Symmetry Based Properties of the Transition Metal Dichalcogenide Nanotubes

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Abstract. The full geometrical symmetry groups (the line groups) of the monolayered, 2Hb and 3R polytypes of the inorganic MoS$_2$ and WS$_2$ micro- and nanotubes of arbitrary chirality are found. This is used to find the coordinates of the representative atoms sufficient to determine completely geometrical structure of tubes. Then some physical properties which can be deduced from the symmetry are discussed: electron band degeneracies, selection rules, general forms of the second rank tensors and potentials, phonon spectra.

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1 Introduction

Layered structures of the transition metal dichalcogenides MS$_2$ (M=Mo,W) are unstable against folding and this can lead to a formation of nanotubes or microtubes. The obtained tubes have high symmetry, which is relevant both for profound insight into their physical properties and for simplification of the calculations. The aim of this paper is to find the symmetry of ideal single-layered rhombohedral 3R and hexagonal 2Hb polytypes of MS$_2$ folded into tubes, and to discuss their general symmetry properties.

In Sect. 2.1, after a brief reminder on the line groups, the symmetry groups for all the chiralities of the monolayered (i.e. consisting of only one sulfur–transition metal–sulfur molecular layer), 2Hb and 3R single-layered polytypes of the MS$_2$ nanotubes are determined. A convenient choice of the lattice vectors enables to perform this task in analogy with single-wall carbon nanotubes. It turns out that the obtained symmetry groups are enough to generate the tubes from only 3, 6 and 9 atoms, respectively; the coordinates of these atoms are given, thus completing determination of the tubes conformations. In Sect. 3 some of many symmetry based physical properties of the nanotubes are discussed: conserved quantum numbers and band degeneracies, normal modes, second-rank tensors and potentials.

2 Symmetry of the MS$_2$ nanotubes

When molecular monolayer exhibiting trigonal symmetry is folded up, the obtained tube is a quasi-1D structure translationally periodic in the direction of tube axis and its Euclidean symmetry is described by the line group. As well as the reported 3R and 2Hb polytypes tubes, built of two and three S-M-S layers. Therefore, after a brief review on the line groups, the geometry of the structures (although still not synthesized) formed by rolling up a monolayer is considered first.

2.1 Line groups

Any quasi-1D system being translationally periodical (with period $a$) along one axis ($z$ axis, by convention) is a regular arrangement of elementary structural units conventionally called monomers. This arrangement is achieved by acting on one of the monomers by the operations forming the generalized translational group $Z$, which is either screw axis $T_{q}(a)$ (here belongs pure translational group $T_{0}(a)$) or glide plane $T_{c}(a)$ group. Also, the monomer itself may have some point group symmetry. Only those point operations leaving $z$-axis invariant are compatible with the 1D translational periodicity, meaning that the maximal axial subgroup $P$ of the monomer point group should be combined with $Z$ to get full symmetry line group. Namely, the candidates for $P$ are groups $C_{n}, S_{2n}, C_{nh}, C_{nv}, D_{n}, D_{nd}, D_{nh}$, where $n = 1, 2, \ldots$ is the principal rotational axis order. Altogether there are 13 infinite families of the line groups $L = ZP$ differing in type of either $Z$ or $P$, and with $n, q$ and $r$ enumerating groups within each family. This means that each element of a line group is of the...
form \( g = z^t C_n^t P \) \((t = 0, 1, \ldots, n-1)\), where the screw notation \( T_q^r \) is generated by \( z = (C_q^t \frac{a_n}{q} \{C_n^t\}) \) (Koster-Seitz notation), while in the glide plane case \( z = (\sigma_h \frac{a_n}{q}) \); \( C_n \) is principal axis rotation of the point group and \( P \) is some of the remaining point group operations \( U \) (the rotation for \( \pi \) around horizontal axis), \( \sigma_v \) and \( \sigma_h \) (vertical and horizontal mirror planes). Monomer is only a part of an elementary cell: the translational period of \( T_q^r \) contains \( q/n \) and 2 monomers, respectively.

Note that the value of \( r \) is not unique: together with \( r \) also \( r + m \frac{q}{n} \), \( m = \pm 1, \pm 2, \ldots \), lead to the same line group. The ambiguity is resolved by convention choosing \( r \) when it is coprime to \( q/n \).

2.2 Monolayered tubes

The monolayer M-S-M \([1]\) is consisted of the pair of the parallel sulfur planes at the distance \( \delta \approx 6\AA \), bisected by the transition metal plane (Fig. 1). All three planes are of the same trigonal lattice, with the basis vectors \( a_1 \) and \( a_2 \) of equal length \( a_0 \approx 3\AA \). While the sulfur atoms in the different planes are exactly one above another, the metal atoms are between the centers of the sulfur triangles. Thus elementary cell of the layer contains two S atoms at \((0, 0)\) (at the heights 0 and \( \delta \)) and the transition metal atom at \((1/3, 1/3)\) (at the height \( \delta/2 \)). This layer has trigonal symmetry of the diperiodic group \( D_6\text{g}_{78}=p\bar{6}m2 \) (isomorphic, with the isogonal group \( D_{3h} \)): horizontal mirror plane coincides with M-plane).

Fig. 1. (a) Perpendicular projection of the monolayer S-M-S \((\circ = \text{M}, \bullet = \text{S})\). (b) The elementary cell of the monolayer containing two overlapping sulfur and one transition metal atom. (c) Single layers of the 2Hb and 3R polytypes.

The monolayered tube \((n_1, n_2)\) is formed when this lattice is rolled up in such a way that the chiral vector \( c = n_1 a_1 + n_2 a_2 \) becomes a horizontal circle on the tube. Analogously to the carbon nanotubes, the chiral angle \( \theta = \arctan \frac{\sqrt{3}n_2}{2n_1} \) is the angle between the lattice vector \( a_1 \) and the chiral vector. Again, the chiral angles from the interval \([0, \pi/6]\) suffice for the description of all the tubes, since those with the angles from \([\pi/6, \pi/3]\) are their optical isomers (the other angles results in the same tubes, due to symmetry of the 2D lattice). Tubes \((n, 0)\), having zero chiral angle are called zig-zag \((Z\) for short), the armchair \((A)\) tubes are \((n, n)\) ones (with \( \theta = \pi/6 \)), while all others are referred as the chiral ones \((C, n_1 > n_2 > 0, \text{with } \theta \in (0, \pi/6))\).

The finite thickness of the monolayer results in different distortions of the interior and exterior parts of the tube. It is proposed \([8]\) that the transition metal cylinder is purely rolled up, while the interior and exterior sulfur ones are additionally shrunk and stretched, respectively, such that their radii are less (greater) then the metallic one for \( \delta/2 \). Although diameter, as well as many other quantitative properties (such as elastic energy or the dispersion relations), of the tube depends on the described distortions, the symmetry group, and consequently the symmetry based properties considered here are not affected by this.

The diameter of the non-distorted cylinder is \(|c|/\pi\) (the length of the chiral vector is \(\sqrt{n_1^2 + n_2^2 + n_3^2a_0} \)). Thus, the interior \(D_{in}\) (sulfur) diameter is

\[
D_{in} = \sqrt{n_1^2 + n_2^2 + n_3^2a_0 - \delta},
\]

and it will be mainly used in the following. The outer diameter is obviously \(D_{out} = D_{in} + 2a\).

The symmetry groups of the MS\(_2\) tubes are found by the procedure established for the carbon nanotubes \([1]\). It is based on the fact that roto-translational tube symmetries emerge from translational periodicity of the unfolded 2D layer. The only modification is the odd order of the diperiodic group principle axis (due to the mutual displacement of the sulfur and metallic sub-lattices), resulting in absence of the \(U\) axis. Here, only the results, obtained by an easy modification according to this difference, will be given. To this end, at first the number of the 2D lattice cells in the elementary cell of the tube \((n_1, n_2)\) is found to be

\[
q = 2\frac{n_1^2 + n_1n_2 + n_2^2}{nR} = \frac{2|c|^2}{Ra_0^2},
\]

where \(n\) is the greatest common divisor of \(n_1\) and \(n_2\), while \(R = 3\) if \(n_1 - n_2\) is multiple of \(3n\), and \(R = 1\) otherwise. Note that \(3q\) is the number of atoms in the elementary cell of the tube.

The symmetry group of the chiral tube \((n_1, n_2)\) is the first family line group

\[
L_c = T_q^r(a)C_n, \quad a = \sqrt{\frac{3q}{2nR}a_0},
\]

\[
r = \frac{n_1 + 2n_2 - \left(\frac{a_0}{n}\right)\varphi(n)}{n_1R} \pmod{\frac{q}{n}}
\]

(the Euler function \(\varphi(x)\) gives the number of coprimes not greater than \(x\)). Each cylinder is one orbit (the set of atoms generated from one of them by the group transformation) of the \(a_1\) type \([\hat{1}]\). The interior sulfur cylinder
is used to fix the coordinate system, choosing the orbit representative atom on the $x$ axis. Thus the cylindrical coordinates of the orbit representatives are

$$(D_{in}^2, 0, 0), \quad (D_{in} + \delta, \phi_0, z_0), \quad (D_{in} + \delta, 0, 0) \quad (4)$$

for interior sulfur, metal and outer sulfur, respectively.

Here, $\phi_0 = \pi n_1' + n_2', z_0 = 2\sqrt{3} \sqrt{n_1' n_2' + n_1 n_2} / n$. This orbit has trivial stabilizer (set of the group elements leaving the representative atom invariant), meaning that at each cylinder the atoms may be enumerated by the group elements.

Precisely, the action of the general element of the group (3) on the point given by the cylindrical coordinates is

$$(C_q \frac{2\pi}{n} \rho, \phi, z) = (\rho, \phi + 2\pi(\frac{n_2}{n} + \frac{2}{q}), z + \frac{2}{q} t a) \quad (5)$$

Thus, any atom in the cylinder (orbit) is given by its orbit representative and pair $(t, s)$: its coordinates are given by (3) with the corresponding representative coordinates from (4) taken for $(\rho, \phi, z)$.

The symmetry group of the zig-zag monolayered tube ($n, 0$) belongs to the eighth line group family:

$$L_z = L(2n)_m c = T_{2n}^1(\sqrt{3}a_0) C_{nv} \quad (6)$$

Again, each cylinder is single $b_1$ orbit, with the coordinates of orbit representatives given by (4), where $\phi_0 = \pi / n$ and $z_0 = \sqrt{3}a_0 / 6$. The stabilizer is $C_{1v}$, meaning that the whole orbit can be generated by the chiral group (3), with $r = 1$ and $q = 2n$. The inner diameter is $D_{in} = na_0 / \pi - \delta$.

For the armchair monolayered tube ($n, n$) the symmetry is described by the fourth line group family:

$$L_A = L(2n)_m c = T_{2n}^1(a_0) C_{nh} \quad (7)$$

The cylinders are orbits of $b_1$ type generated by the atoms positioned as in (3), with $\phi_0 = 2\pi / 3n$ and $z_0 = 0$. The stabilizer is $C_{1h}$, and the orbit is effectively generated by the chiral group again. The inner diameter is $D_{in} = \sqrt{3}a_0 / \pi - \delta$.

### 2.3 Single-layered 2Hb and 3R polytype tubes

Both WS$_2$ and MoS$_2$ crystallize in two forms (space groups P6$_3$/mmc and R3$m$), differing in stacking of the monolayers along the perpendicular direction. The single layer of the hexagonal 2Hb polytype contains two monolayers positioned so that sulfur (metal) atoms of the second monolayer are above the metal (sulfur) atoms of the first one, i.e. the second monolayer is rotated for $\pi / 3$ (around perpendicular axis through S) and then translated for $(a_1 + a_2) / 3$. Single layer of 3R polytype consists of three monolayers: the second is translated for $(a_1 + a_2) / 3$ with respect to the first (S atoms are moved above M atoms of the first monolayer), while the third one is translated for $2(a_1 + a_2) / 3$ (its M atoms get above the S atoms of the first layer). In both cases the distance between monolayers is $\Delta \approx 2A$.

According to the experimental evidence, the walls of MS$_2$ tubes are the 2Hb or 3R polytypes single layers, manifesting high stretchability of the monolayers. The nanotubes ($D_{out} < 0.1 \mu m$) grow in the hexagonal 2Hb polytype, while the microtubes ($D_{out} > 2 \mu m$) grow in rhombohedral 3R polytype. Despite different space groups of crystalline polytypes, the layers symmetry is the same isymmetric diperiodic group Dg69=p31m, with isogonal point group $C_{3v}$. In comparison to the monolayer Dg78, it does not have the horizontal mirror plane. When the layer is rolled up to the tube, such plain produce no tube symmetry, meaning that the same line group is obtained for the monolayered and both polytype single layer tubes of the same chirality. Thus, the only difference is in the number of the orbits out of which these systems are built: while the monolayered tubes have $N = 3$ orbits, the single-layered 2Hb tube consists of $N = 6$ orbits, and the single-layered 3R tube of $N = 9$ orbits.

If the inner monolayer is taken as the referent one, i.e. its orbit representative atoms have coordinates (3), the atoms generating the additional three orbits of the 2Hb single-layered tube are positioned at (in the order from the inner to the outer orbits):

$$\left(\frac{D_{in}^{(2)}}{2}, \phi_0, z_0\right), \quad \left(\frac{D_{in}^{(2)} + 2}{2}, 0, 0\right), \quad \left(\frac{D_{in}^{(2)} + 2}{2} + \delta, \phi_0, z_0\right),$$

where, $D_{in}^{(2)} = D_{in} + 2\delta + 2\Delta$ is the inner diameter of the second monolayer. As for six additional orbit representative atoms of 3R tubes one finds

$$\left(\frac{D_{in}^{(3)}}{2}, \phi_0, z_0\right), \quad \left(\frac{D_{in}^{(3)} + 2}{2}, 2\phi_0, 2z_0\right), \quad \left(\frac{D_{in}^{(3)} + 2}{2} + \delta, \phi_0, z_0\right),$$

for the middle monolayer; the coordinates for the third monolayer having the inner diameter $D_{in}^{(3)} = D_{in} + 4\delta + 4\Delta$, are:

$$\left(\frac{D_{in}^{(3)}}{2}, 2\phi_0, 2z_0\right), \quad \left(\frac{D_{in}^{(3)} + 2}{2} + \delta, 0, 0\right), \quad \left(\frac{D_{in}^{(3)} + 2}{2} + \delta, 2\phi_0, 2z_0\right).$$

These data refer to the arbitrary chiral direction $(n_1, n_2)$. In the special cases of zig-zag and armchair directions, the results are obtained taking by substituting the values given for the corresponding monolayers for $\phi_0$ and $z_0$.

### 3 Symmetry determined properties of MS$_2$ nanotubes

Many physical properties are based on symmetry. Also, the symmetry enables applications of the powerful group theoretical techniques in solving various physical problems. In this paper, the presented symmetry classification of the transition metal dichalcogenide tubes is used to derive some of their physical properties determined by symmetry, postponing the applications to various symmetry based calculations (band structures, selection rules, etc.).
3.1 Quantum numbers and band degeneracies

Symmetry determines quantum numbers extensively used in almost all problems (e.g. selection rules, bands assignment). Translational periodicity is reflected in the conserved quasi-momentum \( k \), taking on the values from the 1D Brillouine zone \((-\pi/a, \pi/a]\). For the armchair tubes, it can be taken from the irreducible domain \([0, \pi/a]\) only since the horizontal mirror plane \( \sigma_h \) makes \( k \) and \(-k\) equivalent. The \( z \)-component of the quasi-angular momentum \( m \) is the quantum number due to the symmetry of the isogonal rotations: since the order of the principle axis of symmetry is \( 4 \), since the horizontal mirror plane \( \sigma_h \) makes \( k \) and \(-k\) equivalent. The \( z \)-component of the quasi-angular momentum \( m \) is the quantum number due to the symmetry of the isogonal rotations: since the order of the principle axis makes \( k \) and \(-k\) equivalent. The quantum numbers are frequently used, at the cost of more complicated selection rules.

Alternatively, the conserved quantum numbers of helical \( (\tilde{k} \in [0, q\pi/na]) \) and pure angular quasi momenta \((\tilde{m})\), taking on the integer values from the interval \((-\frac{\pi}{a}, \frac{\pi}{a}]\) can be used. The former is related to the momentum conjugated to the screw axis generated helix, and it obviously incorporates a part of the angular momentum. The remaining part \( \tilde{m} \) is conserved, since it corresponds to the order \( n \) principle axis of symmetry of the tubes.

The zig-zag (armchair) tubes have additional quantum number \( A/B \) (i.e. +/-) of parity with respect to the vertical (horizontal) mirror plane. Due to this extra symmetry the two dimensional irreducible representations appear, i.e. the degeneracy of the energy bands can be at most double or if the time-reversal symmetry of the (spin-independent) Hamiltonian is taken into account, the maximal degeneracy is fourfold.

Concerning the chiral tubes, their energy bands are nondegenerate (as far as the time-reversal symmetry is not included).

3.2 Normal modes

The classification of the vibrational bands depends only on the symmetry group and the orbits out of which the system is formed. The general classification has been performed already for all orbit types of the line groups \([7]\). Since for the considered tubes are decomposed to the orbits in the previous section, the results for each of the found orbits are to be summed only.

All the tubes considered here consist of a finite number of the orbits of the same type. The symmetry group and (henceforth) orbit type depend on the chiral vector, not on the polytype (monolayer, 2Hb or 3R): \( a_1 \) orbit for the chiral tubes and \( b_1 \) orbits for zig-zag and armchair tubes (recall that these tubes have different symmetries; i.e. while for the zig-zag tube the \( b_1 \) orbit representative lay in the vertical mirror plane, for the armchair tube it is in the horizontal plane). On the contrary, the number of orbits is determined by the polytype: there is \( N = 3, 6, 9 \) orbits in the monolayered, 2Hb, 3R tubes, respectively. Thus the first step in lattice dynamics study can be performed by the classification of the vibrational bands, giving the band quantum numbers. Taking the dynamical representation decomposition \([3]\) for the found orbit types, the phonons (normal modes) are classified. For the chiral tubes one obtains

\[
D^\text{dyn}_C = 3N \sum_k \sum_{m} \tilde{k} A_{\tilde{m}},
\]

where the summation is performed over \( \tilde{k} \in (-\frac{q\pi}{na}, \frac{q\pi}{na}] \) and integers \( \tilde{m} \in (-\frac{\pi}{a}, \frac{\pi}{a}] \). It follows that there are \( 3Nn \) vibrational bands assigned by the quantum number \( \tilde{m} \).

The representations \( \tilde{k} A_{\tilde{m}} \) are one dimensional, meaning that the bands are non-degenerate. Still, since the Hamiltonian is real, the time reversal symmetry leads to the double degeneracy of the bands over \( \tilde{k} \in (0, \frac{\pi}{na}] \): the energies of the phonons with quantum numbers \((\tilde{k}, \tilde{m})\) and \((\tilde{k}, -\tilde{m})\) are equal.

The corresponding decompositions for the zig-zag and armchair tubes are:

\[
D^\text{dyn}_Z = N \sum_{\tilde{k} \in (-\frac{\pi}{a}, \frac{\pi}{a})} \left[ 2kA_0 + 2kA_n + kB_0 + kB_n + N \sum_{m=1}^{n-1} kE_m \right],
\]

\[
D^\text{dyn}_A = N \sum_{m=-n}^{n} \sum_{m=-n+1}^{n} (aA_m + 2aA_n) + 3N \sum_{k \in (0, \frac{\pi}{a})} \sum_{m=-n+1}^{n} kE_m + 3N \sum_{m=1}^{n} \pi E_m,
\]

Here, \( kA_m \) and \( kB_m \) correspond to non-degenerate \( m \)-bands of different vertical mirror parity, while \( kE_m \) denotes the double degenerate band. As for the armchair tubes, the second term classifies the double degenerate bands, while the terms with \( k = 0 \) and \( k = \pi \) give insight in the bands topology (touching at the Brillouine zone boundaries) and horizontal mirror parity of \( k = 0 \) modes.

These decompositions can be used to simplify further vibrational band calculations by standard methods. The obtained bands are automatically assigned by good quantum numbers so that Raman and IR spectra can be directly extracted by selection rules \([4]\), as the relevant line group is found.

3.3 Second rank tensors

As the symmetry classification of the MS\(_2\) tubes has been completed the general matrix forms of the symmetric polar and axial second-rank tensors for systems with line group symmetry \([4]\) can be used to predict many of the
physical properties. Here the optical activity of the isolated nanotubes will be analysed. In order to avoid influence of the other effects, birefringence and anisotropy of absorption, only the activity along the optical axis is discussed. The optically active medium rotates the plane of polarization of a linearly polarized incident light beam incoming along the optical axis, defined by the unit vector e = (e_1, e_2, e_3), through an angle \( \sum a_{ij}e_i e_j a_{ij} \) per unit length, where \( a_{ij} \) denote optical activity tensor elements. As this tensor is axially symmetric second rank tensor, i.e. a polar symmetric second-rank tensor is needed to predict the spatial orientation of the optical axes. The optical activity tensor does not vanish the chirality and of the dielectric tensor for the chiral tubes with \( q = 2n \) and \( r = 1 \), this means that the summation in (11) is performed only over the terms with \( K \) and \( M \) of the same parity. The additional symmetries are manifested as relations between the coefficients \( \omega_K^M(\rho), \epsilon_K^M(\rho) \). The invariance of the potential of the zig-zag (armchair) tubes under vertical (horizontal) mirror plane \( \sigma_v \) (\( \sigma_h \)) means \( V(\rho, \varphi, z) = V(\rho, -\varphi, z) \) (i.e. \( V(\rho, \varphi, z) = V(\rho, -\varphi, -z) \)); this leads to the general form of the potential:

\[
V_Z(\rho, \varphi, z) = \sum_{K = -\infty}^{\infty} \sum_{M = -\infty}^{\infty} \omega_K^M(\rho) \cos \left( M \pi \rho / a \right) e^{i(2\pi / a)Kz} + \\
+ \sum_{K = -\infty}^{\infty} \sum_{M = -\infty}^{\infty} \epsilon_K^M(\rho) \cos \left( M \pi \rho / a \right) e^{i(2\pi / a)Kz};
\]

\[
V_A(\rho, \varphi, z) = \sum_{K = -\infty}^{\infty} \sum_{M = -\infty}^{\infty} \omega_K^M(\rho) e^{iM\varphi} \cos \left( 2\pi / a \right) e^{i(2\pi / a)Kz} + \\
+ \sum_{K = -\infty}^{\infty} \sum_{M = -\infty}^{\infty} \epsilon_K^M(\rho) e^{iM\varphi} \cos \left( 2\pi / a \right) e^{i(2\pi / a)Kz}.
\]

The obtained potentials can be further specified. When the Taylor expansion of \( \alpha_K^M(\rho), \omega_K^M(\rho), \epsilon_K^M(\rho) \) is performed the terms of the same order in \( \rho \) should form the invariant polynomial of the relevant line group, i.e. these coefficients are polynomials over the integrity basis of the line group.

4 Concluding remarks

Geometry of the tubes is completely defined: line groups, number and type of orbits, coordinates of the atom representing orbits are specified generally, i.e. for the tubes of arbitrary chirality. In addition to the rotational, translational and screw axes symmetry of the \( (n_1, n_2) \), \( 0 < n_2 < n_1 \) tubes, the armchair and zigzag tubes are invariant under reflection in the mirror planes: the horizontal and the vertical one, respectively. This leads to the parities of their quantum states which now can be degenerate in contrast to the chiral nanotube quantum states (as far as the time-reversal symmetry is not considered) are non-degenerate. Thus, the complete symmetry groups of the chiral, armchair and zig-zag tubes are:

\[
L_C = T_q^r C_n,
\]

\[
L_A = L_C + \sigma_h L_C = T_q^r C_{nh},
\]

\[
L_Z = L_C + \sigma_v L_C = T_q^r C_{nv}.
\]

Note that the parameters \( q \) and \( r \) of the helical group have the same form as the ones of the corresponding single-wall carbon nanotubes.
properties. First, the good quantum numbers, characterizing the nanotube quantum states are found: the translational, helical and rotational symmetries are reflected in the conserved quasi-momenta $k$, $\tilde{k}$ and $\tilde{m}$. The isogonal angular momentum $m$ is also used in combination with $k$, although it is not a conserved quantity. The ranges of these momenta are given. The vertical (horizontal) mirror plane of zig-zag (armchair) tubes introduces the additional parity quantum numbers denoted by $A$ and $B$ (+ and −) for even and odd states, respectively.

The above enumerated quantum numbers are used in assignment and a priori degeneracy prediction of electronic and vibrational bands. No geometry caused degeneracy is expected for the chiral tubes, and while for the zig-zag and armchair tubes double degeneracy in the interior of the irreducible domain is obligate. Besides the time reversal symmetry, which, when appropriate, doubles these degeneracies, the diameter of the tube is also relevant in this context. Namely, the diperiodic symmetry of the single 2Hb and 3R layers (as well as that of monolayer) imposes six fold degeneracy of the bands in the interior of 2D Brillouine zone. Thus, for the large diameter tubes several (six for chiral and three for achiral ones) bands are to become quasi degenerate. This effect should be observable in microtubes.

Also, the tensors of optical activity and dielectric permeability are studied. The optical activity of the chiral tubes and inactivity of the arm-chair and zig-zag ones is demonstrated. In fact, these results are typical, meaning that the same forms must be obtained for any symmetric axial (polar) second rank tensor.

Finally, the general forms of the potentials in nanotubes are given, thus enabling the generalization of the Bloch theorem to the line group symmetry: by multiplication of the invariant potential functions with irreducible representation matrix elements all the symmetry allowed covariant and wave functions can be obtained.

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