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Symmetry of commensurate double-wall carbon nanotubes

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Abstract
The symmetry groups of double-wall carbon nanotubes (DWCNs) are the line and point groups for the commensurate and incommensurate walls, respectively. For the tubes with diameters between 2.8 Å and 50 Å all possible DWCNs are found. Among them all the 318 commensurate DWCNs are singled out and their symmetry groups are calculated. DWCNs are low symmetry objects with respect to the constituent single-wall tubes, and this symmetry reduction is described by the symmetry breaking groups. Both symmetry and symmetry breaking groups affect the physical properties of the DWCNs. While, e.g., quantum numbers and selection rules are related to the symmetry group, the low interaction between the walls is determined by the breaking group.

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1. Introduction

After the first discovery of carbon nanotubes [1] great interest, both experimental and theoretical, was shown in such materials. The theory of single-wall carbon nanotubes (SWCNs) developed rapidly, since from the very beginning it was facilitated by the high SWCN symmetry [2, 3]. On the other hand, coaxial multishell structures are more complicated for theoretical studies, which emphasizes the necessity of establishing and applying their symmetry. To the best knowledge of the authors, the single step in this direction [3] has been a quite general study of the possible symmetries of double-wall carbon nanotubes (DWCNs). Here we complete this task by the classification of the symmetries of all the commensurate DWCNs (CDWCN).

Each SWCN (n_1, n_2) is a quasi-1D crystal, meaning that its symmetry group is a line (also called monoperiodic or rod) group. If $n_1 = n_2$ the tube is called armchair ($\mathcal{A}$), if $n_2 = 0$ it is zigzag ($\mathcal{Z}$) and all other cases are known as chiral ($\mathcal{C}$). The chiral and achiral tubes have symmetries of different types, described by the line groups [3]:

$$\boldsymbol{L}_{\mathcal{C}} = \boldsymbol{T}_q^r(a)\boldsymbol{D}_n = \boldsymbol{L}q_p22 \qquad \boldsymbol{L}_{\mathcal{ZA}} = \boldsymbol{T}_{2n}^1(a)\boldsymbol{D}_{nh} = \boldsymbol{L}2n_n/mcm. \tag{1}$$

Here, $\boldsymbol{T}_q^r(a)$ is the helical group generated by $\left(C_q^r\middle|na/q\right)$, while $\boldsymbol{D}_n$ and $\boldsymbol{D}_{nh}$ are the point groups: $\boldsymbol{D}_n$ is the group generated by the rotation for $2\pi/n$ around the tube (vertical) axis and the rotation U for π around the perpendicular axis; $\boldsymbol{D}_{nh}$ in addition contains the horizontal mirror plane. The involved parameters depend on n_1 and n_2:

$$n = \mathrm{GCD}(n_1, n_2) \qquad q = 2\left(n_1^2 + n_1n_2 + n_2^2\right)\big/n\mathcal{R} \qquad a = \sqrt{3}\frac{D\pi}{n\mathcal{R}} \tag{2}$$

with $a_0 = 2.461$ Å, $\mathcal{R} = \mathrm{GCD}(2n_1 + n_2, n_1 + 2n_2)/n$, the tube diameter is $D = \frac{n}{\pi}\sqrt{\frac{\tilde{q}\mathcal{R}}{2}}a_0$, while r is a more complicated function of n_1 and n_2 [3]. The corresponding isogonal point groups are $\boldsymbol{D}_q$ for the chiral tubes, and $\boldsymbol{D}_{2nh}$ for the zigzag and armchair tubes. It is useful to note that $\tilde{q} = q/n$ is an integer such that

$$\tilde{q} = 2 \pmod{12}. \tag{3}$$

We use the suitable SWCN reference frame: the z-axis is the tube axis and the x-axis passes through the centre of one of the carbon hexagons. Since each atom of SWCN is obtained as a map of an arbitrary atom C_{000} by the symmetry transformations $\ell_{tsu} = \left(C_q^r\middle|na/q\right)^t C_n^s U^u$ ($t = 0, \pm1, \ldots, s = 0, \ldots, n-1$ and $u = 0, 1$), in this frame the cylindrical coordinates $\boldsymbol{r}_{tsu} = (D/2, \varphi_{tsu}, z_{tsu})$ of the atom $\mathrm{C}_{tsu} = \ell_{tsu}\,\mathrm{C}_{000}$ are

$$\boldsymbol{r}_{tsu} = \left(\frac{D}{2}, (-1)^u\varphi_{000} + 2\pi\left(\frac{tr}{q} + \frac{s}{n}\right), (-1)^u z_{000} + t\frac{n}{q}a\right) \tag{4}$$

with $\varphi_{000} = \frac{n_1+n_2}{\pi D^2}a_0^2$, $z_{000} = \frac{n_1-n_2}{2\sqrt{3}\pi D}a_0^2$ (note that r is missing in [3]). The spatial inversion $\mathcal{I}$ changes the signs of φ_{tsu} and z_{tsu}. It leaves the achiral tubes invariant, being an element of $\boldsymbol{L}_{\mathcal{ZA}}$. In contrast, the chiral tube (n_1, n_2) is transformed into the different tube (n_2, n_1). As their physical properties are neatly related (e.g. same energy spectra, opposite optical activity), only right optical isomers, $n_1 \geqslant n_2$, are considered. The line groups of the left and right chiral tubes are conjugated by $\mathcal{I}$: if ℓ is a symmetry of (n_1, n_2), then $\mathcal{I}\ell\mathcal{I}$ is a symmetry of (n_2, n_1). Therefore, the left and the right groups (1) are isomorphic, with common q, n and a, while the helicity parameters are related by $r_{\mathrm{right}} + r_{\mathrm{left}} = q$.

Double-wall tube will be denoted by W@W′, where $\mathrm{W} = (n_1, n_2)$ and $\mathrm{W}' = (n_1', n_2')$ are the inner and outer coaxially arranged SWCN walls. The interwall distance corresponds roughly [4] to the graphite interlayer distance $\Delta = 3.44$ Å. The spatial inversion applied to the DWCN $(n_1, n_2)@(n_1', n_2')$ gives $(n_2, n_1)@(n_2', n_1')$. On the other hand, the tube $(n_1, n_2)@(n_2', n_1')$ must be independently considered. Therefore, in the study of DWCNs, one has to include both right and left SWCN isomers.

We studied a sample of 318 CDWCNs obtained as follows. At first, we consider all SWCNs with the diameters 2.8 Å $\leqslant D \leqslant$ 50 Å and right chirality. Altogether there are 1280 of them. Each such tube is taken as an interior wall, and we searched for possible outer tubes: their diameters D' must be such that the interlayer distance $(D' - D)/2$ differs from Δ by at most 0.2 Å. There are 42 236 such pairs, but only 240 (about half a per cent!) of them are with commensurate walls. Among them only for 78 CDWCNs are both walls chiral, and their right–left counterparts are to be included independently. This makes a considered sample of 318 CDWCNs. Note that among the selected 1280 SWCNs only 207 (out of which 98 are chiral) have a commensurate pair within the chosen diameter range and allowed interwall distance.

The paper is organized as follows. In section 2 we interrelate the Abelian roto-translational parts of the symmetry groups of CDWCNs and their layers. We also introduce another group, describing the symmetry breaking due to the interaction of the walls. Assuming that the walls are coaxial, these two groups are not dependent on the other details of the relative position of the shells. Then in section 3 we discuss the parities (U-axes, vertical mirror and glide planes, horizontal mirror and roto-reflection planes) which remain symmetries of a CDWCN only in the special relative positions of the walls. Topological arguments point out that some of these special positions should be stable. Finally, we use a specially suited potential for the interlayer interaction [5] to find the stable position and the total symmetry group. In section 4 we analyse CDWCNs with diameters between 2.8 Å and 50 Å. Finally, comments and conclusions are given in section 5.

2. Roto-translational symmetry of CDWCNs

A symmetry of a DWCN W@W′ is any geometrical transformation leaving both walls invariant. Therefore the symmetry group of a DWCN is the intersection $\boldsymbol{L}_{\mathrm{WW}'} = \boldsymbol{L}_{\mathrm{W}} \cap \boldsymbol{L}_{\mathrm{W}'}$ of the groups of the walls. This group depends on the relative position of the walls: even when they are coaxial, there are special high symmetry positions. Nevertheless, this refers only to the parities, while the roto-translational symmetries are the same for all coaxial positions.

2.1. Roto-translational subgroup

Each line group has a subgroup $\boldsymbol{L}^{(1)} = \boldsymbol{T}^r_q(a)\boldsymbol{C}_n$ containing all roto-translational elements. Being generated by $\left(C^r_q\middle|na/q\right)$ and C_n this group is Abelian. Moreover, for any two coaxial tubes their roto-translational symmetries mutually commute. For the chiral and achiral SWCNs, $\boldsymbol{L}^{(1)}$ is an index-2 and an index-4 subgroup of their symmetry groups, respectively.

Obviously, like the full symmetry group, the roto-translational subgroup of a DWCN is the intersection of the walls' symmetry group. A commensurate double-wall tube, being periodical along the tube axis, is a quasi-1D crystal. Thus, for CDWCNs $\boldsymbol{L}^{(1)}_{\mathrm{WW}'}$ is a line group:

$$\boldsymbol{L}^{(1)}_{\mathrm{WW}'} = \boldsymbol{T}^R_Q(A)\boldsymbol{C}_N = \boldsymbol{L}^{(1)}_{\mathrm{W}} \cap \boldsymbol{L}^{(1)}_{\mathrm{W}'}. \tag{5}$$

The parameters Q, R, N and A are functions of the parameters of the walls. The translational period A is the minimal integer multiple of a and a'; it defines co-primes $\hat{a}$ and $\hat{a}'$ such that $A = \hat{a}'a = \hat{a}a'$.

For further purposes here we show that $\mathcal{R} = \mathcal{R}'$ for two commensurate SWCNs, W and W′. Indeed, according to (2), $a = a_0\sqrt{3\tilde{q}/2\mathcal{R}}$, and therefore $a/a' = \sqrt{\tilde{q}\mathcal{R}'/\tilde{q}'\mathcal{R}}$. When $\mathcal{R} \neq \mathcal{R}'$ there appears a factor of 3; due to (3) it can be cancelled neither by $\tilde{q}$ nor by $\tilde{q}'$; thus, a/a' is irrational. Therefore, for CDWCNs $a/a' = \sqrt{\tilde{q}/\tilde{q}'}$; cancelling $\mathrm{GCD}(\tilde{q}, \tilde{q}')$ on the right, one gets that a/a' is a square root of the ratio of the co-primes $\tilde{q}/\mathrm{GCD}(\tilde{q}, \tilde{q}')$ and $\tilde{q}'/\mathrm{GCD}(\tilde{q}, \tilde{q}')$. This is possible if and only if

$$\hat{a} = \sqrt{\tilde{q}/\mathrm{GCD}(\tilde{q}, \tilde{q}')} \qquad \hat{a}' = \sqrt{\tilde{q}'/\mathrm{GCD}(\tilde{q}, \tilde{q}')}. \tag{6}$$

These results are used in the following theorem giving the roto-translational part of the commensurate DWCN symmetry group (for the proof, see appendix A):

Theorem 1. *The roto-translational group of CDWCN is the line group* $\boldsymbol{L}^{(1)}_{\mathrm{WW}'}$ *with*

$$N = \mathrm{GCD}(n, n') \qquad Q = N\mathrm{GCD}\left(r\hat{a}'\frac{n'}{N} - r'\hat{a}\frac{n}{N}, \sqrt{\tilde{q}\tilde{q}'}\right) \qquad A = \hat{a}'a = \hat{a}a'. \tag{7}$$

The helicity parameter R *is determined by the integer* $R_0 = \left(r\hat{a}\tau + \frac{q}{n}s_0\right)Q/q$ *with* $\tau = \sqrt{\tilde{q}\tilde{q}'}/\mathrm{GCD}\left(r\hat{a}'\frac{n'}{N} - r'\hat{a}\frac{n}{N}, \sqrt{\tilde{q}\tilde{q}'}\right)$ *and* $s_0 = \tau(r\hat{a}q' - r'\hat{a}'q)(\hat{n}^{\phi(\hat{n}')} - 1)/n'\tilde{q}\tilde{q}'$ *(here,* ϕ *is the Euler function): then* $R = R_0 + jQ/N$ *where* j *is the minimal non-negative integer for which* R *and* Q *are the co-primes (recall that* $\tilde{q} = q/n$*, and* $\tilde{q}' = q'/n'$*).*

2.2. Breaking group

The interaction potential between the walls is $V(\boldsymbol{R}, \boldsymbol{R}') = \sum_{ij} v(\boldsymbol{r}_i, \boldsymbol{r}'_j)$, where $v(\boldsymbol{r}_i, \boldsymbol{r}'_j)$ are couplings of the atoms of the inner and the outer walls; here $\boldsymbol{R} = \{\boldsymbol{r}_i\}$ and $\boldsymbol{R}' = \{\boldsymbol{r}'_i\}$ are the sets of all the atomic positions. This potential is invariant under the transformations generated by all the symmetries of both walls: $\ell\ell' V(\boldsymbol{R}, \boldsymbol{R}') = V(\ell\ell'\boldsymbol{R}, \ell\ell'\boldsymbol{R}')$ for each $\ell \in \boldsymbol{L}_{\mathrm{W}}$ and $\ell' \in \boldsymbol{L}_{\mathrm{W}'}$. Among them, only the transformations from the intersection $\boldsymbol{L}_{\mathrm{W}} \cap \boldsymbol{L}_{\mathrm{W}'}$ leave both walls invariant. All other transformations change the relative position of the walls, despite the invariance of the potential. Therefore, the symmetry of the potential is the group $\boldsymbol{L}_{\times}$ generated by both $\boldsymbol{L}_{\mathrm{W}}$ and $\boldsymbol{L}_{\mathrm{W}'}$. It appears that the interaction itself imposes the symmetry breaking from the product $\boldsymbol{L}_{\mathrm{W}} \times \boldsymbol{L}_{\mathrm{W}'}$ of the noninteracting systems to $\boldsymbol{L}_{\mathrm{WW}'}$.

Particularly, the roto-translational symmetries form Abelian and mutually commutative groups $\boldsymbol{L}^{(1)}_{\mathrm{W}}$ and $\boldsymbol{L}^{(1)}_{\mathrm{W}'}$. Therefore, their product $\boldsymbol{L}^{(1)}_{\mathrm{W}} \times \boldsymbol{L}^{(1)}_{\mathrm{W}'}$ has $\boldsymbol{L}^{(1)}_{\mathrm{WW}'}$ as an invariant subgroup. The group $\boldsymbol{L}^{(1)}_{\times}$ generated by all roto-translational symmetries of both walls is the Abelian factor group $\boldsymbol{L}^{(1)}_{\times} = \boldsymbol{L}^{(1)}_{\mathrm{W}} \times \boldsymbol{L}^{(1)}_{\mathrm{W}'} \big/ \boldsymbol{L}^{(1)}_{\mathrm{WW}'}$. Analogously to $\boldsymbol{L}^{(1)}_{\mathrm{WW}'}$, this group does not depend on the relative position of the walls. It is the first family line group characterized by the following theorem.

Theorem 2. *The symmetry breaking group of a CDWCN is the line group*

$$\boldsymbol{L}^{(1)}_{\times} = \boldsymbol{T}^{R_\times}_{Q_\times}(A_\times)\boldsymbol{C}_{N_\times} \tag{8}$$

with parameters $N_\times$, $Q_\times$, $A_\times$ and $R_\times$ given by

$$N_\times = \frac{\mathrm{LCM}(n, n')\sqrt{\tilde{q}\tilde{q}'}}{\mathrm{GCD}(r\hat{a}'n'/N - r'\hat{a}n/N, \sqrt{\tilde{q}\tilde{q}'})} \qquad Q_\times = \mathrm{LCM}(q, q') \tag{9}$$

$$A_\times = \frac{aa'\mathrm{GCD}(r\hat{a}'n'/N - r'\hat{a}n/N, \sqrt{\tilde{q}\tilde{q}'})}{A\,\mathrm{GCD}(q, q')} \tag{10}$$

$$\frac{qq'R_\times}{\mathrm{LCM}(q, q')} = \frac{(r\hat{a}'q' - r'\hat{a}q)\hat{a}^{\phi(\hat{a}')} + r'q\hat{a}}{\hat{a}\hat{a}'} \quad (\mathrm{mod}\ \mathrm{GCD}(N\tilde{q}\tilde{q}', r\hat{a}'q' - r'\hat{a}q)). \tag{11}$$

By convention, $R_\times$ is the unique solution of the last equation which is less than $Q_\times$ and co-prime to $Q_\times$ (proof is given in appendix A).

As has been stressed, the breaking group describes the maximal symmetry of the interaction potential. Since the walls' symmetry groups are much larger than the symmetry of the DWCN, the breaking group is very large. This holds also for the roto-translational part $\boldsymbol{L}^{(1)}_{\times}$, and implies that the interaction potential has very fine periodicity along and around the z-axis, i.e. small periods $A_\times$ and $2\pi/N_\times$.

3. Stable positions and full symmetry

Although the walls of a DWCN are coaxial, meaning that the z- and the z'-axes coincide, the x- and x'-axes may differ. Let the x'-axis be obtained from the x-axis by rotation (around the z-axis) by Φ and translation (along the z-axis) by Z. Then Φ and Z completely determine the relative position of the walls. Thus, in the inner wall coordinate system, the atomic coordinates of the outer wall W′ are

$$\boldsymbol{r}'_{tsu} = \left(\frac{D'}{2}, (-1)^u\varphi'_{000} + 2\pi\left(\frac{tr'}{q'} + \frac{s}{n'}\right) + \Phi, (-1)^u z'_{000} + t\frac{n'}{q'}a' + Z\right). \tag{12}$$

3.1. Parities

Additional symmetries (here we shall call them parities) are elements of the full DWCN symmetry group only in the special relative positions (Φ, Z) at which horizontal axes and (in the achiral pairs) mirror, glide or roto-reflection planes coincide.

Let us begin with the U-axis parity. Denoting the U-axis which coincides with the x-axis by U_{00}, the other U-axes are $U_{ts} = \left(C_q^r \middle| na/q\right)^t C_n^s U_{00}$. Their directions are defined in the cylindrical coordinates by $(\varphi_{ts}, z_{ts}) = (\pi(rt + \tilde{q}s)/q, nat/2q)$. Since $\tilde{q}$ is even and r odd, there are two classes of U-axes: U_{e} and U_{o} (i.e. the axes with even and odd t). All the U_{o} axes on both their sides bisect the carbon bonds. Nevertheless, for odd n (such a wall will be referred to as an odd wall) each U_{e}-axis at one side comes through the centre of a carbon hexagon and bisects a bond on the other side. For n even (even wall), there are two types of U_{e}-axes, U_{ee} and U_{eo}, corresponding to even and odd s: U_{ee} passes through the centres of hexagons, and U_{eo} bisects the bonds.

In the achiral cases $q = 2n$ and the U_{ts}-axis is positioned at $(\varphi_{ts}, z_{ts}) = (\pi t/2n + \pi s/n, at/4)$. The U_{e}-axes are the intersections of the vertical and horizontal mirror planes (σ_{ve} and σ_{he}), while the U_{o}-axes are the intersections of the vertical glide planes with the horizontal roto-reflection planes (σ_{vo} and σ_{ho}).

Thus, the coincidence of the axes in (φ, z) and (φ', z') is realized by the relative position of the walls (Φ, Z) with $\Phi = \varphi_{ts} - \varphi'_{t's'}$ and $Z = z_{ts} - z'_{t's'}$. It enlarges the symmetry group by a factor of 2, giving the fifth family line group $\boldsymbol{T}_Q^R(A)\boldsymbol{D}_N$. When both walls are achiral, the coincidence of the U-axes implies the coincidence of some of the symmetry planes: vertical (horizontal) mirror planes with either a mirror or a glide (roto-reflection) plane. In all these cases different groups are obtained [3], but all of them are four times larger than the pure roto-translational group. Also, it is possible to get a symmetry plane even without coincidental U-axes in which case the symmetry is enlarged by a factor of 2 [3].

Without specifying the interaction potential the stable relative position of the walls cannot be predicted. Nevertheless, the topological analysis of the symmetry breaking [6] shows that the extreme points of the invariant functions are on the peripheral strata. This means that the extremes of the interaction will be achieved in the positions with maximal symmetry; particularly this refers to the stable configurations (corresponding to the interaction potential minima).

3.2. Potential and stable configurations

As has been discussed above, to determine the symmetry groups of CDWCNs one has to use the interatomic pairwise potential $v(\boldsymbol{r}, \boldsymbol{r}')$. We take the potential [5] of Lennard-Jones type with the coefficients fitted numerically to the experimental data,

$$v(\boldsymbol{r}_{tsu}, \boldsymbol{r}'_{t's'u'}) = -\frac{18.5426}{|\boldsymbol{r}_{tsu} - \boldsymbol{r}'_{t's'u'}|^6} + \frac{29\,000.4}{|\boldsymbol{r}_{tsu} - \boldsymbol{r}'_{t's'u'}|^{12}} \tag{13}$$

to calculate the potential

$$V(\Phi, Z) = \sum_{tsu} \sum_{t's'u'} v(\boldsymbol{r}_{tsu}, \boldsymbol{r}'_{t's'u'}). \tag{14}$$

The atomic positions are given by (4) and (12). As has been discussed, this potential is invariant under the breaking group $\boldsymbol{L}_\times^{(1)}$, independently of the relative position of the walls. Since rotational and translational periods of this group are $2\pi/N_\times$ and $A_\times$, it suffices to scan only the part $\Phi \in [0, 2\pi/N_\times) Z \in [0, A_\times)$ of the (Φ, Z)-cylinder in order to determine the stable positions as the minima of the potential.

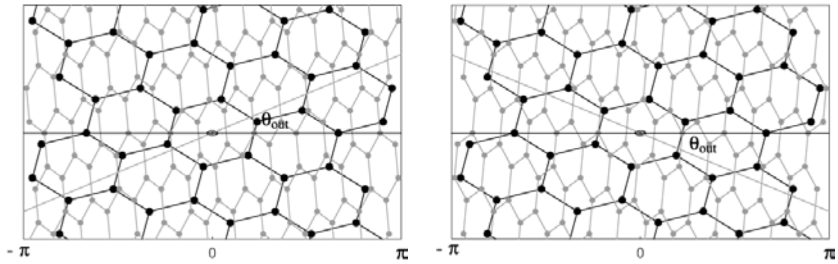

Figure 1. CDWCNs (4,1)@(3,12) (left) and (4,1)@(12,3) (right). The tubes are unfolded, i.e. horizontal and vertical axes are φ and z coordinates. The inner tube, (4, 1), is depicted in black, while the outer ones are grey. The outer tubes chiral angle θ_{out} is indicated. Sign $\otimes$ at the centre highlights the twofold horizontal axis U.

We have performed numerical calculations for the sample of 318 CDWCNs, described in section 1. The results agree with the topological predictions: the single global minimum coincides with one of the highest symmetry positions. Namely, whenever at least one wall is chiral, the minimum is at $(\Phi, Z) = (0, 0)$, and the U_{00}- and U'_{00}-axes coincide, see figure 1.

As for the pair of achiral walls, since $\mathcal{Z}$ and $\mathcal{A}$ tubes are incommensurate, only pairs $\mathcal{ZZ}$ and $\mathcal{AA}$ are considered. The interlayer distance of approximately 3.44 Å is realized [7] for $\mathcal{ZZ}_n = (n, 0)@(n+9, 0)$ and $\mathcal{AA}_n = (n, n)@(n+5, n+5)$. Since the principal axis order is odd for at least one wall (as both n and n' cannot be even), the resulting N is odd. In all these cases the stable configuration is at $Z = A/4$, where $A = a = a'$ is the period of the DWCN: the walls are mutually shifted by $A/4$, resulting in the coincidence of the horizontal mirror plane of one wall with the roto-reflection plane of the other: $\sigma_{\text{he}} = \sigma'_{\text{ho}}$ and $\sigma_{\text{ho}} = \sigma'_{\text{he}}$. Such a plane cannot be a common mirror plane. The product $C_{2N}\sigma_{\text{h}}$ generates a common W and W′ roto-reflection plane. Let n be odd and n' even. Then n/N is odd and the roto-reflection $C_{2N}\sigma_{\text{h}}$ is equal to the element $(C_{2n}\sigma_{\text{ho}})^{n/N}$ of the symmetry of W. Further, σ_{h} itself is a symmetry of W′, but since n' is divisible by $2N$, also $C_{2N} = C_{n'}^{n'/2N}$ is a W′ symmetry.

In most of the cases $\Phi = 0$, i.e. in the stable configuration the walls are not twisted. Therefore, the vertical mirror planes σ_{ve} containing x- and x'-axes coincide. As for the U-axes, due to the vertical shift the only possibility is coincidence of the even axis of one wall with the odd one of the other. One gets the equations $s\pi/n = (2s'+1)\pi/2n'$ for $U_{0s} = U'_{1s'}$ and $(2s+1)\pi/2n = s'\pi/n'$ for $U_{1s} = U'_{0s'}$. The first one, $2sn' = (2s'+1)n$, is solvable only for even n (then n' is odd); one solution is $s = n/2$ and $s' = (n'-1)/2$, giving the axis perpendicular to the common vertical mirror plane. The other equation is solved analogously only for even n'. One concludes that $U_{\text{e}} = U'_{\text{o}}$ for even n, and $U'_{\text{e}} = U_{\text{o}}$ for odd n, giving the common U-axis perpendicular to the common vertical mirror plane, figure 2.

The only exceptions are the achiral CDWCs $\mathcal{AA}_5$ and $\mathcal{ZZ}_9$, where $(\Phi, Z) = (N\pi/2nn', A/4)$: in addition to the translational shift for $A/4$, the outer tube is twisted for $\pi/N_\times$ (i.e. for $\pi/20$ and $\pi/36$, respectively). The vertical mirror and glide planes of the inner shell are at angles $s\pi/n$ and $(2s+1)\pi/2n$, while at angles $s'\pi/n' + N\pi/2nn'$ and $(2s'+1)\pi/2n' + N\pi/2nn'$ in the outer one. The mirror planes do not coincide since the corresponding equation, $N = 2(sn' - s'n)$, has no solution (N is odd). In contrast, a pair of glide planes satisfies $N = 2(sn' - s'n) + (n' - n)$ and coincide. Finally, the conditions $N = 2(sn' - s'n) - n$ for $\sigma_{\text{ve}} = \sigma'_{\text{vo}}$ and $N = 2(sn' - s'n) + n'$ for $\sigma_{\text{vo}} = \sigma'_{\text{ve}}$ are fulfilled by a vertical mirror plane of the odd wall and a glide plane of the even wall, giving a common glide plane. In the odd wall, the intersection of this plane with the horizontal mirror plane gives the

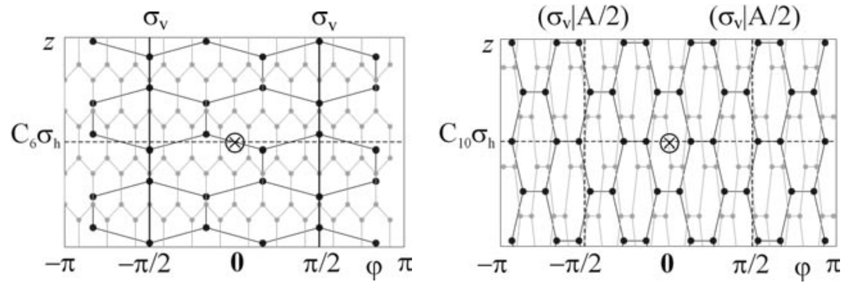

Figure 2. CDWCNs $\mathcal{ZZ}_3$ (left) and $\mathcal{AA}_5$ (right). The tubes are unfolded, i.e. horizontal and vertical axes represent φ and z coordinates. Besides the two-fold horizontal U-axis (⊗), there is either a vertical mirror plane (σ_v, solid line, $\mathcal{ZZ}_3$) or glide plane ($(\sigma_\mathrm{v}|A/2)$, dashed line, $\mathcal{AA}_5$) at $\pm\pi/2$, and a horizontal roto-reflection plane ($C_{2N}\sigma_\mathrm{h}$, horizontal dashed line).

U-axis; simultaneously, in the even wall this is the intersection of the horizontal roto-reflection and vertical glide planes. The obtained common U-axis is again perpendicular to a common glide plane (see figure 2).

3.3. Symmetry groups

Having at our disposal the stable configurations and the corresponding parities, it is easy to deduce the full symmetry groups of CDWCNs. The common U-axis in all CDWCNs enlarges the roto-translational group to $\boldsymbol{T}_Q^R(A)\boldsymbol{D}_N$, while in the $\mathcal{ZZ}$ and $\mathcal{AA}$ there is an additional mirror or glide plane. The common U-axis is, for convenience, taken as the x-axis, while the mirror/glide plane is therefore the yz-plane; the glide plane cyclic group generated by $(\sigma_{\mathrm{v}y}|A/2)$ is here denoted by $\boldsymbol{T}_c$. Thus, the line groups of the CDWCN symmetries are

$$\boldsymbol{L}_\mathcal{C} = \boldsymbol{T}_Q^R(A)\boldsymbol{D}_N = \boldsymbol{L}Q_P2, \boldsymbol{L}Q_P22 \qquad \text{(LG family 5)} \tag{15}$$

$$\boldsymbol{L}_{\mathcal{AA}_5} = \boldsymbol{T}_c(a_0)\boldsymbol{S}_{10} = \boldsymbol{L}\bar{5}c \qquad \text{(LG family 10)} \tag{16}$$

$$\boldsymbol{L}_{\mathcal{ZZ}_9} = \boldsymbol{T}_c(\sqrt{3}a_0)\boldsymbol{S}_{18} = \boldsymbol{L}\bar{9}c \qquad \text{(LG family 10)} \tag{17}$$

$$\boldsymbol{L}_{\mathcal{ZZ}_n} = \boldsymbol{L}_{\mathcal{AA}_n} = \boldsymbol{T}(A)\boldsymbol{D}_{Nd} = \boldsymbol{L}\bar{N}m \qquad \text{(LG family 9).} \tag{18}$$

The group parameters Q, R, N and A are given by theorem 1. In the international notation P is divisible by N, and $P/N = R^{\phi(Q/N)-1}$ (mod Q/N) (i.e. P/N and R inverses modulo Q/N); also, m and c stand for the vertical mirror and glide planes, respectively. The groups $\boldsymbol{L}_\mathcal{C}$ correspond to CDWCNs with one chiral wall at least. The isogonal point groups are

$$\boldsymbol{P}_\mathcal{C} = \boldsymbol{D}_Q \qquad \boldsymbol{P}_{\mathcal{ZZ}} = \boldsymbol{P}_{\mathcal{AA}} = \boldsymbol{D}_{Nd}. \tag{19}$$

4. Sample

As mentioned before, the commensurability of the lattice constants of the layers is a very restrictive condition. Only a few pairs of chiralities match it. However, many CDWCNs correspond to the same pair of chiral angles as many of the corresponding SWCN pairs happen to have the required diameter difference. Therefore, the CDWCNs can be grouped within series, which we call rays. Also, frequently the same SWCN appears as the inner of one, and the outer wall of another CDWCN. The symmetry group of CDWCNs is changed

Table 1. Rays containing five or more CDWCNs with the inner wall diameter 2.8 Å $\leqslant D \leqslant$ 50 Å. The CDWCNs in each ray (given in the first column) are obtained for the values of the parameter z given in the fourth column (the values in parentheses should be omitted). The corresponding line groups and isogonal point groups are given in the second and third columns, respectively. The last column gives the number of found CDWCNs. The table describes 223 of 318 CDWCNs altogether. The translational period is given in units of a_0.

CDWCN ray	Line group	Isogonal	z values	No
$(2+7z)(1,1)@(1+z)(11,2)$ $(1+z)(11,2)@(12+7z)(1,1)$	$\boldsymbol{T}(7)\boldsymbol{D}_1$	$\boldsymbol{D}_1$	0, 1, 2, 3	4 4
	$\boldsymbol{T}(7)\boldsymbol{D}_5$	$\boldsymbol{D}_5$	4	1 1
$(5+7z)(1,0)@(2+z)(5,3)$ $(1+z)(5,3)@(16+7z)(1,0)$	$\boldsymbol{T}(7\sqrt{3})\boldsymbol{D}_1$	$\boldsymbol{D}_1$	0, 2, 3, 5, 6, 8 0, 1, 3, 4, 6, 7	6 6
	$\boldsymbol{T}(7\sqrt{3})\boldsymbol{D}_3$	$\boldsymbol{D}_3$	1, 4 2, 5	2 2
	$\boldsymbol{T}(7\sqrt{3})\boldsymbol{D}_9$	$\boldsymbol{D}_9$	7 8	1 1
$(4+13z)(1,0)@(1+z)(8,7)$ $(1+z)(8,7)@(22+13z)(1,0)$	$\boldsymbol{T}(13\sqrt{3})\boldsymbol{D}_1$	$\boldsymbol{D}_1$	0, 1, 3, 4 0, 1, 3	4 3
	$\boldsymbol{T}(13\sqrt{3})\boldsymbol{D}_3$	$\boldsymbol{D}_3$	2 2	1 1
$z(1,0)@(z+9)(1,0)$	$\boldsymbol{T}(\sqrt{3})\boldsymbol{D}_{1d}$	$\boldsymbol{D}_{1d}$	4, 5, . . . , 62 (6, 9, 12, . . . , 60)	40
	$\boldsymbol{T}(\sqrt{3})\boldsymbol{D}_{3d}$	$\boldsymbol{D}_{3d}$	6, 9, 12, . . . , 60 (9, 18, . . . 54)	13
	$\boldsymbol{T}(\sqrt{3})\boldsymbol{D}_{9d}$	$\boldsymbol{D}_{9d}$	18, 27 . . . , 63	6
	$\boldsymbol{T}(\sqrt{3})\boldsymbol{T}_c\boldsymbol{S}_{18}$		9	1
$z(1,1)@(z+5)(1,1)$	$\boldsymbol{T}(1)\boldsymbol{D}_{1d}$	$\boldsymbol{D}_{1d}$	2, 3, . . . , 36 (5, 10, 15, 20, 25, 30, 35)	29
	$\boldsymbol{T}_c(1)\boldsymbol{S}_{10}$	$\boldsymbol{D}_{5d}$	5	1
	$\boldsymbol{T}(1)\boldsymbol{D}_{5d}$		10, 15, . . . , 35	6
$z(3,2)@(2+z)(3,2)$ $z(3,2)@(2+z)(2,3)$	$\boldsymbol{T}_2^1(\sqrt{57})\boldsymbol{D}_1$	$\boldsymbol{D}_2$	1, 3, . . . , 13	14
	$\boldsymbol{T}(\sqrt{57})\boldsymbol{D}_2$		2, 4, . . . , 14	14
$z(4,1)@(2+z)(4,1)$ $z(4,1)@(2+z)(1,4)$	$\boldsymbol{T}_2^1(\sqrt{7})\boldsymbol{D}_1$	$\boldsymbol{D}_2$	1, 3, . . . , 13 1, 3, . . . , 11	7 6
	$\boldsymbol{T}(\sqrt{7})\boldsymbol{D}_2$		2, 4, . . . , 12 2, 4, . . . , 12 (6)	6 5
	$\boldsymbol{T}_{14}^3(\sqrt{7})\boldsymbol{D}_1$	$\boldsymbol{D}_{14}$	– 13	0 1
	$\boldsymbol{T}_{14}^{13}(\sqrt{7})\boldsymbol{D}_2$		– 6	0 1
$z(7,3)@(1+z)(7,3)$ $z(7,3)@(1+z)(3,7)$	$\boldsymbol{T}(\sqrt{237})\boldsymbol{D}_1$	$\boldsymbol{D}_1$	1, 2, . . . , 7	14
$z(8,1)@(1+z)(8,1)$ $z(8,1)@(1+z)(1,8)$	$\boldsymbol{T}(\sqrt{219})\boldsymbol{D}_1$	$\boldsymbol{D}_1$	1, 2, . . . , 7	14

regularly within a ray; particularly, the translational periods of all tubes in a ray are same. Such rays, with more than six CDWCNs (altogether 223 CDWCNs) are presented in table 1. Thus, we firstly introduce precisely the CDWCN rays.

Let (n_1, n_2) and (n'_1, n'_2) be the walls of a CDWCN. The minimal SWCNs with the same chiral angle are $(\hat{n}_1, \hat{n}_2)$ and $(\hat{n}'_1, \hat{n}'_2)$, where $\hat{n}_i = n_i/n$ $(i = 1, 2)$ are co-primes, as well as $\hat{n}'_i = n'_i/n'$. The CDWCN walls may be written as $n(\hat{n}_1, \hat{n}_2)$ and $n'(\hat{n}'_1, \hat{n}'_2)$. According to (2), the ratio of the CDWCN wall diameters is rational: $D/D' = an/a'n'$; thus, the diameters of the minimal walls are proportional to the walls' periods, $(D/n)/(D'/n') = a/a' = \hat{a}/\hat{a}'$, with the co-primes $\hat{a}$ and $\hat{a}'$ given by (6). It is easy to show that $m(\hat{n}_1, \hat{n}_2)@m'(\hat{n}'_1, \hat{n}'_2)$ is a CDWCN with the same interlayer distance as $n(\hat{n}_1, \hat{n}_2)@n(\hat{n}'_1, \hat{n}'_2)$ only if $m' = n' + (m - n)\hat{a}/\hat{a}'$. Therefore, CDWCNs are grouped in the series

$$m = n + z\hat{a}' \qquad m' = n' + z\hat{a} \qquad z = 0, 1, 2, \ldots. \tag{20}$$

Particularly, if both walls have the same chiral angles, i.e. CDWCN walls are the same minimal tube $(\hat{n}_1, \hat{n}_2)$ multiplied by n and $n' = n + \nu$, this tube $n(\hat{n}_1, \hat{n}_2)@(n + \nu)(\hat{n}_1, \hat{n}_2)$ will be denoted by $(\hat{n}_1, \hat{n}_2)n@(n + \nu)$, and its right–left counterpart by $(\hat{n}_2, \hat{n}_1)n@(n + \nu)$. In such a case $\hat{a} = \hat{a}' = 1$ and according to (20), $(\hat{n}_1, \hat{n}_2)n@(n + \nu)$ is a CDWCN for each n. Such rays are very frequent, and include more than half of all CDWCNs. In our sample, besides 60 zigzag $(1, 0)n@(n + 9)$ and 35 armchair $(1, 1)n@(n + 5)$ there are 41 chiral right–right CDWCNs (and the same number of right–left ones): 14 $(3, 2)n@(n + 2)$, 13 $(4, 1)n@(n + 2)$, seven $(7, 3)n@(n + 1)$ and seven $(8, 1)n@(n + 1)$.

Also the achiral commensurate tubes with interlayer distance closest to 3.44 Å form a $\mathcal{ZZ}$ ray $(1, 0)n@(n + 9)$ (with $\Delta = 3.53$ Å) and an $\mathcal{AA}$ ray $(1, 1)n@(n + 5)$ (with $\Delta = 3.39$ Å). These rays are the most frequent CDWCNs: in our sample they are represented by 60 and 35 tubes, respectively. For all such tubes N is odd: $N = 1, 3, 9$ in $\mathcal{ZZ}$ and $N = 1, 5$ in $\mathcal{AA}$. Further, $a = a' = A$ and therefore $\hat{a} = \hat{a}' = 1$, and since for any achiral SWCN $\tilde{q} = 2$ and $r = 1$, one finds $Q = N$. This means that their roto-translational subgroup is symmorphic: $\boldsymbol{L}^{(1)} = \boldsymbol{T}\boldsymbol{C}_N$. Nevertheless, due to the glide planes, the tenth family groups are non-symmorphic. The roto-translational breaking groups for the tubes $\mathcal{ZZ}$ and $\mathcal{AA}$ are $\boldsymbol{L}^{(1)}_{\times\mathrm{A}} = \boldsymbol{T}(a/2)\boldsymbol{C}_{2nn'/N}$.

It turns out that when at least one layer is achiral the roto-translational symmetry group of a double-wall tube is symmorphic. Besides $\mathcal{ZZ}$ and $\mathcal{AA}$, there are 67 CDWCNs with one achiral wall and the other one chiral. From the remaining 156 $\mathcal{CC}$ CDWCNs (78 right–right and right–left), an additional 99 are with symmorphic symmetry. Thus, altogether there are only 60 tubes with non-symmorphic symmetry: besides $\mathcal{AA}_5$ and $\mathcal{ZZ}_9$, there are 57 $\mathcal{CC}$ with non-symmorphic roto-translational subgroup. Each of these $\mathcal{CC}$ tubes has a layer of one of the following four types: $n(3, 2)$, $n(2, 3)$, $n(4, 1)$ or $n(1, 4)$. The right–right and right–left configurations of $\mathcal{CC}$ tubes may be either both symmorphic, either one symmorphic and the other non-symmorphic, but both right–left pairs cannot be non-symmorphic. In fact, 28 right–right and 29 right–left are with non-symmorphic symmetry. As for $\mathcal{CC}$ CDWCNs, besides the symmorphic groups $\boldsymbol{T}(A)\boldsymbol{D}_N$ for $N = 1, 2, 3, 5, 9$ (international notation $\boldsymbol{L}N2$ for odd N and $\boldsymbol{L}222$ for $N = 2$), there appear only $\boldsymbol{T}^1_2(A)\boldsymbol{D}_1 = \boldsymbol{L}2_122$ (53 CDWCNs), $\boldsymbol{T}^3_{14}(A)\boldsymbol{D}_1 = \boldsymbol{L}14_522$ ((43, 25)@(60, 15), (47, 20)@(60, 15), both with $A = 13\sqrt{7}a_0$ and (52, 13)@(15, 60) with $A = \sqrt{7}a_0$) and $\boldsymbol{T}^{13}_{14}(A)\boldsymbol{D}_2 = \boldsymbol{L}14_622$ (in (24, 6)@(8, 32)).

There is no pure rotational symmetry ($N = 1$) in 243 cases. The twofold principal axis appears in 18 right and 18 left $\mathcal{CC}$ tubes. The higher rotational symmetry is related to the achiral walls: $N = 3$ for 13 $\mathcal{ZZ}$ and 8 $\mathcal{CZ}$; $N = 5$ for 7 $\mathcal{AA}$ and 2 $\mathcal{CA}$ ((30, 30)@(55, 10) and (55, 10)@(40, 40)); $N = 9$ in 7 $\mathcal{ZZ}$ and 2 $\mathcal{CZ}$ ((54, 0)@(45, 27) and (45, 27@(72, 0)) CDWCNs. The order of the isogonal group rotational axis takes on the values $Q = 1, 2, 3, 5, 9, 14$, appearing in 187, 88, 21, 9, 9 and 4 CDWCNs, respectively. It is equal to N in the case of the symmorphic roto-translational groups.

5. Discussion

Commensurate tubes are found to be very rare among possible DWCNs: in the considered sample they make only 0.5%. Their symmetry groups are determined in two steps. Firstly, assuming that the walls are coaxially arranged SWCNs, the roto-translational part is found with the help of theorem 1. The various coaxial relative positions, parametrized by two coordinates Φ and Z, have different symmetry groups, and according to the profound topological principles, one of the maximally symmetric positions should be stable. Calculations with the Lennard-Jones interatomic potential confirm this prediction, and within this model the full symmetry groups are determined. These are the fifth family groups $\boldsymbol{T}_Q^R(A)\boldsymbol{D}_N$ if at least one shell is a chiral SWCN, while if both walls are achiral the groups are either $\boldsymbol{T}(A)\boldsymbol{D}_N$ or $\boldsymbol{T}_c(A)\boldsymbol{S}_{2N}$.

Although the results are derived for the double-wall tubes, they are also valid for the multiwall ones. In fact, due to the negligible interaction of the first and the third shell, the relative position of the second and the third shell should be the same as in the CDWCN. Thus, for the rays $(n_1, n_2)n@(n+\nu)$, the next shell can be $(n+2\nu)(n_1, n_2)$ etc. These multiwall tubes have the same symmetry group as the CDWCNs. This includes all purely achiral tubes. Also, for the other types, despite various possible combinations, no new symmetry appears.

It turns out that the symmetry of a CDWCN is very small in comparison with that of the walls. The tremendous symmetry breaking is described by the breaking group (theorem 2). It is important that the wall–wall interaction $V(\Phi, Z)$ is invariant under this large group. Here, this is used to facilitate numerical determination of the stable positions. Further, the potential, due to the invariance, can be expanded in the breaking group harmonics $\cos(\mu M\Phi + \omega K Z)$ $M = 0, 1, 2, \ldots,$ $K = 0, \pm 1, \ldots.$ The constants μ and ω depend on the breaking group parameters: their product is equal to the symmetry breaking rate, which is defined [8, 7] as $Q_\times/A_\times$ (the number of points per unit cell generated from a single point by the roto-translational part of the line group). Therefore, the harmonics are very rare which results in the reduction of the interlayer interaction. In the incommensurate cases, where the periodicity is completely broken, this is manifested as the superslippery relative displacements of the walls along the DWCN axis.

Another consequence of low symmetry of CDWCNs, i.e. of the large symmetry breaking, is the small order Q of the principal axis of the isogonal group. This would be manifested in the Raman and infrared spectra. Namely, when Q is less than 4 (which is the case for 296, or 93% of the considered CDWCNs), the angular momentum quantum number m is 0 or 1. Therefore, only the parity selection rules can prevent electronic transitions, leaving roughly half of the phonon modes active. This is a huge number, in comparison with 14 or 15 Raman active modes in SWCNs [9]. However, the number of intense Raman peaks is expected to be similar to that of SWCNs, as the Raman features coming from the shells, due to the low interlayer interaction, should remain dominant in the DWCN Raman spectra. Further, as the space inversion is an element of the isogonal point group $\boldsymbol{D}_{Nd}$ of $\mathcal{ZZ}$ and $\mathcal{AA}$ tubes, Raman and infrared scatterings are due to different vibrational modes.

As CDWCNs are built of the walls characterized by the same $\mathcal{R}$ value, the same type walls are more frequent than mixed type walls: there are 132 CDWCNs with both walls metallic, the same number with both semiconducting walls, while only 54 are with different types of walls.

Finally, we point to the lack of chirality of CDWCN symmetry groups. In fact, the roto-translational groups are self-conjugated with respect to the space inversion if and only if $Q = N, 2N$. In other words symmorphic $\boldsymbol{T}\boldsymbol{C}_N$ and $\boldsymbol{T}_{2N}^1\boldsymbol{C}_N$ groups are achiral. Only four CDWCNs, those with $Q = 14$ (listed above), are chiral in this sense, despite the chirality of the wall constituents in most of the CDWCNs. Even in these exceptional cases never are both left–right pairs chiral.

Appendix A. Proofs of the theorems

First we introduce notation. For two real numbers x and x' such that x/x' is rational (x and x' are commensurate) we denote by $\underline{x}$ their greatest common divisor defined as the maximal real such that $x = \hat{x}\underline{x}$ and $x' = \hat{x}'\underline{x}$, with co-prime integers $\hat{x}$ and $\hat{x}'$. With these co-primes the lowest common multiple $\bar{x}$ is defined by $\bar{x} = \hat{x}'x = \hat{x}x' = \hat{x}\hat{x}'\underline{x}$. Further, $f = na/q$ and $f' = n'a'/q'$ denote the fractional translations in the helical generators. Using (6), it can be easily shown that $\hat{f} = \hat{a}'$ and $f' = \hat{a}$ which yield $\bar{a}/\bar{f} = \underline{a}/\underline{f} = \sqrt{\tilde{q}\tilde{q}'}$.

A.1. Proof of theorem 1

Obviously, the common pure rotational and translational subgroups are $\boldsymbol{C}_N$ and $\boldsymbol{T}(A)$, where $N = \underline{n}$ and $A = \bar{a}$. To find Q, we note that the requirement for the common helical generator $\left(C_Q^R\middle|F\right) = \left(C_q^r\middle|f\right)^t C_n^s = \left(C_{q'}^{r'}\middle|f'\right)^{t'} C_{n'}^{s'}$ is fulfilled only for $t = \hat{f}'\tau$ and $t' = \hat{f}\tau$, which yields $t = \hat{a}\tau$ and $t' = \hat{a}'\tau$. As the fractional translation is $F = NA/Q$, it follows that $Q = \sqrt{\tilde{q}\tilde{q}'}N/\tau$. The rotational part implies the identity $rt/q - r't'/q' = s'/n' - s/n$, which reduces to

$$\tau(r\hat{a}q' - r'\hat{a}'q) = \tilde{q}\tilde{q}'N(s'\hat{n} - s\hat{n}'). \tag{A.1}$$

The solution in s and s' exists if and only if τ is a multiple of $\frac{\tilde{q}\tilde{q}'N}{\mathrm{GCD}(r\hat{a}q'-r'\hat{a}'q,\tilde{q}\tilde{q}'N)}$. Since we look for the maximal value for Q, it follows that τ should be minimal, i.e. $\tau = \frac{\tilde{q}\tilde{q}'N}{\mathrm{GCD}(r\hat{a}q'-r'\hat{a}'q,\tilde{q}\tilde{q}'N)}$. Then, it is straightforward to find Q using (6). Finally, the condition for the helical generator gives the equation $(r\hat{a}\tau + \tilde{q}s)/q = R/Q$ with the unique solution in R such that $\mathrm{GCD}(R, Q) = 1$; as follows from (A.1), $s = \tau(r\hat{a}q' - r'\hat{a}'q)(\hat{n}^{\phi(\hat{n}')} - 1)/n'\tilde{q}\tilde{q}' \pmod{n/N}$.

A.2. Proof of theorem 2

The minimal rotation (combined with a translation) in the group generated by the elements of both subgroups is by an angle of $2\pi/\overline{q}$, and therefore $Q_\times = \overline{q}$. Analogously, the minimal fractional translation is $F_\times = \underline{f}$. Each element from the group $L_\times$ can be written as $l_\times = \left(C_n^s C_q^{rt}\middle|tf\right)\left(C_{n'}^{s'}C_{q'}^{r't'}\middle|f't'\right)$. For the pure rotations the translational part vanishes: $ft + f't' = 0$. As in the proof of theorem 1, this gives $t = \hat{a}\tau$ and $t' = \hat{a}'\tau$, which substituted into the rotational part of the requirement gives $s/n + s'/n' + rt/q + r't'/q' = 1/N_\times$. Again, using (6), after some simple algebra one gets $N\tilde{q}\tilde{q}'(\hat{n}'s + \hat{n}s') + N\tau\sqrt{\tilde{q}\tilde{q}'}(r\hat{a}'\hat{n}' - r'\hat{a}\hat{n}) = qq'/N_\times$. Maximal $N_\times$ fulfilling this identity is looked for:

$$N_\times = \frac{qq'}{\mathrm{GCD}(qq', N\tilde{q}\tilde{q}', \sqrt{\tilde{q}\tilde{q}'}(r\hat{a}'n' - r'\hat{a}n))} = \frac{\mathrm{LCM}(n, n')\sqrt{qq'}}{\mathrm{GCD}(\sqrt{\tilde{q}\tilde{q}'}, r\hat{a}'n'/N - r'\hat{a}n/N)}.$$

The fractional translation is now easily found from $Q_\times F_\times = N_\times A_\times$, with the help of the identity $\mathrm{LCM}(a, a') = aa'/A$. Finally, $R_\times$ can be found from the equation $\left(C_n^s C_q^{rt}\middle|tf\right)\left(C_{n'}^{s'}C_{q'}^{r't'}\middle|f't'\right) = \left(C_{Q_\times}^R\middle|F_\times\right)$. Its translation part, $ft + f't' = 1$, is solved by $t = \hat{a}^{\phi(\hat{a}')-1} + z\hat{a}'$ and $t' = -(\hat{a}^{\phi(\hat{a}')} - 1)/\hat{a}' - z\hat{a}$ (for any integer z). When substituted into the rotational part, this yields the following equation in $R_\times$:

$$\frac{qq'R_\times}{\mathrm{LCM}(q, q')} = \frac{(r\hat{a}'q' - r'\hat{a}q)\hat{a}^{\phi(\hat{a}')} + r'q\hat{a}}{\hat{a}\hat{a}'} \quad (\mathrm{mod}\ \mathrm{GCD}(N\tilde{q}\tilde{q}', r\hat{a}'q' - r'\hat{a}q)).$$

Finally, among the solutions, $R_\times$ is the unique one being a co-prime to $Q_\times$.

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