Symmetry of nanotubes rolled up from arbitrary two-dimensional lattices along an arbitrary chiral vector

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The line group describing full symmetry of a nanotube rolled up from an arbitrary layer along an arbitrary chiral vector is found. A helical axis and pure rotations are always present, while mirror and glide planes appear only for special chiral vectors in rhombic or rectangular lattices. Nanotubes are not translationally periodical unless the unit cell of the layer satisfies very specific conditions. Physical consequences, including the incommensurability of carbon nanotubes, are discussed.

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I. INTRODUCTION

The large line group symmetry of carbon nanotubes is crucial[1,2] in predicting their unique properties.[3,4] Knowing the symmetry of carbon nanotubes it was not difficult to determine the symmetry of the inorganic nanotubes,[5] the underlying two-dimensional (2D) lattice of which is also hexagonal. However, apart from recent results on rectangular lattices,[6] the symmetry of tubules related to other kinds of 2D lattices has never been considered, despite a rapidly increasing number of reported types: BC_2N,[7] ternary borides,[8] carbon pentaheptides and Haeckelites,[9] ZnO nanorings,[10] etc.

Here we fill in this gap, presenting a quite general result: full symmetry of a nanotube (NT) obtained by rolling up an arbitrary 2D lattice. Although such a nanotube may have no translational periodicity, its symmetry is always described by a line group. This yields many far-reaching physical consequences including reconsideration of the carbon NT symmetry.

II. LINE GROUPS

To differ from the 2D and 3D crystals, quasi-1D ones do not obey crystallographic restrictions for the rotational axes; further, in some cases helical ordering substitutes translational periodicity. Consequently, the number of different symmetry groups, *line groups*, of quasi-1D systems is infinite, in contrast to 80 diperiodic and 230 space groups. Only 75 line groups are subgroups of the latter; they are known as the rod groups.[11]

Line groups are classified within 13 families (Table I). Each group is a product $\boldsymbol{L}=\boldsymbol{Z}\boldsymbol{P}_n$ of an axial point group $\boldsymbol{P}_n$ and an infinite cyclic group $\boldsymbol{Z}$. Thus $\boldsymbol{P}_n$ is one of $\boldsymbol{C}_n$, $\boldsymbol{S}_{2n}$, $\boldsymbol{C}_{nh}$, $\boldsymbol{D}_n$, $\boldsymbol{C}_{nv}$, $\boldsymbol{D}_{nd}$, and $\boldsymbol{D}_{nh}$, where $n=1,2,\ldots$ is the order of its principal axis (z axis, by convention). The group of the *generalized translations* $\boldsymbol{Z}$ is either a screw axis $\boldsymbol{T}_Q(f)$ or a glide plane $\boldsymbol{T}'(f)$, generated by $(C_Q|f)$ (Koster-Seitz symbol)—i.e., rotation for $2\pi/Q$ around the z axis followed by translation for f along the same axis ($Q\geqslant 1$ is a real number)—and $(\sigma_v|f)$, respectively. While pure translation (for $2f$) pertains to $\boldsymbol{T}'(f)$, group $\boldsymbol{T}_Q(f)=\boldsymbol{T}_q^r(f)$ contains pure translation (for fq) only for rational $Q=q/r$ (r and q integers).

All the combinations $(C_Q|f)^t C_n^s$ of the rotations around the principal axis and the translations form the rotohelical subgroup $\boldsymbol{L}^{(1)}$ (the first family line group) of $\boldsymbol{L}$. In the course of the rolling it emerges from the 2D lattice translations. For the first family line groups $\boldsymbol{L}^{(1)}=\boldsymbol{L}$; for the groups from the families 2–8, $\boldsymbol{L}^{(1)}$, is a halving subgroup, while for the families 9–13, $\boldsymbol{L}^{(1)}$ is a quarter subgroup. Consequently, when $\boldsymbol{L}^{(1)}$ is known, to build up the whole line group it remains to find if there are additional generators (mirror/glide plane and/or U axis) allowed by both the symmetry of the elementary cell of the specific layer and the chosen chiral vector.

Note that Q is not unique, and therefore a convention[6] is introduced: Q is the largest finite number among $Q_s=Qn/(Qs+n)$ for $s=\pm 1$; for the commensurate groups, this Q is written as $Q=q/r$ with q being a multiple of n, $q=\tilde{q}n$, and r is coprime to $\tilde{q}$, while the translational period is $a=\tilde{q}f$. For example, the group combining pure translations $\boldsymbol{T}(f=a)$ with $\boldsymbol{C}_n$ is $\boldsymbol{T}(a)\boldsymbol{C}_n=\boldsymbol{T}_n^1(a)\boldsymbol{C}_n$.

Only the line groups from the first and fifth families may have irrational Q, when they refer to the *incommensurate systems*, helically ordered but without translational periodicity. For the other families Q equals n or $2n$—i.e., $\tilde{q}=1,2$; these *achiral* groups are $\boldsymbol{T}(f)\boldsymbol{P}_n$ (symmorphic groups), $\boldsymbol{T}_{2n}^1(f=a/2)\boldsymbol{P}_n$, or $\boldsymbol{T}'(f=a/2)\boldsymbol{P}_n$.

III. ROTOHELICAL TRANSFORMATIONS

We consider a 2D lattice, with the basis vectors $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ ($A_1\geqslant A_2$) at the angle $\alpha\in(0,\pi/2]$, and define dimensionless parameters X and Y:

$$X=\frac{A_1^2}{A_2^2}\geqslant 1, \quad Y=\frac{A_1}{A_2}\cos\alpha\geqslant 0. \tag{1}$$

A nanotube (n_1,n_2) is obtained by folding the layer in the way that the *chiral vector* $\boldsymbol{c}=(n_1,n_2)=n_1\boldsymbol{A}_1+n_2\boldsymbol{A}_2$ becomes the circumference of the tube (Fig. 1). Alternatively, the NT is defined by the length c (giving the tube's diameter $D=c/\pi$) and the slope (*chiral angle*) θ of $\boldsymbol{c}$:

$$c=A_2\sqrt{n_1^2X+n_2^2+2n_1n_2Y}, \quad \sin\theta=n_2A_2/c. \tag{2}$$

It is enough to consider NT's with $n_2\geqslant 0$—i.e., $0\leqslant\theta<\pi$—as the nanotube $(-n_1,-n_2)$ is the same with (n_1,n_2).

The translations of the layer become rotohelical operations on the tube; i.e., the two-dimensional translational group is folded into $\boldsymbol{L}^{(1)}=\boldsymbol{T}_Q(f)\boldsymbol{C}_n$. Simple geometry and some number theory suffice to find the parameters Q, n, and f (Ref. 12):

$$n = \mathrm{GCD}(n_1, n_2), \tag{3a}$$

$$f = A_1 \frac{\sin\alpha}{\sqrt{\tilde{n}_1^2 X + \tilde{n}_2^2 + 2\tilde{n}_1\tilde{n}_2 Y}}, \tag{3b}$$

$$Q = n \frac{\tilde{n}_1^2 X + \tilde{n}_2^2 + 2\tilde{n}_1\tilde{n}_2 Y}{\tilde{n}_1 z_1 X + \tilde{n}_2 z_2 + (\tilde{n}_1 z_2 + \tilde{n}_2 z_1) Y}. \tag{3c}$$

Here, $\boldsymbol{z}=(z_1,z_2)$ is the closest to the line perpendicular to $\boldsymbol{c}$ (but not on this line, Fig. 1), the lattice vector from the series

$$\boldsymbol{z}_s = (z_{1s}, z_{2s}) = \boldsymbol{z}_0 + s(\tilde{n}_1, \tilde{n}_2), \quad s = 0, \pm 1, \dots, \tag{4}$$

$$\boldsymbol{z}_0 = \begin{cases} (0,1), & \text{if } \boldsymbol{c} = (n,0), \\ (-1,0), & \text{if } \boldsymbol{c} = (0,n), \\ \left(\tilde{n}_2^{\varphi(\tilde{n}_1)-1}, \dfrac{\tilde{n}_2^{\varphi(\tilde{n}_1)} - 1}{\tilde{n}_1} \right), & \text{otherwise}. \end{cases} \tag{5}$$

The Euler function $\varphi(x)$ gives the number of coprimes with x which are less than x.

In conclusion, the rotohelical part $\boldsymbol{L}^{(1)}$ of the NT symmetry generates the whole tube from a single 2D unit cell. The symmetry parameters f and $\tilde{Q}=Q/n$ depend only on the reduced chiral vector $\tilde{\boldsymbol{c}}=\boldsymbol{c}/n=\tilde{n}_1\boldsymbol{A}_1+\tilde{n}_2\boldsymbol{A}_2$, and thus they are same for the ray of the nanotubes $n(\tilde{n}_1,\tilde{n}_2)$ differing by the order n of the principal axis.

A. Commensurability

Instead of analyzing when Eq. (3c) gives rational Q, we find the commensurability condition of a NT directly checking if there is a NT translational period a. Obviously, if it exists, a is the length of the minimal lattice vector $\boldsymbol{a}=a_1\boldsymbol{A}_1+a_2\boldsymbol{A}_2$ orthogonal to the chiral vector. So we examine solvability in coprime integers a_i of

$$\tilde{\boldsymbol{c}} \cdot \boldsymbol{a} = a_2\tilde{n}_2 + a_1\tilde{n}_1 X + (a_2\tilde{n}_1 + a_1\tilde{n}_2) Y = 0. \tag{6}$$

When Eq. (6) is solvable, the period of the tube is

$$a = A_2\sqrt{a_1^2 X + a_2^2 + 2a_1 a_2 Y}. \tag{7}$$

Further, as q is the number of 2D lattice unit cells within the translational period of a NT, the surface area equality $qA_1A_2 \sin\alpha = ca$ gives

$$q = n \frac{\tilde{c}a}{A_2^2\sqrt{X - Y^2}}. \tag{8}$$

Finally, r is to be found from Eq. (3c).

To discuss the solvability Eq. (6), we note that only X and Y may be irrational. As the real numbers are an infinite-dimensional vector space over the rational numbers, for solvability in rational a_i (then also integral solutions exist) it is necessary that 1, X and Y be rationally dependent: either both X and Y are rational or there are rational w, x, and y (with $x \neq y$ as $X > Y$) and irrational J, such that $X=w+xJ$ and $Y=w+yJ$.

For both X and Y rational, Eq. (6) becomes a (rational) proportion between a_1 and a_2. All the nanotubes (n_1,n_2) are commensurate with[12]

TABLE I. Rolling-up correspondence of the line and diperiodic groups. For each family (column 1) of line groups all the different factorizations, rotohelical subgroup $\boldsymbol{L}^{(1)}$, and the isogonal point group $\boldsymbol{P}_q^I$ are given in the columns 2, 3, and 4 (for irrational Q in families 1 and 5, q is infinite; $\boldsymbol{T}_d'$ is a glide plane bisecting the vertical mirror planes or U axes of $\boldsymbol{P}$). The corresponding diperiodic groups enumerated according to Ref. 11 follow: for arbitrary chiral vector rolling gives either the first or fifth family line group; only for the special chiral vector(s) $\boldsymbol{a}=(n,0)$, $\boldsymbol{b}=(0,n)$, $\boldsymbol{c} \in \{(n,0),(0,n)\}$, $\boldsymbol{d}=(n,n)$, $\boldsymbol{e}=(-n,n)$, $\boldsymbol{f} \in \{(n,n),(-n,n)\}$, $\boldsymbol{g} \in \{(n,0),(0,n),(-n,n)\}$, $\boldsymbol{h} \in \{(n,n),(-n,n),(-2n,n)\}$, and $\boldsymbol{i} \in \{(n,0),(0,n),(-n,n),(n,n),(-n,2n),(-2n,n)\}$ do the underlined groups (repeated after the corresponding vectors) give other line group families below.

F	Factorizations	$\boldsymbol{L}^{(1)}$	$\boldsymbol{P}_q^I$	DG
1	$\boldsymbol{T}_Q\boldsymbol{C}_n$	$\boldsymbol{T}_Q\boldsymbol{C}_n$	$\boldsymbol{C}_q$	$1,2,4,5,8,9,10,\underline{11},\underline{12},\underline{13},\underline{14},\underline{15},\underline{16},\underline{17},\underline{18},\underline{27},\underline{28},\underline{29},\underline{30},\underline{31},\underline{32},\underline{33},\underline{34},\underline{35},\underline{36},65,66,67,68,\underline{69},\underline{70},\underline{71},\underline{72},74,\underline{78},\underline{79}$
5	$\boldsymbol{T}_Q\boldsymbol{D}_n$	$\boldsymbol{T}_Q\boldsymbol{C}_n$	$\boldsymbol{D}_q$	$3,6,7,\underline{19},20,21,22,\underline{23},\underline{24},\underline{25},\underline{26},\underline{37},\underline{38},\underline{39},\underline{40},\underline{41},\underline{42},\underline{43},\underline{44},\underline{45},\underline{46},\underline{47},\underline{48},49,50,51,52,53,54,\underline{55},\underline{56},\underline{57},\underline{58},\underline{59},\underline{60},\underline{61},\underline{62},\underline{63},\underline{64},73,75,76,\underline{77},\underline{80}$
2	$\boldsymbol{T}\boldsymbol{S}_{2n}$	$\boldsymbol{T}\boldsymbol{C}_n$	$\boldsymbol{S}_{2n}$	$\boldsymbol{a}$: 17, 33, 34; $\boldsymbol{b}$: 12, 16, 29, 30
3	$\boldsymbol{T}\boldsymbol{C}_{nh}$	$\boldsymbol{T}\boldsymbol{C}_n$	$\boldsymbol{C}_{nh}$	$\boldsymbol{a}$: 11, 14, 15, 27, 31, 32; $\boldsymbol{b}$: 28
4	$\boldsymbol{T}_{2n}^1\boldsymbol{C}_{nh}, \boldsymbol{T}_{2n}^1\boldsymbol{S}_{2n}$	$\boldsymbol{T}_{2n}^1\boldsymbol{C}_n$	$\boldsymbol{C}_{2nh}$	$\boldsymbol{e}$: 13, 18, 35; $\boldsymbol{d}$: 36; $\boldsymbol{h}$: 69, 72, 78; $\boldsymbol{g}$: 70, 71, 79
6	$\boldsymbol{T}\boldsymbol{C}_{nv}, \boldsymbol{T}_d'\boldsymbol{C}_{nv}$	$\boldsymbol{T}\boldsymbol{C}_n$	$\boldsymbol{C}_{nv}$	$\boldsymbol{a}$: 28; $\boldsymbol{b}$: 11, 14, 15, 27, 31, 32
7	$\boldsymbol{C}_n\boldsymbol{T}'$	$\boldsymbol{T}\boldsymbol{C}_n$	$\boldsymbol{C}_{nv}$	$\boldsymbol{a}$: 12, 16, 29, 30; $\boldsymbol{b}$: 17, 33, 34
8	$\boldsymbol{T}_{2n}^1\boldsymbol{C}_{nv}, \boldsymbol{T}_d'\boldsymbol{C}_{nv}$	$\boldsymbol{T}_{2n}^1\boldsymbol{C}_n$	$\boldsymbol{C}_{2nv}$	$\boldsymbol{e}$: 36; $\boldsymbol{d}$: 13, 18, 35; $\boldsymbol{h}$: 70, 71, 79; $\boldsymbol{g}$: 69, 72, 78
9	$\boldsymbol{T}\boldsymbol{D}_{nd}, \boldsymbol{T}'\boldsymbol{D}_{nd}$	$\boldsymbol{T}\boldsymbol{C}_n$	$\boldsymbol{D}_{nd}$	$\boldsymbol{a}$: 42, 45; $\boldsymbol{b}$: 24, 38, 40
10	$\boldsymbol{T}'\boldsymbol{S}_{2n}=\boldsymbol{T}_d'\boldsymbol{D}_n$	$\boldsymbol{T}\boldsymbol{C}_n$	$\boldsymbol{D}_{nd}$	$\boldsymbol{c}$: 25, 39, 43, 44, 56, 60, 62, 63
11	$\boldsymbol{T}\boldsymbol{D}_{nh}, \boldsymbol{T}'\boldsymbol{D}_{nh}$	$\boldsymbol{T}\boldsymbol{C}_n$	$\boldsymbol{D}_{nh}$	$\boldsymbol{c}$: 23, 37, 41, 46, 55, 59, 61, 64
12	$\boldsymbol{T}'\boldsymbol{C}_{nh}, \boldsymbol{T}'\boldsymbol{D}_n$	$\boldsymbol{T}\boldsymbol{C}_n$	$\boldsymbol{D}_{nh}$	$\boldsymbol{a}$: 24, 38, 40; $\boldsymbol{b}$: 42, 45
13	$\boldsymbol{T}_{2n}^1\boldsymbol{D}_{nh}, \boldsymbol{T}_{2n}^1\boldsymbol{D}_{nd}, \boldsymbol{T}_d'\boldsymbol{D}_{nh}, \boldsymbol{T}_d'\boldsymbol{D}_{nd}$	$\boldsymbol{T}_{2n}^1\boldsymbol{C}_n$	$\boldsymbol{D}_{2nh}$	$\boldsymbol{f}$: 26, 47, 48, 55, 56, 57, 58, $\boldsymbol{f}$: 61, 62, 63, 64; $\boldsymbol{i}$: 77, 80

$$q = n \frac{2\tilde{n}_1\tilde{n}_2\underline{X}\bar{Y} + \tilde{n}_1^2\bar{X}\underline{Y} + \tilde{n}_2^2\underline{X}\underline{Y}}{\mathrm{GCD}(\tilde{n}_1\underline{X}\bar{Y} + \tilde{n}_2\underline{X}\underline{Y}, \tilde{n}_2\underline{X}\bar{Y} + \tilde{n}_1\bar{X}\underline{Y})}, \tag{9}$$

$$\boldsymbol{a} = \frac{(\tilde{n}_1\underline{X}\bar{Y} + \tilde{n}_2\underline{X}\underline{Y}, -\tilde{n}_2\underline{X}\bar{Y} - \tilde{n}_1\bar{X}\underline{Y})}{\mathrm{GCD}(\tilde{n}_1\underline{X}\bar{Y} + \tilde{n}_2\underline{X}\underline{Y}, \tilde{n}_2\underline{X}\bar{Y} + \tilde{n}_1\bar{X}\underline{Y})}. \tag{10}$$

In the other case, rational and irrational parts of Eq. (6) make a system of two homogeneous equations in a_i, solvable when its determinant vanishes:

$$\tilde{n}_1^2 w(y - x) - \tilde{n}_1\tilde{n}_2 x - \tilde{n}_2^2 y = 0. \tag{11}$$

This constraint on $\tilde{n}_1$ and $\tilde{n}_2$ singles out a subset of the chiral vectors yielding commensurate NT's. Note that solutions may not exist (rational numbers are not algebraically closed). When they exist, all the chiral vectors $n\tilde{\boldsymbol{c}}(n=1,2,\dots)$ give

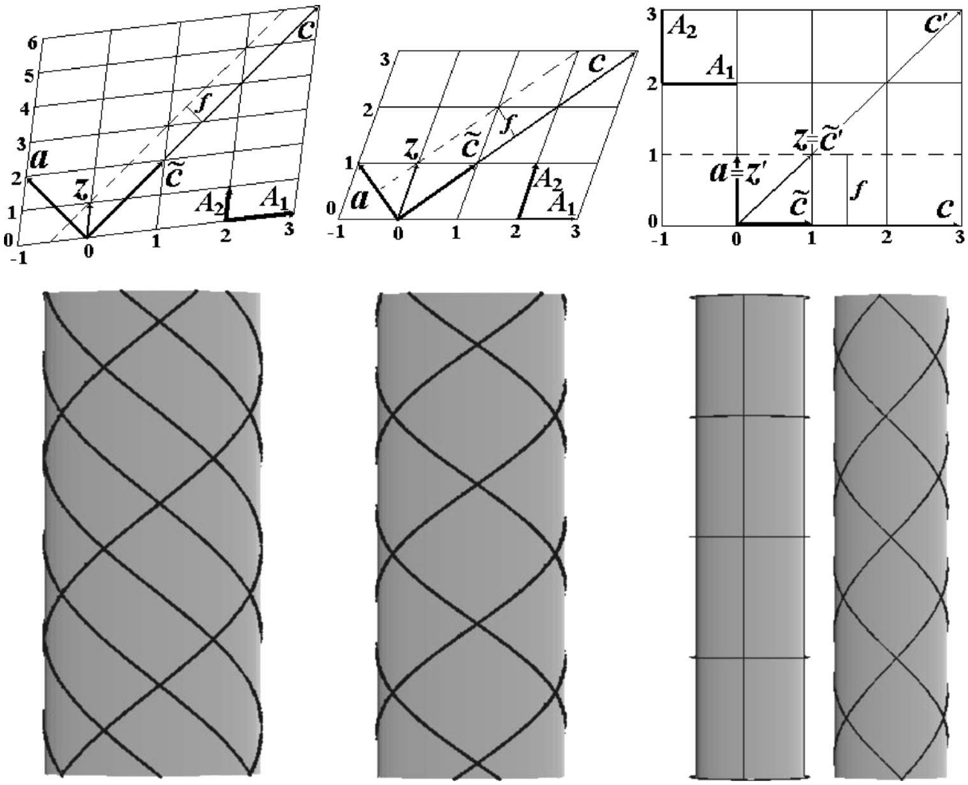

FIG. 1. Top: chiral vectors $\boldsymbol{c}$, with corresponding $\boldsymbol{a}$ (in the commensurate cases), z (all z_s are on the dashed line), and f. Left: $\boldsymbol{A}_1=(12,\sqrt{2})$ and $\boldsymbol{A}_2=\left(\frac{1}{\sqrt{2}},6\right)$ ($X=w=4$, $Y=J+X=24\sqrt{2}/73$, $x=0$, $y=1$), with $\boldsymbol{c}=(3,6)$, $\boldsymbol{z}=(0,1)$, and $\boldsymbol{L}^{(1)}=\boldsymbol{T}^1_{12}\left(3\sqrt{2}-\frac{1}{2}\right)\boldsymbol{C}_3$. Middle: rhombic layer with $\alpha=70°$, $\boldsymbol{c}=(3,3)$, $z=(0,1)$, and $\boldsymbol{L}^{(1)}=\boldsymbol{T}^1_6(a/2\approx 0.57A_1)\boldsymbol{C}_3$. Right: rectangular layer with $A_1/A_2=\pi/3$, $\boldsymbol{c}=(3,0)$, $z=(1,1)$, $\boldsymbol{L}^{(1)}=\boldsymbol{T}^1_3(a=A_2)\boldsymbol{C}_3$, $\boldsymbol{c}'=(3,3)$, $z'=(0,1)$, and $\boldsymbol{L}^{(1)'}=\boldsymbol{T}^1_{(9+\pi^2)/3}(3\pi/\sqrt{9+\pi^2}A_1)\boldsymbol{C}_3$. Bottom: corresponding nanotubes.

commensurate NT's with period $\boldsymbol{a}$, being fully determined by the reduced chiral vector $\tilde{\boldsymbol{c}}$. Besides, interchanging the roles of $\tilde{\boldsymbol{c}}$ and $\boldsymbol{a}$, we get NT's with period $\tilde{\boldsymbol{c}}$, orthogonal to chiral vectors $n\boldsymbol{a}$. Hence, in such lattices chiral vectors of commensurate NT's are on two perpendicular lines.

For $\tilde{n}_2\neq 0$, the constraint (11) becomes

$$\frac{\tilde{n}_1}{\tilde{n}_2}=\frac{x\pm\sqrt{x^2-4wxy+4wy^2}}{2w(y-x)}=\nu_\pm \tag{12}$$

and $\tilde{n}_1/\tilde{n}_2$ is rational only if $\sqrt{x^2-4wxy+4wy^2}$ is. The commensurate NT's are $\boldsymbol{c}^\pm=n\tilde{\boldsymbol{c}}^\pm$ with mutually orthogonal $\tilde{\boldsymbol{c}}^\pm=\boldsymbol{a}^\mp=(\bar{\nu}_\pm,\underline{\nu}_\pm)$, giving $q=n(\underline{\nu}_+\bar{\nu}_- - \underline{\nu}_-\bar{\nu}_+)$ and $a^\pm=A_2\sqrt{\underline{\nu}_\mp^2+\bar{\nu}_\mp^2X+2\underline{\nu}_\mp\bar{\nu}_\mp Y}$.

The case $\tilde{n}_2=0$ appears if and only if $w=0$, meaning $Y=yX$ (i.e., $J=X$ and $x=1$). Then the ray orthogonal to $\tilde{\boldsymbol{c}}^+=(1,0)$ is obtained as $\tilde{\boldsymbol{c}}^-=(\bar{y},\underline{y})$. The periods are $a^+=A_1\bar{y}|\tan\alpha|$ and $a^-=A_1$, while $q=n\underline{y}$.

IV. ADDITIONAL SYMMETRIES

Apart from the translational symmetry, a 2D lattice has a rotational $\boldsymbol{C}_2$ symmetry which is generated by the rotation of π around the axis perpendicular to the layer. In addition, rhombic and rectangular lattices have vertical mirror and glide planes and also, in the rhombic rectangular and hexagonal lattices, the order of the rotational axis is 4 and 6, respectively. However, atomic arrangements within the lattice unit cell may reduce the symmetry group to one of 80 diperiodic groups.[11] Additional symmetries, preserved after rolling up a layer into a NT, may appear: twofold rotational axis and mirror and glide planes. When combined with the rotohelical group $\boldsymbol{L}^{(1)}$ given by Eqs. (3), they yield a line group which belongs to one of the remaining 12 families.

The rotation C_2 of a layer becomes a horizontal twofold axis, the U axis, of the tube. Thus, whenever the order of the principal axis of the layer is 2, 4, or 6, the symmetry of the NT is the fifth family line group $\boldsymbol{T}_Q(f)\boldsymbol{D}_n$ at least. Note that the higher-order rotational symmetries of the layer do not give rise to the symmetry of NT's.

The vertical mirror (glide) plane is preserved in the NT only if the chiral vector is perpendicular to it. When $\boldsymbol{c}$ is parallel to the plane, the NT obtains a horizontal mirror (rotoreflectional) plane. All these transformations can be combined (Table I) only with the rotohelical groups $\boldsymbol{T}(a)\boldsymbol{C}_n$ or $\boldsymbol{T}^1_{2n}(a)\boldsymbol{C}_n$ (i.e., $\tilde{q}=1,2$) of the achiral NT's.

First, we consider rectangular lattices $\alpha=\pi/2$ (i.e., $Y=0$). For irrational $X=J$, we have $w=y=0$ (then $\underline{y}=1$) and $x=1$, yielding $\tilde{c}^+=(1,0)$ and $\tilde{c}^-=(0,1)$, with $\tilde{q}=1$; i.e., the helical factor reduces to the pure translational group. For X rational, from Eq. (9) we get $\tilde{q}=(\tilde{n}_1^2\bar{X}+\tilde{n}_2^2\underline{X})/\mathrm{GCD}(\tilde{n}_1,\underline{X})\mathrm{GCD}(n_2,\bar{X})$. Thus, for $X\neq 1$, the same result as for X irrational is achieved, while in the case $X=1$ (square lattice) additionally $\tilde{q}=2$ is obtained for $\tilde{c}^\pm=(\pm 1,1)$.

Second, for the rhombic lattices, $A_1=A_2$—i.e., $X=1$. For Y irrational, taking $J=Y-1$, we have $w=y=1$ and $x=0$ (then $\underline{x}=1$), yielding $\tilde{c}^\pm=(\pm 1,1)$ with $\tilde{q}=2$—i.e., $\boldsymbol{L}^{(1)}=\boldsymbol{T}^1_{2n}(a/2)\boldsymbol{C}_n$. For rational Y, from Eq. (9) we get $\tilde{q}=[2\tilde{n}_1\tilde{n}_2\bar{Y}+(\tilde{n}_1^2+\tilde{n}_2^2)\underline{Y}]/\mathrm{GCD}(\tilde{n}_1\bar{Y}+\tilde{n}_2\underline{Y},\tilde{n}_1\underline{Y}+\tilde{n}_2\bar{Y})$, allowing the same $\tilde{c}^\pm$ as for Y irrational. Only if $Y=0$ or $Y=1/2$ does the additional pair $\tilde{\boldsymbol{c}}^+=(1,0)$ and $\tilde{\boldsymbol{c}}^-=(0,1)$ appear, giving $\tilde{q}=1$ in the case of the square lattice and, again, $\tilde{q}=2$ for the hexagonal lattice.

Additional symmetries of the layer reduce the number of the different NT's. For the layers with the principal axis order $n=1,2,3,4,6$, the effective interval of the chiral angle is $[0,2\pi/n')$, where $n'=\mathrm{LCM}(2,n)=2,2,6,4,6$, respectively. Further, a vertical mirror plane of the layer intertwines the chiral vectors of the optically isomeric tubes, enabling us to halve this range to $[0,\pi/n']$. However, if there is not such a plane, the optical isomer of the tube (n_1,n_2) is again the tube (n_1,n_2) but obtained from the layer reflected in the plane perpendicular to $\boldsymbol{A}_1$.

V. DISCUSSION

The full symmetries of NT's rolled up from arbitrary 2D lattices along an arbitrary chiral vector are described by line groups. Depending on the type of 2D lattice and chiral vector direction, NT's may be commensurate or incommensurate (in the latter case the line group belongs to the first or fifth family).

The so-called achiral tubes have no optical isomers, and their helical factors are either trivial (translations only) or of the zigzag type. Hence, they are always commensurate. They are obtained from rectangular and rhombic 2D lattices, respectively, for the special directions of the chiral vector, which allow mirror and glide planes. The results presented here agree with the previously reported ones in the cases of hexagonal[1,2] and rectangular[6] lattices.

The conserved quantum numbers related to the rotohelical symmetries of NT's are quasimomenta:[1,2] helical, $\tilde{k}$, from the helical Brillouin zone (HBZ) $(-\pi/f,\pi/f]$, and remaining (nonhelical part) angular $\tilde{m}$, taking integer values from the interval $(-n/2,n/2]$. When the U axis or vertical or horizontal mirror or glide plane is a symmetry, the corresponding parity (Π^U, Π^v, and Π^h, taking values $+1$ and -1 for even and odd states) is conserved. More conventional quantum numbers for commensurate nanotubes are linear and total angular quasimomenta, k varying within the BZ $(-\pi/a,\pi/a])$ and m (integers from $(-q/2,q/2]$), where q is the order of the principal axis of the isogonal point group. However, m is not conserved in the umklapp processes.

These quantum numbers assigning energy bands $E^{\Pi}_{\tilde{m}}(\tilde{k})$ [or $E^{\Pi}_{m}(k)$] of (quasi)particle spectra correspond to irreducible representations of the NT line group; the dimension of the representation is the degeneracy of the band. Thus, for incommensurate NT's, the degeneracy is either 1 or 2, while for the commensurate ones also fourfold degeneracy is possible (families 9–13). In the families 2–5 and 9–13, z-reversing elements (U axis, horizontal mirror and rotoreflectional planes) intertwine $\tilde{k}$ and $-\tilde{k}$ (k and $-k$), causing at least twofold band degeneracy in the interior of the reduced HBZ $[0,\pi/f]$ (reduced BZ $[0,\pi/a]$). Only at its boundaries 0 and π/f (0 and π/a) is this degeneracy absent (but the U axis, simultaneously intertwining $\pm\tilde{m}$ and $\pm m$, preserves degeneracy for $\tilde{m}\neq 0,n/2$ and $m\neq 0,q/2$). Thus only these boundaries are special $\tilde{k}$ and k points, where the bands joining and van Hove singularities systematically appear. As the Jahn-Teller theorem holds for the line groups,[13] the NT electronic subsystem is in the nondegenerate state (excluding spin).

Groups of the same family with the same n are isomorphic for any Q. Thus, a change of this continual parameter does not diminish the symmetry, and it should be varied in numerical relaxation. For the most exhaustively studied NT's, carbon NT's, the graphene lattice is a rhombic hexagonal ($X=1$ and $Y=\frac{1}{2}$), giving commensurate chiral NT's of fifth family or achiral (zigzag and armchair) tubes of the 13th family.[2] However, for the chiral tubes, the relaxation slightly changes the helical axis, and there is no *a priori* physical reason for commensurability. Incommensurability affects the physical properties: quasimomentum fails to be conserved, and only the selection rules of the helical quantum numbers[1,13] are applicable. This effect must be taken into account, particularly when external fields or a mechanical influence[3] like twisting is studied. As closely related to symmetry,[14] diffraction patterns may be a significant tool in resolving (in)commensurability and other related issues.

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