv (m + \frac{1}{2}n)/L_1$. These allowed values of \vec{k} therefore form parallel lines in the (k_x, k_y) plane, and the locations at

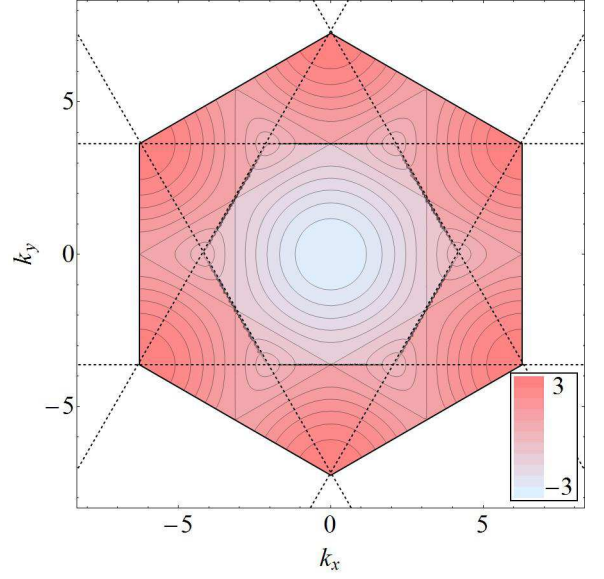


FIG. 1: Contour plot of the rescaled dispersion relation $E(\vec{k})/\gamma_0$ of the infinite graphene sheet for \vec{k} within the first Brillouin zone and expressed in units of $R_{cc}^{-1}/\sqrt{3}$. The dotted lines indicate the lowest-order Bragg “planes”, and the six points with $E = 0$ at which these planes have pairwise intersections constitute the corresponding Fermi “surface”.

which these lines intersect the Bragg planes in Fig. 1 determine whether the corresponding (m, n) nanotube is metallic, semiconducting, or insulating. Nanotubes for which $n = 0$ (i.e., $\beta = 0$) or $m = n$ (i.e., $\beta = \pi/6$) are dubbed “zigzag” or “armchair” respectively; nanotubes with other values of (m, n) are generally referred to as “chiral”. In general, the vector \vec{T} perpendicular to \vec{V}_1 is the tube axis.

We now consider imposing *two* non-parallel identifications on the graphene sheet, as illustrated in Fig. 2. In general, we consider two arbitrary lattice identification

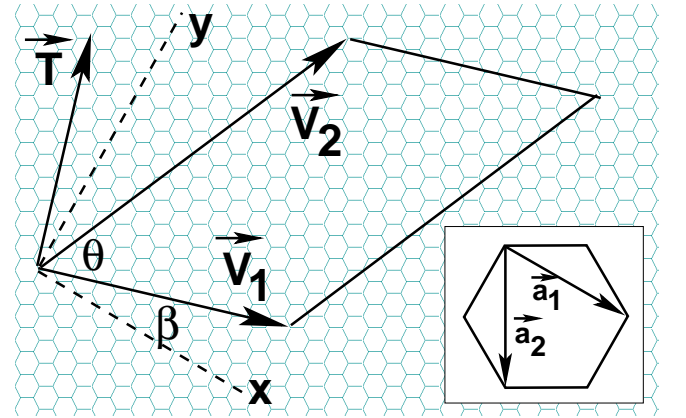


FIG. 2: Coordinate system (x, y) , lattice vectors $\vec{a}_{1,2}$, compactification vectors $\vec{V}_{1,2}$, and tube axis vector \vec{T} on the graphene sheet.

vectors $\vec{V}_1 = m\vec{a}_1 + n\vec{a}_2$ and $\vec{V}_2 = p\vec{a}_1 + q\vec{a}_2$; without loss of generality we shall assume that $-\pi/3 < \beta \leq \pi/3$. We shall also assume without loss of generality that the quantity $N_{\text{hex}} \equiv np - mq$ is positive, or equivalently that the relative angle θ from \vec{V}_1 to \vec{V}_2 lies in the range $0 < \theta < \pi/2$, as illustrated in Fig. 2. Such identifications together result in a so-called (m, n, p, q) nanotorus which may be viewed as a (m, n) nanotube in which opposite ends are joined to each other, potentially with a relative twist angle θ . This description is especially appropriate if $L_2^2 \equiv |\vec{V}_2|^2 = p^2 + pq + q^2 \gg L_1^2$. Note that N_{hex} describes the number of hexagonal cells which tile the surface of the resulting donut, and is equal to precisely half the number of carbon atoms in the nanotorus. Imposing the double periodicity condition $\psi(\vec{r}) = \psi(\vec{r} + \vec{V}_1) = \psi(\vec{r} + \vec{V}_2)$ on the electron wavefunction $\psi(\vec{r})$ in conjunction with the Bloch condition then leads to the constraint in Eq. (2) as well as the additional constraint

$$k_x L_2 \cos \delta + k_y L_2 \sin \delta = 2\pi \ell_2, \quad \ell_2 \in \mathbb{Z}, \quad (3)$$

where $\delta \equiv \theta + \beta$. Solving Eqs. (2) and (3) simultaneously then yields

$$\begin{aligned} k_x &= \frac{2\pi}{L_1 L_2 \sin \theta} [\ell_1 L_2 \sin \delta - \ell_2 L_1 \sin \beta] \\ k_y &= \frac{2\pi}{L_1 L_2 \sin \theta} [-\ell_1 L_2 \cos \delta + \ell_2 L_1 \cos \beta] \end{aligned} \quad (4)$$

or equivalently

$$\begin{aligned} k_x &= \frac{2\pi}{N_{\text{hex}}} [-\ell_1 q + \ell_2 n] \\ k_y &= \frac{2\pi}{\sqrt{3} N_{\text{hex}}} [-\ell_1 (2p + q) + \ell_2 (2m + n)] \end{aligned} \quad (5)$$

Thus, we see that the allowed electron wavevectors now form a two-dimensional grid of points in the (k_x, k_y) plane. Note that there are always exactly N_{hex} allowed wavevectors lying inside the fundamental region bounded by the Bragg planes in Fig. 1, where points lying on a single Bragg plane itself are counted as half and where points lying at the intersections of two Bragg planes are counted as a third.

Whether such nanotori are metallic, semiconducting, or insulating depends on whether these points hit or come particularly close to the intersections of the Bragg planes in Fig. 1. It is found that nanotori in which both $m - n$ and $p - q$ are multiples of three are metallic, with solutions to Eqs. (4) and (5) that lie precisely on the Fermi surface. For practical applications, it proves useful to focus on only those nanotori with $L_2 \gg L_1 \gg R_{cc}$, as this condition allows one to bend the nanotube into a nanotorus without excessive strain or deformation of the underlying graphene sheet (the effects of which would otherwise distort the dispersion relation in Fig. 1, and hence the band structure of the torus). Within this limit, it is then conventional to regard nanotori with $m - n = 0 \pmod{3}$ but $p - q \neq 0 \pmod{3}$ as semiconducting, since the allowed wavevectors come “close” to the Fermi surface in this limit. All other nanotori are then considered insulating.

III. MODULAR SYMMETRIES AND SPECTRAL EQUIVALENCES OF THE CARBON NANOTORUS

All of the above results are completely standard, and are well known in the carbon-nanotorus literature. In particular, tori with different values of (m, n, p, q) are physically distinct: they have entirely different arrangements of hexagons tiling their surfaces, with different values of the physical radii $L_{1,2}$, chiral angle β , and twist angle θ . We shall take this to be our definition of “physically distinct”. There are, of course, certain trivial identifications which relate different nanotori to each other: for example, the (m, n, p, q) torus and the $(m + n, -m, p + q, -p)$ torus are actually identical, since they correspond to (\vec{V}_1, \vec{V}_2) pairs which are related to each other by a uniform 60° rotation. Such trivial identifications reflect the underlying hexagonal lattice symmetries of the graphene sheet from which these nanotori are constructed, and result in identical carbon nanotori with identical patterns of carbon atoms on their surfaces. Such nanotori are therefore not physically distinct.

By contrast, an important question is whether there exist physically *distinct* nanotori (*i.e.*, tori which are *not* related by symmetries of the hexagonal lattice) which nevertheless yield identical grids of allowed wavevectors (k_x, k_y) . If so, we will have found cases of physically distinct tori with different values of $(L_1, L_2, \theta, \beta)$ which are nevertheless spectrally identical. In other words, such tori will have identical energy spectra and electrical conducting properties.

At first sight, it might appear that no such spectral equivalences exist for carbon nanotori. After all, the results in Eq. (4) for carbon nanotori may initially appear to be nothing more than a two-dimensional generalization of the results in Eq. (2) for carbon nanotubes, and no such spectral equivalences exist for carbon nanotubes. However, it is important to realize that this is not true for carbon nanotori. In particular, it turns out that the set of allowed values of (k_x, k_y) in Eq. (5) is actually invariant under two additional symmetry transformations which we shall denote S and T :

$$S: \begin{cases} m \rightarrow -p \\ n \rightarrow -q \\ p \rightarrow m \\ q \rightarrow n \end{cases} \quad T: \begin{cases} m \rightarrow m \\ n \rightarrow n \\ p \rightarrow p + m \\ q \rightarrow q + n \end{cases} \quad (6)$$

Under these transformations, it is straightforward to demonstrate that $N_{\text{hex}} \equiv np - mq$ is invariant, while the physical parameters L_1 , L_2 , θ , and β transform in the following manner:

$$S: \begin{cases} L_1 \rightarrow L_2 \\ L_2 \rightarrow L_1 \\ \theta \rightarrow \pi - \theta \\ \beta \rightarrow \beta + \theta - \pi \end{cases}$$

$$T : \begin{cases} L_1 & \rightarrow L_1 \\ L_2 & \rightarrow \sqrt{L_1^2 + L_2^2 + 2L_1L_2 \cos \theta} \\ \cot \theta & \rightarrow \cot \theta + (L_1/L_2) \csc \theta \\ \beta & \rightarrow \beta \end{cases} \quad (7)$$

It is important to stress that the individual equations in Eqs. (4) and (5) are not invariant under S or T , rather, what is invariant is the *set* of values of (k_x, k_y) to which these equations lead. Moreover, since these sets of solutions for (k_x, k_y) are invariant under S and T individually, they are also invariant under any sequence of S and T transformations. For example, under the $ST^{-1}ST(TS)^2$ transformation we find $(m, n, p, q) \rightarrow (3m - 2p, 3n - 2q, 2m - p, 2n - q)$, and this too is a symmetry of the solutions to Eq. (5).

It then follows from these observations that any two tori whose defining vectors \vec{V}_1 and \vec{V}_2 differ through S and T transformations share the same electronic spectra but are intrinsically different from each other — *i.e.*, that they are isospectral but physically distinct. That they are isospectral follows from the fact that the same set of (k_x, k_y) solutions are selected in each case. By contrast, that they are physically distinct follows from the fact that the fundamental identifications between carbon atoms on the graphene sheet are altered by S and T transformations in a manner that transcends trivial hexagonal lattice symmetries. This is perhaps easiest to see in the case of the T transformation, which corresponds to the action $(\vec{V}_1, \vec{V}_2) \rightarrow (\vec{V}_1, \vec{V}_1 + \vec{V}_2)$. This changes not only L_2 but θ , and thus produces a new torus which has a greater “twist” when the ends of the nanotube are joined.

It may be less obvious that the S transformation also connects physically distinct tori. Indeed, this transformation corresponds to the action $(\vec{V}_1, \vec{V}_2) \rightarrow (-\vec{V}_2, \vec{V}_1)$, and at first glance it might appear that this is merely a trivial relabeling of the two independent periodicities, along with a reflection (sign flip). However, we must remember that the S transformation also changes the associated θ and β angles in non-trivial ways. Alternatively, we can also appreciate the non-trivial nature of S by considering the combination

$$T' \equiv ST^{-1}S^{-1} = TST \quad (8)$$

which corresponds to the action $(\vec{V}_1, \vec{V}_2) \rightarrow (\vec{V}_1 + \vec{V}_2, \vec{V}_2)$. [The second equality in Eq. (8) follows as a result of the identity $(ST)^3 = -\mathbf{1}$, or equivalently $(T^{-1}T')^3 = -\mathbf{1}$.] Note that T' is in some sense “dual” to T : each performs a full twist around a different cycle of the torus. In other words, as illustrated in Fig. 3, while T corresponds to cutting through one side of the torus and re-attaching the two edges along with a twist, T' corresponds to cutting the torus in half like a bagel and then twisting each half relative to the other before re-attaching. Thus, T' results in a physically distinct torus, just as T does, and furthermore these resulting tori are not related to each other through hexagonal lattice symmetries. It then follows from Eq. (8) that S also cannot correspond to a

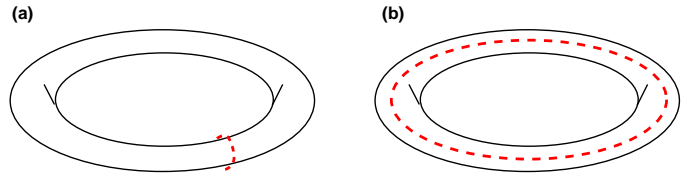


FIG. 3: Sketch of (a) the T transformation, and (b) the T' transformation, as actions on the carbon nanotorus. In each case, one should imagine affixing the carbon atoms to the surface of the torus, then cutting the torus along the dashed (red) line (thereby breaking those carbon/carbon bonds which cross this line), twisting one half of the torus by a full 2π rotation relative to the other half, and then reattaching these bonds to reconstruct a new nanotorus. The original and final nanotori will be related by the T or T' modular transformations respectively, while much more complex spectral equivalences can be generated through combinations of these two fundamental operations.

lattice symmetry — *i.e.*, S must connect physically distinct tori as well. Indeed, S and T' are interchangeable in the sense that the two generators of the modular group can be considered to be either $\{S, T\}$ or $\{T, T'\}$.

Note that if we define the complex quantity $\tau \equiv (L_2/L_1)e^{i\theta}$, then the S and T transformations correspond to $\tau \rightarrow -1/\tau$ and $\tau \rightarrow \tau + 1$ respectively. Together, these transformations generate the so-called “modular group”, which is one of the primordial symmetries associated with toroidal compactifications. In general, any transformation which takes the form $\tau \rightarrow (a\tau + b)/(c\tau + d)$ where $a, b, c, d \in \mathbb{Z}$ and $ad - bc = 1$ is a modular transformation. What we have shown, then, is that any two carbon nanotori whose defining parameters are related by a modular transformation are spectrally identical even though they are physically distinct. In other words, any transformation which can be generated through repeated actions of the S and T generators leads to a spectral equivalence between physically distinct tori.

It is important to emphasize that the appearance of these modular symmetries is not a total surprise. Modular symmetries often arise in the presence of toroidal compactifications, and are a direct consequence of the underlying geometry of the carbon nanotorus. Indeed, the zone-folding of a macroscopic lattice necessarily introduces periodic equivalences of the sort discussed here, and in the case of two dimensions with non-parallel identifications, such periodicities generically lead to modular symmetries. In other words, the underlying toroidal graph is not altered by modular symmetries, and thus the adjacencies of the graph (and the isospectrality which results) are preserved intact. However, when applied to the case of carbon nanotori, these symmetries are *physical*, in the sense that the nanotori they relate are isospectral but physically distinct. As we shall see, this is particularly significant, allowing these symmetries to have profound effects on the physics of these nanotorus systems and in particular on the range of behaviors they may exhibit.

In a sense, these modular symmetries can be viewed

as a generalization of a similar set of symmetries that emerge for Möbius graphs. To see this, let us imagine taking a long strip of hexagons and gluing opposite ends of this strip together with an arbitrary number of half-twists. At first glance, one might suspect that the resulting spectrum should depend on the actual number of half-twists. However, it turns out that the resulting spectrum depends only on whether this number is even or odd²¹. This Möbius case is, of course, a relatively trivial example of this phenomenon, since it deals with only a single possible kind of twist corresponding to the single periodicity that defines the Möbius strip. Indeed, for the case of carbon nanotori, our point is that there exists a whole *group* of transformations — the modular group — which is built upon the actions of *two* non-commuting underlying generators (S and T) which can be combined and performed in a variety of inequivalent ways. This leads to “sewing” and “gluing” configurations on the torus which are much more complex than on the Möbius strip, and which require greater mathematical machinery to study — and this in turn leads to distinctions between the notions of “physically distinct” and “spectrally distinct” which are even more pronounced than in the Möbius case. However, even the relatively simple Möbius case illustrates one of our basic themes: there can be lots of physically distinct twisted hexagon strips, yet very few of them are spectrally distinct. It is the preservation of the underlying graph in each case which makes this possible.

As a result of these modular symmetries, we can henceforth establish an unambiguous convention for uniquely describing the spectral properties of a given carbon nanotorus: we calculate its complex parameter τ as defined above, and then use a sequence of S and T modular transformations as needed in order to bring τ into a special region of the complex τ -plane known as the “fundamental domain” \mathcal{F} defined by

$$\mathcal{F} \equiv \{ \tau : -\frac{1}{2} < \tau_1 \leq \frac{1}{2}, \tau_2 > 0, |\tau| \geq 1 \} \quad (9)$$

where $\tau_1 \equiv \text{Re } \tau$ and $\tau_2 \equiv \text{Im } \tau$. Note that the condition $N_{\text{hex}} \equiv np - mq > 0$ already ensures that $\tau_2 > 0$. We can then use the underlying symmetries of the hexagonal graphene lattice in order to bring the resulting angle β into the range $0 \leq \beta < \pi/3$. Note that this convention is tantamount to describing the spectrum of a given carbon nanotorus in terms of that spectrally equivalent nanotorus which is as close to being rectangular as possible. Following this procedure therefore provides an unambiguous test of whether any two physically distinct carbon nanotori in fact have the same spectral properties.

IV. PHYSICAL IMPLICATIONS

The existence of these modular symmetries and the spectral equivalences they induce has profound implications for the physics of carbon nanotori. Indeed, as

we shall see, the use of these modular symmetries will sharpen our ability to classify nanotori on the basis of those physical properties (such as their metallicities, *etc.*) which ultimately stem from their band structures. Furthermore, use of these modular symmetries can even provide *statistical* insights into the properties of randomly produced carbon nanotori — insights which may ultimately have practical consequences for the manufacture of such objects in environments in which their resulting properties often cannot be controlled or engineered in advance.

As discussed above, the first and most direct implication of these modular symmetries is that there exist physically distinct nanotori — often with markedly different radii and chiral angles — which nevertheless possess identical energy spectra and conductivity properties. As an example of this phenomenon, let us consider the $(3, 2, 24, 10)$, $(7, 3, -22, -12)$, and $(8, 6, -25, -21)$ carbon nanotori. Clearly, we see that these nanotori are physically distinct and are characterized by different sets of cycle lengths $L_{1,2}$, different chiral angles β , and different twist angles θ . As a result, these three tori have entirely different patterns of carbon atoms tiling their surfaces. Yet, the latter two nanotori are in fact related to each another by S and T transformations, and consequently they each yield the same spectrum of allowed \vec{k} vectors shown in Fig. 4. Similarly the first nanotorus is related to the second two through not only S and T transformations, but also trivial 60° rotations of the underlying graphene sheet. Thus, these tori all share identical spectra, and according to the convention specified above, we can describe this spectrum uniquely as having $N_{\text{hex}} = 18$, $\tau = (2 + 9\sqrt{3}i)/13$, and $\tan \beta = \sqrt{3}/7$.

Second, as a corollary to this observation, we also learn that the usual notions of “zigzag” and “armchair” — notions which are critical for describing the chirality and metallicity of carbon nanotubes — no longer hold as special indicators of the spectral properties of corresponding carbon nanotori. In other words, nanotori built from zigzag or armchair nanotubes might have spectral properties which are identical to those of nanotori built from non-zigzag or non-armchair nanotubes; moreover, these spectral properties might or might not correspond to the special zigzag or armchair angles $\beta = 0, \pi/6$. As an example, the $(6, 0, -17, -6)$ nanotorus is built from a zigzag nanotube while the $(9, 9, -40, -44)$ nanotorus is built from an armchair nanotube and the $(3, 15, 13, 53)$ and $(4, 8, 21, 33)$ nanotori are built from chiral nanotubes with different chiralities. Yet all four nanotori have identical spectral properties which are the same as those of a chiral nanotorus with $N_{\text{hex}} = 36$, $\tau = 12(1 + \frac{3}{2}\sqrt{3}i)/31$, and $\tan \beta = 5\sqrt{3}/7$ (or $\beta \approx 51.05^\circ$). Indeed, using the mathematical results of Ref.¹⁶, we can show that any carbon nanotorus is spectrally equivalent to one built from a zigzag carbon nanotube.

Conversely, a carbon nanotorus can have a spectrum which exhibits a zigzag or armchair property that is lacking in the original nanotube from which it is constructed.

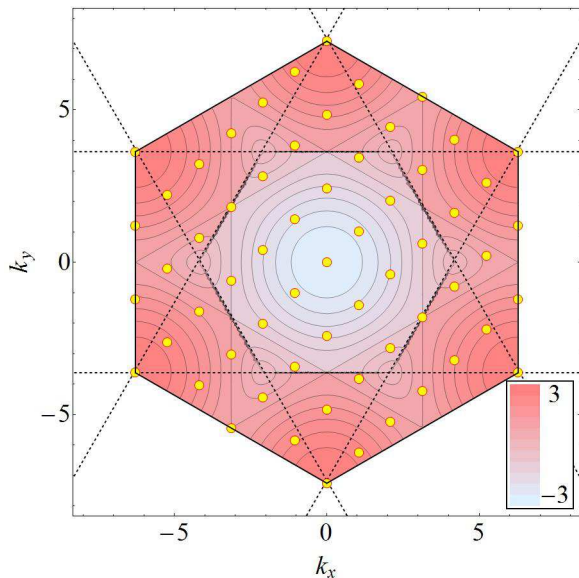


FIG. 4: A plot of the energy spectrum common to the $(3, 2, 24, 10)$, $(7, 3, -22, -12)$, and $(8, 6, -25, -21)$ carbon nanotori, with allowed wavevectors indicated by (yellow) dots superimposed over the energy contours in Fig. 1. Note that these nanotori are not metallic, as none of the allowed wavevectors coincide with any of the six points which constitute the Fermi “surface”.

As an example, the $(9, 0, -25, -4)$ nanotorus is built from a zigzag nanotube and the $(4, 7, -12, -30)$ nanotorus is built from a chiral nanotube. Yet both nanotori have the spectral properties of an armchair nanotorus, with $N_{\text{hex}} = 36$, $\tau = 3\sqrt{3}/2i$, and $\beta = \pi/6$. Likewise, the $(9, 9, -27, -31)$ nanotorus is built from an armchair nanotube and the $(3, 6, -11, -34)$ nanotorus is built from a chiral nanotube. Yet both nanotori have the spectral properties of a zigzag nanotorus, with $N_{\text{hex}} = 36$, $\tau = (3 + 9\sqrt{3}i)/8$, and $\beta = 0$.

Third, it turns out that not every possible spectral signature $(N_{\text{hex}}, \tau, \beta)$ can be realized, even in principle. Instead, these three quantities experience internal constraints and correlations which ultimately reflect the fixed hexagonal lattice structure of the underlying graphene sheet and which require that any allowed spectral signature $(N_{\text{hex}}, \tau, \beta)$ originate from four real integers (m, n, p, q) . These correlations amongst $(N_{\text{hex}}, \tau, \beta)$ can take a variety of different forms. For example, for odd values of N_{hex} , it turns out that there exist no self-consistent spectral signatures with purely imaginary values of τ . Similarly, for $N_{\text{hex}} = 24$, there are solutions with $\text{Re } \tau \in \{\pm 1/2, \pm 1/3, \pm 1/4, \pm 1/7\}$, but no other inverse integers; likewise, all of these except for $\text{Re } \tau = 1/7$ have $\beta = 0$. In fact, these internal constraints amongst the four real parameters embodied in $(N_{\text{hex}}, \tau, \beta)$ are sufficiently strong that they effectively eliminate one real degree of freedom from within this parametrization. In other words, although four real degrees of freedom are required in order to parametrize a given physically distinct

nanotorus, only three real degrees of freedom are required in order to uniquely describe its spectral properties¹⁶.

It is easy to understand why such constraints arise. Ordinarily, as a question of topology, tori can exist with all shapes and volumes, for there are literally an infinite number of ways in which we can construct a torus by rolling up an unmarked sheet of paper. However, in the case of carbon nanotori, our original “sheet of paper” is not unmarked: it is actually a graphene sheet of carbon atoms which has its own hexagonal lattice structure. The existence of such a lattice structure has a number of critical consequences: it forces our toroidal defining vectors \vec{V}_1 to \vec{V}_2 to be *lattice vectors*; it restricts the resulting possible combinations of N_{hex} and τ to those values consistent with the periodicity of the lattice; and it breaks the rotational symmetry of our original uncompactified two-dimensional sheet and necessitates the introduction of a new measurable parameter, the angle β defined in Fig. 2, which describes the orientation of the torus relative to the underlying lattice. Conversely, the presence of the hexagonal lattice gives a clear meaning to the twist angle θ . This quantity would have had no meaning when rolling up an unmarked sheet of paper.

Fourth, it is clear that the existence of spectral equivalences between different nanotori implies that the number of *spectrally* distinct nanotori in any set will necessarily be smaller than the number of *physically* distinct nanotori in that set. However, it turns out that the magnitude of this truncation can easily become quite staggering. As an example, let us consider the set of physically distinct (m, n, p, q) nanotori with fixed $N_{\text{hex}} = np - mq = 18$ which can be formed from integers in the range $|m|, |n|, |p|, |q| \leq \Lambda$ for some cutoff Λ . For concreteness, we shall take $\Lambda = 100$. In order to count only physically distinct nanotori, we shall require that (m, n) be chosen such that $-\pi/3 < \beta \leq \pi/3$. We shall also require, as a rough measure of their physical consistency in three-dimensional space, that each such nanotorus have an outer circumference L_2 which is at least triple its inner cross-sectional circumference L_1 ; note that other similar mathematical conditions may alternatively be imposed, but the qualitative results to follow are essentially unchanged. Given these constraints, we then find through direct enumeration that there are exactly 12 205 physically distinct carbon nanotori which have $N_{\text{hex}} = 18$. Yet, as a result of these spectral equivalences, it turns out that these 12 205 physically distinct carbon nanotori give rise to only 14 distinct energy spectra! These distinct energy spectra are listed in Table I, along with a representative carbon nanotorus in each class.

This is clearly a major truncation. Even with the relatively small value $N_{\text{hex}} = 18$ and relatively small cutoff $\Lambda = 100$, each spectral signature listed in Table I is shared by literally hundreds or thousands of physically distinct carbon nanotori.

Fifth, it is also worth noting that this truncation does not treat metallic and non-metallic nanotori equally. In general, a given (m, n, p, q) carbon nanotorus will be

τ_1	τ_2	$\tan \beta$	metal?	sample (m, n, p, q)
0	$\sqrt{3}$	0	yes	(12, 15, 42, 51)
0	$3\sqrt{3}$	$\sqrt{3}/3$	yes	(10, 13, -34, -46)
0	$9\sqrt{3}$	0	no	(10, 8, -39, -33)
0	$9\sqrt{3}$	$\sqrt{3}/27$	no	(19, 17, -66, -60)
$1/3$	$\sqrt{3}$	0	no	(10, -6, -33, 18)
$-1/3$	$\sqrt{3}$	0	no	(10, -4, 33, -15)
$1/4$	$3\sqrt{3}/4$	$\sqrt{3}/3$	yes	(10, 16, -32, -53)
$-1/4$	$3\sqrt{3}/4$	$\sqrt{3}/3$	yes	(10, 1, -32, -5)
$1/4$	$9\sqrt{3}/4$	0	no	(10, -1, 32, -5)
$-1/4$	$9\sqrt{3}/4$	0	no	(10, 18, -34, -63)
$3/7$	$9\sqrt{3}/7$	$\sqrt{3}/2$	no	(10, 14, 32, 43)
$-3/7$	$9\sqrt{3}/7$	$\sqrt{3}/5$	no	(10, 12, 34, 39)
$2/13$	$9\sqrt{3}/13$	$\sqrt{3}/7$	no	(10, 11, -32, -37)
$-2/13$	$9\sqrt{3}/13$	$3\sqrt{3}/5$	no	(10, 14, -33, -48)

TABLE I: For $N_{\text{hex}} = 18$ and $\Lambda = 100$, there are 12 055 physically distinct carbon nanotori (m, n, p, q) with $L_2 > 3L_1$. However, these exhibit only 14 spectrally distinct energy spectra and band structures, and only four of these correspond to metals. These 14 spectrally distinct values of $\tau \equiv \tau_1 + i\tau_2 = |\tau|e^{i\theta}$ and β are listed above, along with a sample (m, n, p, q) nanotorus in each class.

metallic if at least one of its allowed wavevectors \vec{k} lies on the Fermi surface, or in this case on one of the six points at which two Bragg planes intersect. As is well known, this occurs only when the differences $m - n$ and $p - q$ are each a multiple of three. This implies that in any large set of physically distinct carbon nanotori, approximately one-ninth of the nanotori should be metallic. However, we see from Table I that four out of the fourteen possible distinct spectral signatures are metallic. This is almost triple what would have been expected, implying that the fraction of spectrally distinct nanotori which are metallic is nearly triple the fraction of physically distinct nanotori which are metallic. In other words, the truncation from the four-parameter space of physically distinct nanotori to the three-parameter space of spectrally distinct nanotori is remarkably sensitive to the metallicity of the nanotori in question.

One might argue that both of these effects — the huge truncation in the number of distinct spectral signatures and the relative abundance of those which are metallic — merely reflect the fact that we restricted our integers (m, n, p, q) to lie within a fixed range bounded by $\pm\Lambda$, or that we took a relatively small value of N_{hex} . However, it is easy to demonstrate that the second of these effects is relatively insensitive to the choice of Λ , and that the first of these effects only becomes even more dramatic as Λ is increased. For example, if we restrict our attention to carbon nanotori with $N_{\text{hex}} = 36$, we find that the number of physically distinct nanotori and the number of spectrally distinct nanotori both rise as a function of Λ .

However, we see from Fig. 5 (left panel) that the number of physically distinct nanotori with fixed N_{hex} grows as Λ^2 , as expected, while the number of spectrally distinct nanotori quickly hits a plateau (right panel) which remains flat for an increasingly long interval in Λ before a new, hitherto-unrealizable spectral signature becomes possible and a new plateau develops. [This growth in the number of physically distinct nanotori as a function of Λ can easily be deduced from the observation that the number of quadruplets of integers (m, n, p, q) grows as Λ^4 , while the corresponding number of attainable values of $N_{\text{hex}} = np - mq$ grows as Λ^2 .] As a result, the number of physically distinct nanotori quickly outpaces the number of spectrally distinct nanotori. Moreover, we see from Fig. 5 that the number of distinct metallic spectral signatures remains roughly one third (and not one ninth) the total number of distinct spectral signatures.

We may also consider how these results vary with the choice of N_{hex} . This is shown in Fig. 6 where, as functions of N_{hex} and for $\Lambda = 100$, we have plotted the number of spectrally distinct carbon nanotori as well as the number of those spectrally distinct carbon nanotori which are metallic. It is clear from these results that the numbers of spectrally distinct nanotori remain relatively small, even though they rise with N_{hex} , as expected.

It is also easy to understand the jagged, oscillating nature of the results in Fig. 6. Nanotori must have $N_{\text{hex}} \in 3\mathbb{Z}$ in order to be metallic, while they must have $N_{\text{hex}} \in 2\mathbb{Z}$ if they are rectangular, with $\theta = \pi/2$. Thus, one difference between tori with $N_{\text{hex}} \in 6\mathbb{Z}$ and those with $N_{\text{hex}} \notin 6\mathbb{Z}$ is the existence of additional non-rectangular carbon nanotori with $\theta \neq \pi/2$. However, it must also be borne in mind that a random selection of four integers (m, n, p, q) is $5/3$ times more likely to result in an even value for $N_{\text{hex}} = np - mq$ than an odd one. As we see from Fig. 6, the combined effect from these two features is fairly significant.

Finally, another important implication of these spectral equivalences between physically distinct carbon nanotori concerns the traditional rules of thumb which allow us to determine whether a given carbon nanotorus is metallic, semiconducting, or insulating. Throughout the existing literature on this topic, one finds what we shall call the “rule of three”: a given (m, n, p, q) carbon nanotorus with $L_2 \gg L_1 \gg 1$ will be metallic if both $m - n$ and $p - q$ are multiples of three, semiconducting if $m - n$ is multiple of three while $p - q$ is not, and insulating in all other cases. It is, of course, easy to verify that this characterization of a metallic nanotorus is modular invariant. Specifically, if a given nanotorus has (m, n, p, q) parameters which are metallic according to the rule of three, then all other nanotori to which it is spectrally equivalent will also have parameters which are metallic according to the rule of three. In other words, if $m - n$ and $p - q$ are both multiples of three, modular transformations of these parameters will not disturb this property.

By contrast, the rule-of-three definition of semiconduc-

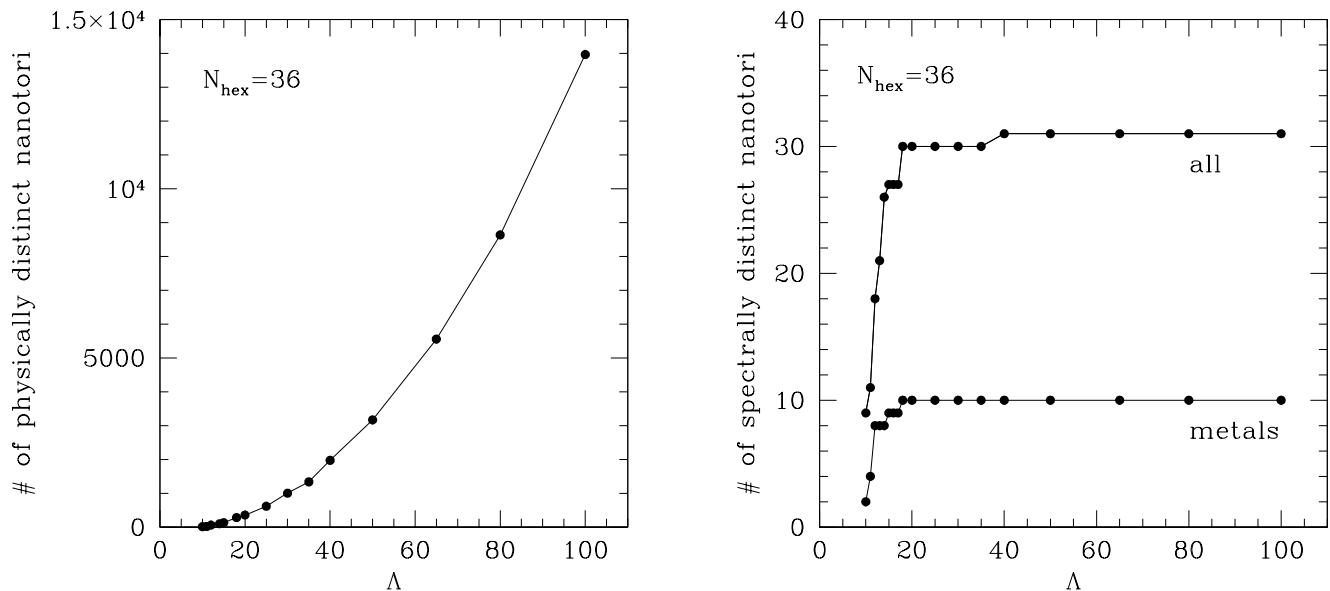


FIG. 5: Dramatic reduction in the number of *spectrally* distinct carbon nanotori (right panel) compared with the number of *physically* distinct carbon nanotori (left panel). This illustrates the ubiquity and power of spectral equivalences amongst arbitrary sets of allowed nanotori. Also shown (right panel) is the number of spectrally distinct nanotori which are metallic, indicating that metallic properties appear approximately three times more frequently amongst *spectrally* distinct nanotori than amongst *physically* distinct nanotori.

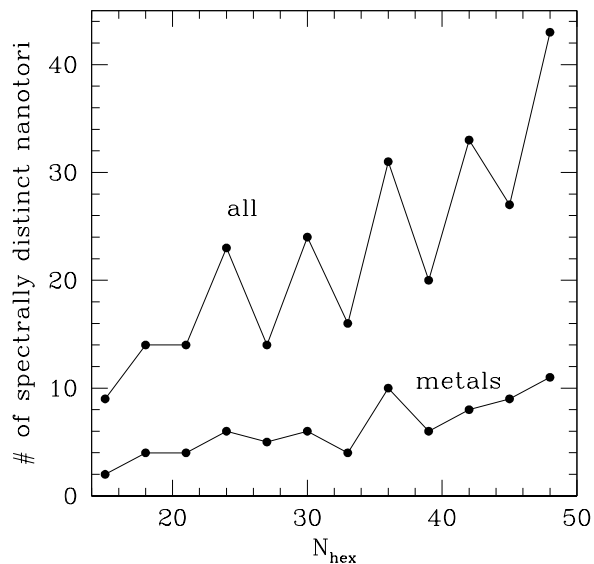


FIG. 6: The numbers of spectrally distinct carbon nanotori (upper curve) and metallic spectrally distinct carbon nanotori (lower curve), plotted as functions of $N_{\text{hex}} \in 3\mathbb{Z}$ for $\Lambda = 100$. Both numbers remain relatively small. The “oscillating” nature of these plots reflects in part the importance of the twist angle θ , since only non-rectangular tori can exist when N_{hex} is odd.

tors is *not* modular invariant — even when we preserve the condition that $L_2 \gg L_1$. As a graphic illustration of this point, consider the $(3, 0, 20, 21)$ torus. Note that indeed $L_2 \gg L_1$ for this torus. According to the standard rule of three, such a torus can be identified as a semi-conductor because $m - n$ is a multiple of three. By contrast, let us now consider the $(23, 21, 2320, 2121)$ nanotorus. This torus also clearly has $L_2 \gg L_1$. However, because $m - n$ is not a multiple of three, we would expect this nanotorus to be an insulator. Indeed, the rule of three tells us to expect this even though our first impression might be that the second nanotorus has larger radii in both directions, and therefore might have energy levels which are more closely spaced.

However, even though these tori have very different physical parameters, it turns out that they are related through modular transformations and therefore have identical energy spectra. They therefore also have identical metallicity properties. This provides a graphic illustration that as a mathematical statement, the standard “rule of three” fails to characterize the conductivity properties of such nanotori because it is inconsistent with the modular transformations which reflect the additional symmetries of the compactified graphene sheet. In other words, the standard definition for a semiconducting carbon nanotorus fails to be modular invariant, and thus cannot be complete as a description of the underlying conductivity properties of the nanotorus. This is yet another consequence of the fact that modular invariance in this context is an actual physical symmetry relating the

spectra of physically distinct nanostructures.

We close this section with an important comment. Throughout this section, our goal has been to illustrate various mathematical ramifications of the modular symmetries which govern the spectra of different carbon nanotori. The specific examples we have provided throughout this section were therefore chosen for their mathematical simplicity as opposed to their phenomenological practicality. For example, we restricted our attention in this section to nanotori with relatively small values of N_{hex} , while realistic carbon nanotori can be expected to have $N_{\text{hex}} \approx \mathcal{O}(10^2 - 10^3)$. Likewise, realistic carbon nanotori will generally be quite long and thin, with quantities such as $L_2 \sin \theta$ exceeding L_1 by an order of magnitude or more. However, all of the conclusions we have drawn in this section continue to hold even when more realistic tori are considered. As an example, let us restrict our attention to carbon nanotori with $N_{\text{hex}} = 600$ for which $L_2 \sin \theta \geq 10L_1$. The latter condition guarantees that our nanotorus remains relatively long and thin even if there are multiple windings of the hexagonal carbon lattice around the tube axis of the torus. Taking $\Lambda = 400$, we find there are 15 027 physically distinct nanotori which satisfy these conditions, but only 52 of these are spectrally distinct. Furthermore, of these 52 spectral equivalence classes, 14 correspond to metals. We see, then, that even for realistic nanotori, our modular symmetries continue to lead to large classes of spectrally equivalent nanotori and a relative overabundance of classes which are metallic. Indeed, in the limit $\Lambda \rightarrow \infty$, it is straightforward to show that the number of physically distinct carbon nanotori in each spectral equivalence class also grows to infinity.

V. MODULAR INVARIANCE AND MAGNETIC FLUXES

With an eye towards potential implications of modular symmetries for the magnetic phenomena associated with twisted carbon nanotori^{12,17}, we now consider the introduction of magnetic fluxes. For full generality, we consider the possibility of *two* distinct fluxes: one which travels all the way around (and through) the length of the nanotube which forms the torus; and another, namely the usual Aharonov-Bohm flux, which pierces the plane of the nanotorus, coming up through the donut hole. We shall denote these fluxes ϕ_1 and ϕ_T respectively, as their associated vector potentials \vec{A}_1 and \vec{A}_T lie parallel to the vectors \vec{V}_1 and \vec{T} in Fig. 2, respectively. As is typical for such systems, we then find that we can incorporate the effects of these fluxes by keeping our previous band-structure energy function $E(\vec{k})$ in Eq. (1) unchanged, and simply modifying our constraint equations for (k_x, k_y) in Eqs. (2) and (4) so that the integers ℓ_i are shifted ac-

cording to

$$\ell_i \rightarrow \ell_i + \frac{\phi_i}{\phi_0} \quad (10)$$

where ϕ_0 is the flux quantum and where

$$\phi_2 \equiv \phi_T + \tau_1 \phi_1. \quad (11)$$

Note that it is the possible existence of a non-trivial twist angle θ which is responsible for the distinction between ϕ_2 and ϕ_T . We then find that the resulting system continues to exhibit a spectral equivalence under the modular transformations in Eqs. (6) and (7) as long as we allow (ϕ_1, ϕ_T) to remain invariant under the T transformation and to mix with each other under the S transformation:

$$S: \begin{pmatrix} \phi_1 \\ \phi_T \end{pmatrix} \rightarrow \begin{pmatrix} \phi'_1 \\ \phi'_T \end{pmatrix} \equiv \begin{pmatrix} -\tau_1 & -1 \\ \tau_2^2/|\tau|^2 & -\tau_1/|\tau|^2 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_T \end{pmatrix}. \quad (12)$$

Thus, a carbon nanotorus parametrized by $(m, n, p, q, \phi_1, \phi_T)$ will have the same spectral properties as one parametrized by $(m', n', p', q', \phi'_1, \phi'_T)$, where these two sets of parameters are related through the modular transformations discussed above.

VI. DISCUSSION

In this paper, we have highlighted and investigated the implications of a geometric symmetry — modular invariance — which emerges upon the compactification of a graphene sheet to form a carbon nanotorus. Although not traditionally considered in the carbon-nanotorus literature, modular invariance plays a critical role in describing the spectral properties of these nanotori and leads to spectral equivalences between physically distinct nanotori. As we have shown, this has profound implications for the classification of carbon nanotori, indicating that large numbers of seemingly unrelated nanotori are in fact completely identical in terms of their spectral properties. Along the way, we also showed that the traditional “rule of three” classification rubric is incomplete, as it is based on quantities which do not respect these spectral equivalences. We also found that the fraction of spectrally distinct carbon nanotori which are metals is approximately three times greater than would naively be expected on the basis of standard results in the literature. Finally, we also showed that these spectral equivalences can easily be extended to cases in which non-trivial magnetic fluxes are present.

The existence of these spectral symmetries also provides a deeper theoretical underpinning to certain results which already exist in the literature. For example, it is well known that many carbon nanotori exhibit persistent currents in the presence of a non-zero magnetic flux ϕ . As functions of ϕ/ϕ_0 , these currents typically follow complicated “sawtooth” patterns which have a natural periodicity under shifts $\phi \rightarrow \phi + \phi_0$. It has

also separately been observed (see, *e.g.*, Ref.¹⁷) that any such sawtooth pattern is preserved but shifted horizontally upon the introduction of a nanotorus twist in which $\vec{V}_2 \rightarrow \vec{V}_2' \equiv \vec{V}_2 + f\vec{V}_1$, where f is chosen such that \vec{V}_2' is also a lattice vector. Indeed, when $f \in \mathbb{Z}$, the magnitude of this horizontal shift exactly matches the periodicity of the sawtooth pattern and the net result is unchanged.

Remarkably, this coincidence is now easy to understand from the point of view of modular transformations: when $f \in \mathbb{Z}$, the mapping from $\vec{V}_2 \rightarrow \vec{V}_2'$ is nothing but the T modular transformation, and as we have shown, modular transformations preserve the electrical properties of the torus, including its persistent currents. We thus see that the periodicity of the sawtooth pattern for persistent currents under shifts $\phi \rightarrow \phi + \phi_0$ — a periodicity which can be understood on elementary grounds having nothing to do with modular transformations — can now also be interpreted as a spectral equivalence under the T modular transformation. Moreover, we now see that this is merely the tip of the iceberg, and that these sorts of spectral equivalences actually have a richer structure and context that not only corresponds to the entire modular group but also transcends the specific example of persistent currents.

As we have discussed above, the traditional “rule of three” is not formulated in a modular-invariant way and is therefore incomplete as a description of the electronic properties of carbon nanotori. However, the full implications of these modular symmetries are significantly broader than just the rule of three: no theoretical result concerning the electronic properties of carbon nanotori can be correct unless it respects these modular symmetries. In other words, no calculation of any electronic property of a given carbon nanotorus in terms of its fundamental defining parameters (m, n, p, q) can be correct unless it yields a result which is invariant under the modular transformations in Eq. (6). In this respect, modular invariance functions for carbon nanotori in much the same way as gauge invariance functions for electromagnetic systems: no theoretical result can be correct unless it can be phrased in terms of quantities which are invariant under the symmetry in question. Of course, at a mathematical level, both modular invariance and gauge invariance rest on relatively simple algebraic identities. However, they both provide powerful organizing principles, and have significant physical manifestations and implications for the symmetry structures of the systems in which they appear.

Needless to say, several additional comments are in order. First, it should be noted that in this paper we have focused on what might be called the “ideal” nanotorus. In particular, we have not accounted for the fact that the actual physical construction of such a torus in three-dimensional space requires that we introduce both an intrinsic and extrinsic curvature onto our otherwise flat graphene sheet. In this sense, the construction of a carbon nanotorus is different from that of a carbon nanotube (in which only the extrinsic curvature is non-vanishing).

The introduction of intrinsic curvature requires that we subject our underlying graphene sheet to considerable strain, deforming not only the positions of carbon atoms but also their relative spacings. These effects have been addressed by a number of authors, using a variety of different techniques¹⁸.

That said, these spectral equivalences should continue to hold, even in the presence of such deformations. There are several reasons for this. First, in the limit $L_1, L_2 \gg R_{cc}$, all effects due to these deformations will be suppressed. However, this is precisely the limit in which nanotori can be constructed from purely hexagonal graphene sheets without the introduction of curvature-inducing pentagonal or heptagonal carbon rings. Second, it can be shown that even when such strain is present, maximum toroidal stability occurs when this strain is uniformly distributed along the nanotorus¹⁹, and this is precisely the situation in which the techniques of Ref.¹⁴ can be used in order to mathematically rewrite the effects of such strain as arising due to a fictitious magnetic flux. As we have seen, the spectral equivalences we have found continue to exist even when such fluxes are introduced. But most importantly, while *any* deformations of the underlying graphene sheet can be expected to have effects on the corresponding band-structure energy function $E(\vec{k})$ shown in Fig. 1, such deformations will not disturb the symmetries inherent in the constraint equations for $\vec{k} = (k_x, k_y)$ derived in Eqs. (2) and (3). Indeed, these equations reflect nothing more than the effects of toroidal compactification, and their structure leads directly to the modular symmetries inherent in Eqs. (4) and (5). Thus, since these spectral equivalences ultimately stem from these symmetry properties, we are assured that any two tori related by modular transformations will sample the same set of wavevectors \vec{k} . Such tori will therefore continue to be spectrally identical regardless of the function $E(\vec{k})$, provided the deformations to $E(\vec{k})$ for the two tori are themselves identical. Moreover, as we have argued above, even in cases where these deformations are not identical, they can at most differ by terms which are suppressed by factors of the presumably large nanotori radii. Such differences can therefore be safely neglected.

A similar conclusion also holds for thermal effects. It might seem, at first glance, that thermal effects could also destroy the spectral equivalences, since they too can have a dramatic effect on the band structure of the underlying graphene sheet²⁰. However, as noted above, these spectral equivalences are a consequence of the geometric symmetries that arise upon *compactifying* this sheet; they are largely independent of the symmetries of the sheet itself. Indeed, these modular symmetries exist for *any* choices of identification vectors \vec{V}_1 and \vec{V}_2 , even if those vectors are altered by other effects. Therefore, as long as the temperature is sufficiently low that the electron coherence length exceeds both the inner and outer toroidal circumferences, the spectral equivalences we have been discussing should remain intact up to terms suppressed by the large nanotori radii.

These comments notwithstanding, it still remains true that not all such nanotori are equally likely to appear in nature. In particular, those nanotori whose constructions implicitly involve large numbers of twists are likely to be rather difficult to construct or stabilize, as the carbon atoms that constitute the underlying graphene sheet are likely to experience significant strain, leading to major deformations of the underlying carbon bond lengths and angles away from their ideal values. This is especially relevant, given that our statistical discussions in Sect. IV implicitly assume that each of the relevant (m, n, p, q) nanotori can appear with equal probability.

At a mathematical level, it is difficult to draw a firm boundary between those carbon nanotori which are realizable in nature as *bona-fide* molecules and those which are not. However, in this paper we have restricted ourselves to statistical examinations of only those nanotori which already obey certain critical constraints. For example, we have limited ourselves to nanotori in which L_1 and L_2 are both significantly bigger than the carbon-carbon bond length R_{cc} . Thus each twist experienced for the whole nanotorus has only a minor effect on the bond lengths and angles corresponding to each individual carbon atom. In addition, we have further limited ourselves to nanotori which also satisfy $L_2 \gg L_1 \sin \theta$. This ensures that each such nanotorus can be realized in three-dimensional space, without the unphysical self-overlapping that would arise if this condition were not met. Together, these conditions help to ensure that the strains induced by these modular transformations are not too severe.

Needless to say, there are many implications of these spectral equivalences which we have not yet explored. It would be interesting, for example, to consider the implications of these symmetries for the existence or absence of persistent currents as well as the existence or absence of colossal magnetic moments. This work is currently in progress. It would also be interesting to understand these modular transformations in terms of fictitious fluxes, using analogues of the techniques presented in Ref.¹⁴.

In closing, we would like to make two final remarks, one of primarily mathematical interest and one of more practical applicability.

First, as we have seen, modular invariance is the symmetry which underlies most of the results we have presented in this paper. At a mathematical level, modular invariance is normally just a relabelling symmetry in the sense that two sets of torus parameters related by a modular transformation normally correspond to the same physical torus. This is certainly the case in string theory, and in most other situations in theoretical high-energy physics in which modular transformations have played a significant role (see, *e.g.*, Ref.²²).

However, the case of carbon nanotori is quite different. Here, modular transformations relate parameters corresponding to carbon nanotori which are physically distinct. As we have discussed, this is because we are not merely rolling up an unmarked sheet of paper when

we subject it to two non-parallel identifications; we are rolling up a graphene sheet which already has a hexagonal carbon lattice imprinted on it. Viewed from this perspective, it is therefore somewhat remarkable that modular transformations continue to play a role, indicating when two distinct nanotori will have the same spectral properties. Indeed, in the case of carbon nanotori, we see that modular invariance is thus promoted from a mere relabeling symmetry to something far deeper: *modular invariance becomes an outright physical symmetry between physically distinct entities*. We know of no other physical situation in which modular invariance plays such a role.

Second, it is also exciting at a practical level that physically distinct carbon nanotori can have identical energy spectra and electrical properties. Since these nanotori are physically distinct, some are likely to be far more complicated to construct in the laboratory than others. Nevertheless, these spectral equivalences suggest that it may not be necessary to fabricate a very complex nanotorus (or generate sizable magnetic fluxes) in order to obtain a desired spectral property; there are likely to be far simpler nanotori and/or fluxes which can perform the same function. This could have significant implications for the production and use of such nano-materials.

This work was supported in part by the Department of Energy under Grant DE-FG02-04ER-41298. We are happy to thank P. McEuen, D. Ralph, C. Stafford, and H. Tye for discussions, and we wish to acknowledge the hospitality of the Kavli Institute for Theoretical Physics (KITP) in Santa Barbara, California, where this paper was completed.

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- ¹ S. Iijima, *Nature* **354**, 56 (1991).
 - ² B. I. Dunlap, *Phys. Rev. B* **46**, 1933 (1992); S. Itoh, S. Ihara, and J. Kitakami, *Phys. Rev. B* **47**, 1703 (1993); *Phys. Rev. B* **47**, 12908 (1993).
 - ³ J. Liu, H. Dai, J. H. Hafner, D. T. Colbert, R. E. Smalley, S. J. Tans, and C. Dekker, *Nature* **385**, 780 (1997).
 - ⁴ R. Martel, H. R. Shea, and P. Avouris, *Nature* **398**, 299 (1999); *J. Phys. Chem. B* **103**, 7551 (1999).
 - ⁵ M. Ahlskog, E. Seynaeve, R. J. M. Vullers, C. van Haesendonck, A. Fonseca, K. Hernadi, and J. B. Nagy, *Chem. Phys. Lett.* **300**, 202 (1999).
 - ⁶ M. Terrones, W. K. Hsu, J. P. Hare, H. W. Kroto, H. Terrones, and D. R. M. Walton, *Phil. Trans. R. Soc. A* **354**, 2025 (1996); H. R. She, R. Martel, and P. Avouris, *Phys. Rev. Lett.* **84**, 4441 (2000); M. Sano, A. Kamino, J. Okamura, and S. Shinkai, *Science* **293**, 1299 (2001); H. Watanabe, C. Manabe, T. Shigematsu, and M. Shimizu, *Appl. Phys. Lett.* **78**, 2928 (2001).
 - ⁷ R. C. Haddon, *Nature* **388**, 31 (1997).
 - ⁸ M. F. Lin and D. S. Chuu, *Phys. Rev. B* **57**, 6731 (1998).
 - ⁹ L. Liu, G. Y. Guo, C. S. Jayanthi, and S. Y. Wu, *Phys. Rev. Lett.* **88**, 217206 (2002).
 - ¹⁰ C. C. Tsai, F. L. Shyu, C. W. Chiu, C. P. Chang, R. B. Chen, and M. F. Lin, *Phys. Rev. B* **70**, 075411 (2004).
 - ¹¹ A. Ceulemans, L. F. Chibotaru, S. A. Bovin, and P. W. Fowler, *J. Chem. Phys.* **112**, 4271 (2000).
 - ¹² M. Margańska and N. Szopa, *Acta Phys. Pol. B* **32**, 427 (2001).
 - ¹³ R. Saito, M. Fujita, G. Dresselhaus, and M. S. Dresselhaus, *Appl. Phys. Lett.* **60**, 2204 (1992); *Phys. Rev. B* **46**, 1804 (1992).
 - ¹⁴ C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **78**, 1932 (1997).
 - ¹⁵ S. A. Bovin, L. F. Chiboratu, and A. Ceulemans, *J. Mol. Cat. A* **166**, 47 (2001).
 - ¹⁶ E. C. Kirby, R. B. Mallion, and P. Pollak, *J. Chem. Soc. Faraday Trans.* **89**(12), 1945 (1993); S. Negami, *Discrete Math.* **44**, 161 (1983).
 - ¹⁷ K. Sasaki and Y. Kawazoe, *Prog. Theor. Phys.* **112**, 369 (2004).
 - ¹⁸ M. F. Lin, R. B. Chen, and F. L. Shyu, *Solid State Commun.* **107**, 227 (1998); A. A. Odintsov, W. Smit, and H. Yoshioka, *Europhys. Lett.* **45** (5), 598 (1999); K. Sasaki, *Phys. Rev. B* **65**, 155429 (2002); S. Latil, S. Roche, and A. Rubio, *Phys. Rev. B* **67**, 165420 (2003); Z. Zhang, Z. Yang, X. Wang, J. Yuan, H. Zhang, M. Qiu, and J. Peng, *J. Phys. Condens. Matter* **17**, 4111 (2005); C. Feng and K. M. Liew, *Carbon* **47**, 1664 (2009).
 - ¹⁹ V. Meunier, P. Lambin, and A. A. Lucas, *Phys. Rev. B* **57**, 14886 (1998); J. Han, *Chem. Phys. Lett.* **282**, 187 (1998).
 - ²⁰ C. P. Liu, H. B. Chen, and J. W. Ding, *J. Phys. Condens. Matter* **20**, 015206 (2008).
 - ²¹ P.W. Fowler and H.S. Rzepa, *Phys. Chem. Chem. Phys.* **8**, 1775 (2006).
 - ²² K. R. Dienes, *Phys. Rev. Lett.* **88**, 011601 (2002); K. R. Dienes and A. Mafi, *Phys. Rev. Lett.* **88**, 111602 (2002).