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Modified group projectors: tight-binding method

M Damnjanović, T Vuković and I Milošević

Faculty of Physics, University of Belgrade, PO Box 368, 11001 Belgrade, Yugoslavia

E-mail: yqoq@afrodita.rcub.bg.ac.yu

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Abstract. The symmetry implantation in the tight-binding method is analysed. A transparent algorithm is proposed to calculate eigenvalues and eigenvectors with automatic assignment by the complete set of conserved quantum numbers. For crystals, the energy bands are obtained with no summation over the lattice, while the eigenvectors are symmetry-adapted generalized Bloch states. The method is applied to the electronic π -bands of single-wall carbon nanotubes: together with the dispersion relations, their assignment by the full symmetry (line group) quantum numbers (linear, helical and angular momenta and parities) is performed and the corresponding symmetry-adapted eigenstates are found. It is argued that these novel quantum numbers prevent conductivity in all but armchair tubes.

1. Introduction

The tight-binding approach is one of the most frequently used and developed techniques in research on complex molecular and especially solid state systems [1]. Although based on deep (but *a posteriori* justified) physical approximations (e.g. one-particle concept, short-range interactions), its efficiency promotes it as the first-choice tool in almost all energy band calculations, frequently immediately giving satisfactory final results. Incorporation of symmetry in such calculations is important: besides the reduction of the calculations, the obtained assignment of the eigenenergies by the conserved quantum numbers enables further qualitative analyses utilizing selection rules.

The aim of this paper is to give a complete formalism of the symmetry implantation within the tight-binding method. Besides the formal rigorousness enlightening the whole context and scope of applicability, the benefits of this approach are that from the beginning it uses the full symmetry group (still allowing us to restrict it to a subgroup for some particular needs), and results in a precisely defined minimal algorithm. The full group treatment yields assignment by the maximal set of conserved quantum numbers, enabling usage of all possible selection rules. The mentioned minimality refers both to the set of necessary input data and to the procedure itself: only the minimal subsystem, i.e. the atoms which generate the whole system by the action of the group, is used (e.g. not the elementary cell of a crystal, but its basic domain which by the total space group generates the crystal; this is a single atom in the case of carbon nanotubes [2]).

Let S be the system with the symmetry group G . The set of group transformations (rotations, reflections, translations, ...) leaving an atom of S , say x , invariant form a stabilizer subgroup of x . The other transformations of G map x into other atoms forming a subsystem of S called the orbit of x . Thus, the group action divides the system into disjoint orbits.

Within the tight-binding model, each atom contributes to the total state space by its own space; this, so-called *interior*, space is usually of low dimension and depends on the problem considered. For example, this is the space spanned by the (several) relevant atomic orbitals when electronic structure is studied, the three-dimensional space of the ion displacements from the stable configuration in studies of vibrations, the spin space when magnons are looked for etc. Due to symmetry, all the atoms of the same orbit introduce the same interior space into the total space. While the conformation of the system is obviously completely defined when one (arbitrary) atom from each orbit, the *orbit representative*, is given, the interior spaces of these representatives completely determine the total state space of the considered tight-binding model. It is then intuitively plausible to expect that the complete calculations can be reduced to the interior spaces of orbit representatives only.

We realize this task rigorously in section 2, using modified group projector technique [3] for induced representations (sketched in subsection 2.1). The analysis of the structure of the total state space (in subsection 2.2) shows that it is the sum of the induced spaces, thus requiring further development of the technique. The transfer operators, generalizing the Bloch procedure for translational periodicity to the full symmetry group, interrelate total space with the orbit representative subspace. This strongly affects the structure of the Hamiltonian, so that its eigenvalue problem can be completely solved using part of the orbit representative space only, namely the range of the modified projector. To illustrate the main points of the procedure, the single-wall carbon nanotube (SWCT) electronic bands are found in section 3. The application of their recently determined full symmetry group [4] within the proposed method results in the simple derivation of the dispersion relations (given in table 2), automatically assigned by the complete set of quantum numbers: in addition to the linear (or helical) and angular momenta commonly used [5, 6], the parities are introduced. The main characteristics of the presented method are summarized in section 4, where also some general consequences of the novel parity quantum numbers in physics of nanotubes are discussed.

2. Tight-binding Hamiltonian in the multi-orbit induced spaces

Introducing adjusted notation, we start with a reminder on the necessary notions of the modified group projector technique [3]. Then these results are generalized to the multi-orbit case, which is sufficient to treat any tight-binding problem.

2.1. Reminder on the modified group projector technique for induced representations

In the state space $\mathcal{S} = \mathcal{S}_D$ let the group act by the representation $D(\mathbf{G})$ decomposing onto the irreducible components $D^{(\mu)}(\mathbf{G})$ of dimension $|\mu|$ as $D(\mathbf{G}) = \oplus_{\mu} a_{\mu} D^{(\mu)}(\mathbf{G})$, i.e. a_{μ} is its frequency number. The symmetry-adapted or standard basis (SAB) $\{|\mu t_{\mu} m\rangle\}_{\mu}$; $t_{\mu} = 1, \dots, a_{\mu}$; $m = 1, \dots, |\mu|$ is a basis satisfying

$$D(g)|\mu t_{\mu} m\rangle = \sum_{m'=1}^{|\mu|} D_{m'm}^{(\mu)}(g)|\mu t_{\mu} m'\rangle \quad \forall g \in \mathbf{G}. \quad (1)$$

The SAB can be found by the modified group projector technique (to avoid summation over group in the commonly used group projector method, which makes it inappropriate for direct numerical implementations and introduces conceptual problems when non-compact groups are dealt with). For each irreducible component $D^{(\mu)}(\mathbf{G})$ with $a_{\mu} > 0$, the initial space \mathcal{S}_D is directly multiplied by the dual $\mathcal{H}^{(\mu)*}$ of the space of $D^{(\mu)}(\mathbf{G})$, giving the space carrying the auxiliary representation $\Gamma^{\mu}(\mathbf{G}) \stackrel{\text{def}}{=} D(\mathbf{G}) \otimes D^{(\mu)*}(\mathbf{G})$. The range $\mathcal{R}(\Gamma^{\mu})$ of the

modified group projector $G(\Gamma^\mu) \stackrel{\text{def}}{=} \frac{1}{|G|} \sum_g \Gamma^\mu(g)$ is its fixed point subspace. Any basis $\{|\mu t_\mu\rangle \mid \mu = 1, \dots, a_\mu\}$ of $\mathcal{R}(G(\Gamma^\mu))$ yields the μ -part of the SAB as the partial scalar products with the standard basis $\{|\mu^* m\rangle \mid m = 1, \dots, |\mu|\}$ of $\mathcal{H}^{(\mu^*)}$:

$$|\mu t_\mu m\rangle = \langle \mu^* m \mid \mu t_\mu \rangle \quad t_\mu = 1, \dots, a_\mu \quad m = 1, \dots, |\mu|. \quad (2)$$

If the basis is required to be simultaneously a symmetry-adapted and eigenbasis (SAEB) of the Hamiltonian H (naturally, H commutes with $D(G)$), the vectors $|\mu t_\mu\rangle$ should be chosen as the eigenvectors of $H \otimes I_\mu$ (the identity operator in $\mathcal{H}^{(\mu^*)}$ is denoted by I_μ).

The method is especially powerful when $D(G)$ has inductive structure $D(G) = \delta(S \uparrow G) \otimes d(G)$, where $\delta(S)$ is a representation (called interior) of the subgroup S and $d(G)$ any representation (called exterior) of G . In the problem considered here no external representation appears, and it should be omitted (i.e. substituted by the trivial representation). Let $Z = \{z_p \mid p = 0, \dots, |Z| - 1\}$ (with $|Z| = |G|/|S|$) be a left transversal of S , i.e. a chosen set of coset representatives in the partition $G = \sum_{p=0}^{|Z|-1} z_p S$ of G onto the cosets $z_p S$. By convention, z_0 is the identity element e . Then for any fixed $g \in G$ and $z_p \in Z$ there are unique $s(g, z_p) \in S$ and the index $p(g)$ satisfying $g = z_p s(g, z_p) z_{p(g)}^{-1}$ (e.g. for $g = z_p$, $s(z_p, z_p) = z_{p(z_p)} = e$, i.e. $p(z_p) = 0$). Given the interior representation $\delta(S)$ (in the space \mathcal{S}_δ with the basis $\{|\psi\rangle \mid \psi = 1, \dots, |\delta|\}$), we look for the SAB of the induced representation $D(G) = \delta(S \uparrow G)$. The modified procedure deals with two auxiliary representations for each irreducible component $D^{(\mu)}(G)$: $\Gamma^\mu(G) = D(G) \otimes D^{(\mu)*}(G)$ in the space $\mathcal{S}_{\Gamma^\mu} = \mathcal{S}_D \otimes \mathcal{H}^{(\mu^*)} = \oplus_p \mathcal{S}_{p\gamma^\mu}$ (its operators are $\Gamma^\mu(g) = \sum_p E_{p(g)}^p \otimes \beta_p^\mu \gamma^\mu(s(g, z_p)) \beta_{p(g)}^{\mu\dagger}$), and its pulled down subgroup representation $\gamma^\mu(S) = \delta(S) \otimes D^{(\mu)*}(G \downarrow S)$ (the restricted representation is denoted by \downarrow) in $\mathcal{S}_{\gamma^\mu} = \mathcal{S}_\delta \otimes \mathcal{H}^{(\mu^*)}$. The spaces $\mathcal{S}_{p\gamma^\mu}$ are the replicas of $\mathcal{S}_{0\gamma^\mu} \equiv \mathcal{S}_{\gamma^\mu}$. The matrices E_q^p (with vanishing all but pq th element, which equals one) are used to switch between these spaces; together with the operators $\beta_p^\mu = I_\delta \otimes D^{(\mu)*}(z_p)$ in \mathcal{S}_{γ^μ} they give the transfer operators $E_0^p \otimes \beta_p^\mu : \mathcal{S}_{\gamma^\mu} \rightarrow \mathcal{S}_{p\gamma^\mu}$. The modified group projector $G(\Gamma^\mu)$ is essentially equivalent to the pulled down projector $S(\gamma^\mu)$ (onto the fixed point space of $\gamma^\mu(S)$) by the partial isometry $B^\mu : \mathcal{S}_{\gamma^\mu} \rightarrow \mathcal{S}_{\Gamma^\mu}$:

$$G(\Gamma^\mu) = B^\mu \{E_0^0 \otimes S(\gamma^\mu)\} B^{\mu\dagger} \quad B^\mu = \frac{1}{\sqrt{|Z|}} \sum_t E_t^0 \otimes \beta_t^\mu. \quad (3)$$

Finally, the basis $|\mu t_\mu\rangle^0$ of the range of $S(\gamma^\mu)$ determines the vectors $|\mu t_\mu\rangle = B^\mu |\mu t_\mu\rangle^0$, giving the SAB $|\mu t_\mu m\rangle$ by (2):

$$|\mu t_\mu m\rangle = \langle \mu^* m \mid (B^\mu |\mu t_\mu\rangle^0) \rangle. \quad (4)$$

2.2. Multi-orbit systems and tight-binding Hamiltonian

As explained in the introduction, a complex system S (e.g. molecule, crystal, multi-layer, polymer etc) with the symmetry group G is composed of several subsystems S^P ($P = 1, 2, \dots$), each being an orbit of G . Let the corresponding stabilizers and transversals be S^P and Z^P . When an atom from a subsystem S^P is taken as the orbit representative, the transversal elements z_p^P biuniquely map it to all the other atoms of the same orbit. Thus the atoms of the system are enumerated by the pairs (Pp) of the orbit and the transversal element indices; especially, the chosen orbit representative is $(P0)$.

In the tight-binding analysis each atom of the orbit S^P contributes to the relevant state space \mathcal{S} by δ^P atomic orbitals $|(Pp)\psi\rangle$ ($\psi = 1, \dots, \delta^P$) spanning the interior space $\mathcal{S}_{p\delta^P}$; the action of the stabilizer element s^P on $|(Pp)\psi\rangle$ gives the linear combination of the orbitals from the same atom, $\sum_{\phi=1}^{\delta^P} \delta_{\phi\psi}^P (s^P) |(Pp)\phi\rangle$, defining the interior representation $\delta^P(S^P)$ (thus

$\delta^P = |\delta^P(S^P)|$. The direct sum of the interior spaces gives the total state space $\mathcal{S} = \mathcal{S}_D$, with a basis $\{|(Pp)\psi\rangle \mid \forall P, p, \psi\}$. In this space the group acts by its representation $D(G)$, which is naturally reduced into the orbit subspaces: given the basis vector $|(P0)\psi\rangle$, each group element g is uniquely written in the form $z_p^P s^P$ with $s^P \in S^P$, and therefore

$$D(g)|(P0)\psi\rangle = D(z_p^P)(\delta^P(s^P)|(P0)\psi\rangle) = \sum_{\phi}^{\delta^P} \delta_{\phi\psi}^P(s^P)|(Pp)\phi\rangle. \quad (5)$$

Since the orbit representative choice is arbitrary, this relation shows that the group action interrelates the orbitals from the same orbit only. Thus, the direct sum of the interior spaces over each orbital is an invariant space for $D(G)$. Further, (5) shows that in each of these invariant subspaces the group action is inductive [7], implying the final conclusion that the total representation is of multi-orbit induced type, i.e. it is the direct sum $D(G) = \oplus_P D^P(G)$ of several induced representations. Therefore, the results of the previous section are to be generalized to such a case, with each $D^P(G) = \delta^P(S^P \uparrow G)$ being an induced representation from the subgroup S^P (with the transversal Z^P) and the interior representation $\delta^P(S^i)$.

Considering the SAB only, the generalization of the procedure is straightforward. In fact, the corresponding auxiliary representation of the modified technique is itself partially reduced in the inductive spaces $\mathcal{S}_{\Gamma^{P\mu}}$:

$$\Gamma^\mu(G) = D(G) \otimes D^{(\mu)*}(G) = \oplus_P \Gamma^{P\mu}(G) \quad \Gamma^{P\mu}(G) = D^P(G) \otimes D^{(\mu)*}(G).$$

Therefore it is pulled down into the orbit representative space $\mathcal{S}_{\gamma^\mu} = \oplus_P \mathcal{S}_{\gamma^{P\mu}}$ for each component (orbit) $\Gamma^{P\mu}$ independently, and the transfer operator, mapping \mathcal{S}_{γ^μ} into \mathcal{S}_{Γ^μ} , is an obvious generalization of (3):

$$B^\mu = \sum_P B^{P\mu} \quad B^{P\mu} = \frac{1}{\sqrt{|Z^P|}} \sum_{p \in Z^P} E_{P0}^{Pp} \otimes \beta_p^{P\mu} \quad (6)$$

with $\beta_p^{P\mu} = I_{\delta^P} \otimes D^{(\mu)*}(z_p^P)$. Finally, the pulled down projector is

$$G^\downarrow(\Gamma^\mu) = \sum_P B^{P\mu\dagger} G(\Gamma^{P\mu}) B^{P\mu} = \sum_P E_{P0}^{P0} \otimes S^P(\gamma^{P\mu}). \quad (7)$$

Note the possibility of obtaining the SAB independently in each subspace \mathcal{S}_{D^P} using (4).

Further, let the Hamiltonian be given and SAEB is looked for. By the modified prescription the auxiliary operator $H_\mu = H \otimes I_\mu$ (in $\mathcal{S}_D \otimes \mathcal{H}^{(\mu)*}$) is pulled down to the space \mathcal{S}_{γ^μ} by B^μ , giving

$$H_\mu^\downarrow \stackrel{\text{def}}{=} B^{\mu\dagger} H_\mu B^\mu = \sum_{PQ} E_{Q0}^{P0} \otimes \frac{\sum_{pq} \beta_p^{P\mu\dagger} h_{Qq}^{Pp} \beta_q^{Q\mu}}{\sqrt{|Z^P||Z^Q|}} \quad (8)$$

where

$$h_{Qq}^{Pp} = \left(\sum_{\phi, \psi} h_{Qq\psi}^{Pp\phi} |\phi\rangle \langle \psi| \right) \otimes I_\mu \quad (9)$$

are the (rectangular) submatrices in the decomposition $H_\mu = \sum_{PQ} \sum_{pq} E_{Qq}^{Pp} \otimes h_{Qq}^{Pp}$. Commutativity of H with $D(G)$ interrelates these matrices: for the transversal elements the conditions $[H, D(z_p^P)] = 0$ give $h_{Qq}^{Pp} = (\delta^P(s^P(z_q^Q, z_p^P)) \otimes I_\mu) h_{Q0}^{Pp(z_q^Q)}$, and (8) becomes

$$H_\mu^\downarrow = \sum_{PQ} E_{Q0}^{P0} \otimes \frac{\sum_{pq} \gamma^{P\mu\dagger}(s^P(z_q^{Q^{-1}}, z_p^P)) \beta_p^{P\mu\dagger} h_{Q0}^{Pp}}{\sqrt{|Z^P||Z^Q|}}. \quad (10)$$

Since H_μ^\downarrow commutes with the projector $G^\downarrow(\Gamma^\mu)$, the vectors $|\mu t_\mu\rangle^0$ should be chosen as the eigenvectors of H_μ^\downarrow from the range of $S(\gamma^\mu)$: $H_\mu^\downarrow|\mu t_\mu\rangle^0 = \epsilon_{\mu t_\mu}|\mu t_\mu\rangle^0$ and $G^\downarrow(\Gamma^\mu)|\mu t_\mu\rangle^0 = |\mu t_\mu\rangle^0$. Finally, the expansion (4) gives the vectors $|\mu t_\mu m\rangle$. It can be directly checked that the obtained basis is the required SAEB of H , with the same eigenvalues $\epsilon_{\mu t_\mu}$. Vectors $|\mu t_\mu\rangle^0$ are linear combinations of the vectors from various $S_{\gamma^p\mu}$, i.e. vectors of the SAEB mix the states from different orbit spaces \mathcal{S}_{D^p} .

In particular, if all the subgroups S^P have common transversal Z , and Z is itself a subgroup of G (i.e. when $G = ZS^P$ is a weak direct product), then $s^P(z_q^{-1}, z_p) = e$ for any p and q , simplifying the form of the pulled down Hamiltonian:

$$H_\mu^\downarrow = \sum_{PQ} E_{Q0}^{P0} \otimes \sum_p \beta_p^{\mu^\dagger} h_{Q0}^{Pp}. \quad (11)$$

Besides the single-electron approximation yielding the inductive multi-orbit structure of the state space, the tight-binding model involves also the assumptions on the mutually interacting neighbours. This Hamiltonian determining approximation is to be incorporated in (10) and (11). Precisely, it is assumed that each atom (Pp) interacts with N^P neighbours ($Pp; n$) ($n = 1, \dots, N^P$) through coupling coefficients $V_{\psi\phi}^{Pn}$ between the involved orbitals (the numbers of interacting neighbours and coupling coefficients are the same for all the atoms from the same orbit). So, the Hamiltonian is

$$H = \sum_P \sum_{n=1}^{N^P} \sum_{p=0}^{|Z^P|-1} \sum_{\psi=1}^{\delta^P} \sum_{\phi=1}^{\delta^{[Pp;n]}} V_{\phi\psi}^{Pn} |(Pp; n)\phi\rangle \langle (Pp)\psi| \quad (12)$$

where $[Pp; n]$ is the orbit to which the neighbour ($Pp; n$) belongs. Therefore, using in (9) the matrix elements $h_{Q0\psi}^{Pp\phi} = \sum_{n=1}^{N^Q} V_{\phi\psi}^{Qn} \delta_{(Q0;n)}^{(Pp)}$ (δ_j^i is the Kronecker delta) determined by (12), the pulled down Hamiltonian becomes

$$H_\mu^\downarrow = \sum_Q \sum_{n=1}^{N^Q} E_{Q0}^{[Q0;n]0} \otimes \left\{ \gamma_{Q(Q0;n)}^{[Q0;n]\mu} \beta_{(Q0;n)}^{[Q0;n]\mu^\dagger} \left(\sum_{\phi=1}^{\delta^{[Q0;n]}} \sum_{\psi=1}^{\delta^Q} V_{\phi\psi}^{Qn} |\phi\rangle \langle \psi| \otimes I_\mu \right) \right\} \quad (13)$$

where

$$\gamma_{Qp}^{P\mu} = (|Z^Q| |Z^{[Q0;n]}|)^{-1/2} \sum_q \gamma^{P\mu^\dagger}(s^P(z_q^{-1}, z_p^P)).$$

Finally, when there is a common transversal, being a subgroup in G , (11) reduces to the simple sum over neighbours:

$$H_\mu^\downarrow = \sum_Q \sum_{n=1}^{N^Q} E_{Q0}^{[Q0;n]0} \otimes \left\{ \beta_{(Q0;n)}^{[Q0;n]\mu^\dagger} \left(\sum_{\phi=1}^{\delta^{[Q0;n]}} \sum_{\psi=1}^{\delta^Q} V_{\phi\psi}^{Qn} |\phi\rangle \langle \psi| \otimes I_\mu \right) \right\}. \quad (14)$$

3. SWCN bands

Symmetry groups L_C of chiral (n_1, n_2) , and $L_{Z,A}$ of zig-zag $(n, 0)$ and armchair (n, n) SWCTs (C , Z and A tubes for short) are the line groups [4] given in the factorized and international notation

$$L_C = T_q^r D_n = L_{q_p} 22 \quad L_{Z,A} = T_{2n}^1 D_{nh} = L_{2n_n} / mcm \quad (15)$$

with the translational period $a = a_0 \sqrt{3q/2n\mathcal{R}}$. Here $a_0 = 2.461 \text{ \AA}$ is the honeycomb lattice period, while n , q , p , r and \mathcal{R} are defined in terms of n_1 and n_2 . The parameters $\tilde{q} = q/n$ and q are even since $\tilde{q} = 2 \pmod{12}$, while n and p are even iff both n_1 and n_2 are even; also $q > 10$ for the realistic tubes (having diameters $D = a_0 \sqrt{\mathcal{R}nq/2}/\pi > 3.4 \text{ \AA}$).

The factorized notation shows that these groups are weak direct products of the cyclic groups generated by $(C_q^r | a/\tilde{q})$, C_n and U for L_C , and additionally σ_x for $L_{Z,A}$ (the horizontal axis U and vertical mirror plane σ_x define the coordinate system, as presented in the figure 1, showing a fragment of honeycomb lattice which is rolled up to form the nanotube). Thus, their elements are monomials

$$\ell(t, s, u, v) = \left(C_q^r \left| \frac{a}{\tilde{q}} \right. \right)^t C_n^s U^u \sigma_x^v \quad (16)$$

with $t = 0, \pm 1, \dots, s = 0, \dots, n-1, u = 0, 1$ and $v = 0$ for L_C and $v = 0, 1$ in $L_{Z,A}$.

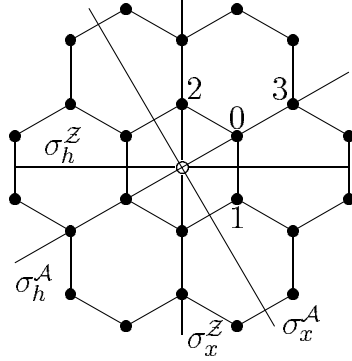


Figure 1. The nearest neighbours of the C atom $0 = (000)$ are the atoms $i = (000, i)$ ($i = 1, 2, 3$). Perpendicular to the figure at \circ is the U -axis taken as the x -axis of the coordinate system; $\sigma_{x/h}^{Z/A}$ represents the vertical (xz) and the horizontal (xy) mirror planes of Z and A tubes.

Each SWCT is a single-orbit system. The type of the orbit according to the classification in [8], the stabilizer and the transversal are given in table 1. In all cases the transversal is the group $T_q^r D_n$. It is used to enumerate the atoms: the transversal element $\ell(t, s, u) = \ell(t, s, u, 0)$ maps the orbit representative atom C_{000} , with the radius vector in the cylindrical coordinate system of figure 1

$$r_{000} = \left(\frac{D}{2}, \phi_0, z_0 \right) \quad \phi_0 = 2\pi \frac{n_1 + n_2}{nq\mathcal{R}} \quad z_0 = \frac{n_1 - n_2}{\sqrt{6nq\mathcal{R}}} a_0 \quad (17)$$

into the atom C_{tsu} with the coordinates $r_{tsu} = (D/2, (-1)^u \phi_0 + 2\pi(t/q + s/n), (-1)^u z_0 + tna/q)$. Experimental data justified the plausibility of the simple tight-binding nearest-neighbour model. Each C atom contributes one p^\perp (i.e. graphene p_z) orbital $|tsu\rangle$ (the notation is simplified: the capital and the Greek indices for orbits and interior space vectors, taking on only the value 1, are omitted). The orbital $|tsu\rangle$ spans the (one-dimensional) interior space carrying the trivial stabilizer representation $\delta(\mathcal{S}) = 1(\mathcal{S})$, since the p^\perp orbital is obviously invariant under the stabilizer elements. Thus in the total tight-binding space \mathcal{S} , being spanned by all these orbitals, the symmetry group acts by the induced representation $D(\mathcal{G}) = 1(\mathcal{S} \uparrow \mathcal{G})$. The pulled down modified projector with the irreducible representation $D^{(\mu)}(\mathcal{G})$ (see the appendix) becomes $\mathcal{S}(D^{(\mu)*}) = \sum_{s \in \mathcal{S}} D^{(\mu)*}(s) / |\mathcal{S}|$, and the dimension of its range gives the frequency number a_μ of $D^{(\mu)}(\mathcal{G})$ in $D(\mathcal{G})$.

The model assumes the interaction with three nearest neighbours (see figure 1). Therefore, the pulled down Hamiltonian reads

$$H_\mu^\downarrow = \sum_{i=0}^3 V_i D^{(\mu)*}(\ell(t_i, s_i, u_i)). \quad (18)$$

Table 1. Orbits and neighbours of SWCTs. For \mathcal{C} , \mathcal{Z} and \mathcal{A} tubes their line group, orbit type, stabilizer and transversal group are in the columns G , O , S and Z . Then follow the parameters t_i and s_i ($u_i = 1$) defining the nearest neighbours of the initial atom in the form $(000; i) = C_{t_i s_i}$.

	G	O	S	Z	(000; 1)	(000; 2)	(000; 3)
\mathcal{C}	$L_{\mathcal{C}}$	a_1	$\{e\}$	$T_q^r D_n$	$t_1 = -\frac{n_2}{n}$ $s_1 = \frac{2n_1 + (1+r\mathcal{R})n_2}{q\mathcal{R}}$	$t_2 = \frac{n_1}{n}$ $s_2 = \frac{(1-r\mathcal{R})n_1 + 2n_2}{q\mathcal{R}}$	$t_3 = t_1 + t_2$ $s_3 = s_1 + s_2$
\mathcal{Z}	$L_{\mathcal{Z}\mathcal{A}}$	b_1	$\{e, C_n \sigma_x\}$	$T_{2n}^1 D_n$	$t_1 = 0$ $s_1 = 1$	$t_2 = 1$ $s_2 = 0$	$t_3 = 1$ $s_3 = 1$
\mathcal{A}	$L_{\mathcal{Z}\mathcal{A}}$	d_1	$\{e, \sigma_h\}$	$T_{2n}^1 D_n$	$t_1 = -1$ $s_1 = 1$	$t_2 = 1$ $s_2 = 0$	$t_3 = 0$ $s_3 = 1$

Here, $\ell(t_i, s_i, u_i)$ is the transversal element which maps the initial atom into its neighbour $(000; i)$; it is given in table 1. By $i = 0$ in equation (18) the initial atom itself is included (the diagonal term of the Hamiltonian); nevertheless, its contribution to the energy is reduced to the additive constant V_0 , and hereafter it is omitted. Further, since the distortions of the honeycomb lattice induced by rolling up are nearly homogeneous, all the remaining coupling constants are taken to be equal: $V_1 = V_2 = V_3 = V$ (estimated between -2.7 and -2.5 eV).

Finally, using the irreducible representations from the appendix and the data from table 1, the Hamiltonian and the modified projectors are pulled down and the results are presented in table 2 (the projectors are given by the bases of their ranges in the last column). The general dispersion relations for the bands of \mathcal{C} , \mathcal{Z} and \mathcal{A} tubes are, respectively,

$$\epsilon_{E_m}^{\pm}(k) = \pm|V| \sqrt{\sum_{i=1}^3 (1 + 2 \cos \psi_i)} \quad (19a)$$

$$\epsilon_{G_m}^{\pm}(k) = \pm|V| \sqrt{1 + 4 \cos \frac{ka}{2} \cos \frac{m\pi}{n} + 4 \cos^2 \frac{m\pi}{n}} \quad (19b)$$

$$\epsilon_{\tilde{G}_m}^{\pm}(k) = \pm|V| \sqrt{1 + 4 \cos \frac{ka}{2} \cos \frac{m\pi}{n} + 4 \cos^2 \frac{ka}{2}}. \quad (19c)$$

The angles used in (19a) are

$$\psi_1 = -ka \frac{n_2}{q} + 2\pi m \frac{2n_1 + n_2}{qn\mathcal{R}} \quad \psi_2 = ka \frac{n_1}{q} + 2\pi m \frac{n_1 + 2n_2}{qn\mathcal{R}} \quad (20)$$

while $\psi_3 = \psi_2 - \psi_1$. Substituting them in (19a) by

$$\tilde{\psi}_1 = -\tilde{k}a \frac{n_2}{q} + 2\pi \tilde{m} \frac{2n_1 + (1+r\mathcal{R})n_2}{qn\mathcal{R}} \quad \tilde{\psi}_2 = \tilde{k}a \frac{n_1}{q} + 2\pi \tilde{m} \frac{(1-r\mathcal{R})n_1 + 2n_2}{qn\mathcal{R}} \quad (21)$$

($\tilde{\psi}_3 = \tilde{\psi}_2 - \tilde{\psi}_1$) one obtains the $\epsilon_{E_m}^{\pm}(\tilde{k})$ bands assigned by the helical quantum numbers $\tilde{k}\tilde{m}$ alternatively used in the literature. To find the standard basis $|\mu t_{\mu} m\rangle$ it suffices to apply (4), with β_{tsu}^{μ} and $|\mu t_{\mu}\rangle^0$ given in table 2. For example, the bands of the representations ${}_k E_m^{\mathcal{A}}$ of the \mathcal{Z} tubes correspond to the symmetry adapted generalized Bloch states:

$$|kmA\rangle_{\pm} = \frac{1}{\sqrt{|Z|}} \sum_{ts} e^{-i(\frac{m\pi}{n} + \frac{ka}{2})t} (|(ts0)\rangle \pm e^{ih_m^k} |(ts1)\rangle) \quad (22a)$$

$$|-k, m, A\rangle_{\pm} = \frac{1}{\sqrt{|Z|}} \sum_{ts} e^{-i(\frac{m\pi}{n} - \frac{ka}{2})t} (|(ts1)\rangle \pm e^{ih_m^k} |(ts0)\rangle) \quad (22b)$$

where $h_m^k = \arg\{V(e^{i\psi_1} + e^{i\psi_2} + e^{i(\psi_1+\psi_2)})\}$.

Table 2. Bands and symmetry-adapted eigenvectors of the carbon nanotubes. For each irreducible component $D^{(\mu)}(L)$ of $D(L) = 1(S \uparrow L)$ its frequency number a_μ , energy $\epsilon_{\mu t_\mu}$, the transfer operator β_{tsu}^μ and the pulled down standard eigenbasis $|\mu t_\mu\rangle^0$ (in terms of the SAB of tables A1 and A2) are presented. The matrices M_2, K_2, O_2, M_4, K_4 and O_4 are given in the appendix; $\gamma = \arg(1 + 2e^{i\frac{ka}{2}} \cos \frac{\pi m}{n})$.

\mathcal{C}	a_μ	$\epsilon_{\mu t_\mu}$	β_{tsu}^μ	$ \mu t_\mu\rangle^0$
$0A_m^\Pi$	1	$V\Pi(1 + 2e^{2i\frac{m\pi}{q}})$	$\Pi^u e^{-im(rt+s\tilde{q})\frac{2\pi}{q}}$	$ 0m\Pi\rangle$
πA_m^Π	1	$-V\Pi$	$\Pi^u e^{-i(m(rt+s\tilde{q})\frac{2\pi}{q} + \frac{t\pi}{q})}$	$ \pi m\Pi\rangle$
kE_m	2	(19a)	$K_2^*(\frac{kt}{q})M_2^*(m\frac{tr+s\tilde{q}}{q})O_2^u$	$\frac{ km\rangle \pm e^{i\frac{h_k^k}{m}} -k, -m\rangle}{\sqrt{2}}$
$0\tilde{A}_m^\Pi$	1	$V\Pi(1 + 2e^{2i\frac{\tilde{m}\pi}{n}})$	$\Pi^u e^{-i\tilde{m}s\frac{2\pi}{n}}$	$ 0\tilde{m}\Pi\rangle$
$\tilde{\pi}A_m^\Pi$	1	$-V\Pi$	$\Pi^u (-1)^t e^{-i\tilde{m}s\frac{2\pi}{n}}$	$ \tilde{\pi}\tilde{m}\Pi\rangle$
$\tilde{k}E_{\tilde{m}}$	2	(19a)	$K_2^*(\frac{\tilde{k}t}{q})M_2^*(s\tilde{m})O_2^u$	$\frac{ \tilde{k}\tilde{m}\rangle \pm e^{i\frac{h_{\tilde{k}}^{\tilde{k}}}{\tilde{m}}} -\tilde{k}, -\tilde{m}\rangle}{\sqrt{2}}$
\mathcal{Z}	a_μ	$\epsilon_{\mu t_\mu}$	β_{tsu}^μ	$ \mu t_\mu\rangle^0$
$0A_m^\Pi$	1	$V\Pi(1 + 2e^{i\frac{m\pi}{n}})$	$\Pi^u e^{-i\frac{m\pi}{n}t}$	$ 0m\Pi A\rangle$
$0E_m^\Pi$	1	$V\Pi(1 + 2\cos \frac{m\pi}{n})$	$\Pi^u M_2(-\frac{2s+t}{2}m)O_2^u$	$\frac{ 0m\Pi\rangle + e^{i\frac{m2\pi}{n}} 0, -m, \Pi\rangle}{\sqrt{2}}$
kE_m^A	2	$\pm V \sqrt{5 + 4e^{i\frac{m\pi}{n}} \cos \frac{ka}{2}}$	$e^{-i\frac{m\pi}{n}t} K_2(-\frac{kt}{2})O_2^u$	$\frac{ kmA\rangle \pm e^{i\frac{h_k^k}{m}} -k, m, A\rangle}{\sqrt{2}}$
$\pi E_{\frac{n}{2}}^\Pi$	1	$-V\Pi$	$(-i)^t (-1)^s \Pi^u K_2(-\frac{t\pi}{2a})$	$\frac{ \frac{\pi}{a}, \frac{n}{2}, \Pi\rangle - \frac{\pi}{a}, -\frac{n}{2}, \Pi\rangle}{\sqrt{2}}$
kG_m	2	(19b)	$K_4(-\frac{kt}{2}, -m\frac{t+2s}{2})O_4^u$	$\frac{ km\rangle + e^{i\frac{m2\pi}{n}} k, -m\rangle}{2}$ $\pm e^{i\gamma} \frac{ -k, m\rangle + e^{i\frac{m2\pi}{n}} -k, -m\rangle}{2}$
\mathcal{A}	a_μ	$\epsilon_{\mu t_\mu}$	β_{tsu}^μ	$ \mu t_\mu\rangle^0$
$0\Pi_m^+$	1	$V\Pi(1 + 2e^{i\frac{m\pi}{n}})$	$\Pi^u e^{-i\frac{m\pi}{n}t}$	$ 0, m, +, \Pi\rangle$
$0E_m^+$	2	$\pm V \sqrt{5 + 4\cos \frac{m\pi}{n}}$	$M_2(-\frac{2s+t}{2}m)O_2^u$	$\frac{ 0m+\rangle \pm e^{i\frac{h_0^0}{m}} 0, -m, +\rangle}{\sqrt{2}}$
kE_m^Π	1	$V\Pi(1 + 2e^{i\frac{m\pi}{n}} \cos \frac{ka}{2})$	$\Pi^u e^{-i\frac{m\pi}{n}t} K_2(-\frac{kt}{2})O_2^u$	$\frac{ km\Pi\rangle + -k, m, \Pi\rangle}{\sqrt{2}}$
$\pi E_{\frac{n}{2}}^\Pi$	1	$-V\Pi$	$(-i)^t (-1)^s \Pi^u K_2(-\frac{t\pi}{2a})$	$\frac{ \frac{\pi}{a}, \frac{n}{2}, \Pi\rangle + \Pi \frac{\pi}{a}, -\frac{n}{2}, \Pi\rangle}{\sqrt{2}}$
kG_m	2	(19c)	$K_4(-\frac{kt}{2}, -m\frac{t+2s}{2})O_4^u$	$\frac{ km\rangle \pm e^{-i\frac{h_k^k}{m}} k, -m\rangle}{2}$ $+ \frac{ -k, m\rangle \pm e^{-i\frac{h_k^k}{m}} -k, -m\rangle}{2}$

4. Summary

The modified group projector technique is applied to find the SAB for the sum $D(G) = \bigoplus_P \delta^P(S^P \uparrow G)$ of the induced interior representations $\delta^P(S^P)$ of arbitrary subgroups S^P of G . It is shown that this basis is the expanded basis $|\mu t_\mu\rangle^0$ of the range of the pulled down projector $G^\downarrow(\Gamma^\mu) = \sum_P E_{P0}^P \gamma^{P\mu}(S^P)$ in the low-dimensional auxiliary space (orbit representative spaces multiplied by dual irreducible space). The same procedure is applied when the standard basis, being also the eigenbasis of the Hamiltonian H , is looked for: then in the range of $G^\downarrow(\Gamma^\mu)$ the eigenvectors $|\mu t_\mu\rangle^0$ of the pulled down Hamiltonian H_μ^\downarrow are to be found. For the tight-binding Hamiltonian the general expression for the operators H_μ^\downarrow is found.

These results enable calculation of the crystal energy bands, by a transparent procedure. The inputs are orbit stabilizers (these may be generally tabulated for the group with no reference to the system, column 3 of table 1 in the example studied here) and the system-dependent coupling coefficients and the data characterizing neighbours in terms of the group

elements (columns 4–6 of table 1). The bands, automatically assigned by the full set of symmetry quantum numbers, are found as the eigenvalues of the Hamiltonian pulled down to the orbit representative subspace. The corresponding eigenvectors (the last column in table 2) are straightforwardly transferred to the generalized Bloch eigenstates with the help of the operators (6) (being the sum of the operators β^μ given in table 2). Note that the modified procedure enables us to find the SAEB using the subgroup generators only [3], i.e. no summation over group elements appears in the procedure, since the completely symmetry adapted states are used from the very beginning. In the standard prescriptions [1], one starts with partially adapted states, e.g. Bloch functions adapted to the translational subgroup, which enlarges the dimension of the eigenproblem (the elementary cell may contain a large number of atoms from each orbit), while the remaining symmetry is independently analysed afterwards. The physical contents of the operator $\gamma_{Qp}^{P\mu}$ from (13) is essentially geometrical: the different transversals Z^P and Z^Q arrange the atoms on the corresponding orbits differently. Even when the two orbits have the same transversal, since in general it is not a subgroup, the successive elements are not arranged homogeneously. Thus, the sum over the orbit S^Q involved in $\gamma_{Qp}^{P\mu}$ averages relative positions of S^Q and S^P atoms. The terms in the sum are mutually equal when the relative positions of the corresponding atoms on the two orbits are constant, provided by homogeneous action of the same transversal when it is a subgroup. In any case, this geometrical factor depends only on the involved pair of orbits, and can be calculated (and tabulated) *a priori*, independently of the system under study.

The method is applied to find energy bands and corresponding eigenfunctions of the carbon nanotubes [2]. Although the band dispersion relations have been already calculated in the literature for both km [5] and $\tilde{k}\tilde{m}$ quantum numbers [6], only a part of the symmetry group (screw axis and principal rotational axis) has been used, while the parities have been neglected. Such incomplete band assignation can produce errors in studying various processes, since the selection rules incorporating parities are more severe, forbidding some otherwise allowed interband transitions. Also the generalized Bloch eigenfunctions have the most precise form only when the full symmetry is used. The necessity for full symmetry group treatment is enforced by the fact that the peaks of the density of states mostly correspond to the even or odd states, i.e. to the representations with parities. An illustration of the profound importance of this novel quantum number arises from conductivity analysis: it is known that the simplest tight-binding model predicts conductivity in all the tubes (n_1, n_2) with $n_1 - n_2$ divisible by three, since the pair of bands with the same $m = m_F$ is crossed at $k_F = 2\pi/3a$ if $\mathcal{R} = 3$ or $k_F = 0$ if $\mathcal{R} = 1$ (the Fermi level is $E_F = 0$). On the other hand, the non-crossing rule prevents crossing of bands having all the quantum numbers the same. Since U -parity characterizes bands only at $k = 0$ and π , the bands differing only by this parity at $k = 0$ should attain a secondary gap in any more accurate analysis (this gap must be finite for $k \neq 0$, and continuity implies the gap at $k = 0$). Looking at table 2 one easily concludes that only the armchair tubes may be conductive, since only for them are there bands with the same m differing in σ_x parity: these are the bands with $m = 0, n$. Finally, one checks that for $m_F = n$ the bands corresponding to ${}_k E_n^A$ and ${}_k E_n^B$ indeed cross (at $k_F = 2\pi/3a$). Of course, this method can be easily performed for the less simplified model, where the coupling coefficients are not mutually equal. Then the dispersion relation (19a) is generalized to

$$\epsilon_m^\pm(k) = \pm \sqrt{\sum_i \left(V_i^2 + 2 \frac{V_1 V_2 V_3}{V_k} \cos \psi_k \right)}. \quad (23)$$

The band crossing appears now only for the armchair tubes, when $V_1 = V_2 < V_3$ (again $m_F = n$). Further advantages of the band assignation by the complete set of quantum numbers, e.g. influence on the band topology and density of states, will be analysed elsewhere.

Table A1. Irreducible representations of L_C classified by the km and $\tilde{k}\tilde{m}$ quantum numbers. For the irreducible representations denoted in the first column, possible values of k and m (\tilde{k} and \tilde{m}) are given in the second column, and then the matrices of the generators follow. Finally, the SAB is given in terms of quantum numbers. Only for integer $m = n/2, q/2, -p/2, (q-p)/2$ do the corresponding representations appear. (*) $k = 0$ with $m \in (0, \frac{q}{2})$, and $k = \frac{\pi}{a}$ with $m \in (-\frac{p}{2}, \frac{q-p}{2})$ and $k \in (0, \frac{\pi}{a})$ with $m \in (-\frac{q}{2}, \frac{q}{2}]$.

IR	(k, m)	$\left(C_q^r \left \frac{a}{\tilde{q}} \right.\right)$	C_n	U	SAB
${}_k A_m^{\Pi^U}$	$k = 0, m = 0, \frac{q}{2}$ $k = \frac{\pi}{a}, m = -\frac{p}{2}, \frac{q-p}{2}$	$e^{i(mr \frac{2\pi}{q} + k \frac{a}{\tilde{q}})}$	$e^{im \frac{2\pi}{n}}$	Π^U	$ km \Pi^U\rangle$
${}_k E_m$	(*)	$M_2\left(\frac{mr}{\tilde{q}}\right) K_2\left(\frac{k}{\tilde{q}}\right)$	$M_2(m)$	O_2	$ km\rangle$ $ -k, -m\rangle$
${}_{\tilde{k}} A_{\tilde{m}}^{\Pi^U}$	$\tilde{k} = 0, \tilde{q} \frac{\pi}{a}, \tilde{m} = 0, \frac{n}{2}$	$e^{i\tilde{k} \frac{a}{\tilde{q}}}$	$e^{i\tilde{m} \frac{2\pi}{n}}$	Π^U	$ \tilde{k}\tilde{m} \Pi^U\rangle$
${}_{\tilde{k}} E_{\tilde{m}}$	$\tilde{k} = 0, \tilde{q} \frac{\pi}{a}, \tilde{m} \in (0, \frac{n}{2})$ $\tilde{k} \in (0, \tilde{q} \frac{\pi}{a}), \tilde{m} \in (-\frac{n}{2}, \frac{n}{2}]$	$K_2\left(\frac{\tilde{k}}{\tilde{q}}\right)$	$M_2(\tilde{m})$	O_2	$ \tilde{k}\tilde{m}\rangle$ $ -\tilde{k}, -\tilde{m}\rangle$

Table A2. Irreducible representations of $L_{\mathcal{Z}\mathcal{A}}$ classified by the km quantum numbers. For the irreducible representations denoted in the first column allowed values of k and m are given in the second column, and then the matrices of the generators follow. Finally, the SAB is given in terms of quantum numbers. Only for n even does ${}_{\pi} E_{n/2}^{\Pi^U}$ appear.

IR	(k, m)	$\left(C_{2n}^1 \left \frac{a}{2} \right.\right)$	C_n	U	σ_x	SAB
${}_0 A/B_m^{\Pi^h}$	$k = 0, m = 0, n$	$e^{im \frac{\pi}{n}}$	1	$\Pi^h \Pi^v$	Π^v	$ 0m \Pi^h \Pi^v\rangle$
${}_0 E_m^{\Pi^h}$	$k = 0, m \in (0, n)$	$M_2\left(\frac{m}{2}\right)$	$M_2(m)$	$\Pi^h O_2$	O_2	$ 0m \Pi^h\rangle$ $ 0, -m, \Pi^h\rangle$
${}_k E_m^{A/B}$	$k \in (0, \frac{\pi}{a}), m = 0, n$ $k = \frac{\pi}{a}, m = 0$	$e^{i \frac{m\pi}{n}} K_2\left(\frac{k}{2}\right)$	I_2	$\Pi^v O_2$	$\Pi^v I_2$	$ km \Pi^v\rangle$ $ -k, m, \Pi^v\rangle$
${}_{\pi} E_{\frac{n}{2}}^{\Pi^U}$	$k = \frac{\pi}{a}, m = \frac{n}{2}$	$i K_2\left(\frac{\pi}{2a}\right)$	$-I_2$	$\Pi^U I_2$	O_2	$\left\{ \frac{\pi}{a}, \frac{n}{2}, \Pi^U \right\}$ $\left\{ \frac{\pi}{a}, -\frac{n}{2}, \Pi^U \right\}$
${}_k G_m$	$k \in (0, \frac{\pi}{a}), m \in (0, n)$ $k = \frac{\pi}{a}, m \in (0, \frac{n}{2})$	$K_4\left(\frac{k}{2}, \frac{m}{2}\right)$	$M_4(m)$	O_4	V_4	$ km\rangle, k, -m\rangle,$ $ -k, m\rangle, -k, -m\rangle$

Appendix. Irreducible representations of L_C and $L_{\mathcal{Z}\mathcal{A}}$

There are two physically based classification of the irreducible representations of the non-symorphic line groups (such as the considered ones), differing in the quasi-momenta used: quantum numbers labelling representations may be either k and m of linear and angular quasi-momenta, or \tilde{k} and \tilde{m} of helical (includes linear and a part of angular) and remaining angular momenta. As for the \mathcal{C} tubes, both are used in the literature (see e.g. [5] for km and [6] for $\tilde{k}\tilde{m}$ classification), while for the \mathcal{Z} and \mathcal{A} tubes only the former, as has been done in this paper.

Note that m is not a conserved quantum number, since it emerges in the isogonal point group: it is not a subgroup of the non-symorphic symmetry group.

Due to the U -axis in L_C and $L_{Z,A}$ the linear quasi-momentum k runs over the irreducible domain $[0, \pi/a]$ (and $\tilde{k} \in [0, \tilde{\pi}]$ with $\tilde{\pi} = \tilde{q}\pi/a$), being half of the Brillouin zone. In its interior the representations are grouped in the k -series differing by m (or \tilde{k} -series differing by \tilde{m}). At the boundaries some representations of L_C have U -parity quantum number $\Pi^U = \pm 1$ denoted as the superscript $+/-$. As for the group $L_{Z,A}$ the superscript $+/-$ stands for σ_h -parity (with respect to the horizontal mirror plane $\sigma_h = U\sigma_x$) $\Pi^h = \pm 1$, except for the representations ${}_{\pi}E_{n/2}^{\pm}$, where it corresponds to $\Pi^U = \pm 1$; additionally, some of the k -series and boundary representations of $L_{Z,A}$ have a quantum number of σ_x -parity $\Pi^v = \pm 1$, denoted by A/B , respectively. The representations are given by the matrices of the group generators. In the tables I_n and O_n stand for n -dimensional diagonal and off-diagonal unit matrices respectively; the two-dimensional diagonal matrices are $M_2(m) = \text{diag}[e^{im2\pi/n}, e^{-im2\pi/n}]$, $K_2(k) = \text{diag}[e^{ika}, e^{-ika}]$, while $M_4(m) = I_2 \otimes M_2(m)$, $K_4(k, m) = K_2(k) \otimes M_2(m)$ and $V_4 = I_2 \otimes O_2$ are four dimensional.

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