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Generalized Bloch states and potentials of nanotubes and other quasi-1D systems II

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Abstract
A generalized Bloch theorem for systems with line group symmetry (e.g., nanotubes, stereo-regular polymers, quasi-one-dimensional crystals) shows that single-particle eigenfunctions are essentially composed of two factors: a function which is invariant under the symmetry transformations and a function which determines the symmetry of the state. Here we derive the representative functions for all irreducible representations of the line groups.

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The discoveries of various types of nanotubes [1–3] and other quasi-one-dimensional nanostructures such as nanowires and nanosprings [4] stressed the necessity of applying line groups in nanophysics [6].

The line groups [11] describe symmetries of systems with periodicity in one direction only (the z-axis by convention) and due to the lack of the crystallographic restrictions there are infinitely many such groups (in contrast to the finite number of the diperiodic and space groups). Eighty of them can be seen as subgroups of the space groups and they are also called *rod groups* [12].

The symmetry adapted basis (SAB) of the single-particle quantum state space $\mathcal{L}(\mathbb{R}^3)$ is a necessary prerequisite in any quantum mechanical study. The generalized Bloch theorem for systems with symmetry described by line groups shows that single-particle eigenfunctions are essentially composed of two factors [13]: a function which is invariant under the symmetry transformations and a function which determines the symmetry of the state. This paper addresses the problem of finding representative functions for all irreducible representations of the line groups.

After a brief reminder about the line groups, the covariant functions are derived and explicitly incorporated into the generalized form of the Bloch theorem.

The line groups consist of symmetries of structures that are periodic along a single direction. The periodicity of the line groups is not restricted to the translational one, but includes generalizations to regular incommensurate structures. Namely, each line group is a product $\boldsymbol{L} = \boldsymbol{Z}\boldsymbol{P}_n$ of an axial point group $\boldsymbol{P}_n$ (n is the order of its principal axis) and an infinite cyclic group of generalized translations $\boldsymbol{Z}$, which may be either a screw axis $\boldsymbol{T}_Q(f)$ or a glide plane $\boldsymbol{T}_c(f)$, generated by $(C_Q|f)$ (where the Koster–Seitz symbol denotes rotation by $2\pi/Q$ around the principal axis, which is conveniently chosen as the z-axis, followed by translation by f along the same axis) and $(\sigma_v|f)$, respectively.

There are infinitely many line groups and they are gathered into 13 families. Only the groups from the first family are Abelian while the groups from the other families have a first family group as a halving subgroup or as an index four subgroup.

Transformation ℓ of the line group $\boldsymbol{L}$ acts on a function $F(\boldsymbol{r})$ according to the coordinate representation $D(\boldsymbol{L})$ defined as

$$D(\ell)F(\boldsymbol{r}) \stackrel{\text{def}}{=} F(\ell^{-1}\boldsymbol{r}). \tag{1}$$

It is a reducible representation and each irreducible representation $D^{(\lambda)}(\boldsymbol{L})$ (of the dimension $|\lambda|$) of $\boldsymbol{L}$ is a component of $D(\boldsymbol{L})$ with frequency number $f^{\lambda} = f$. A symmetry adapted basis of $\mathcal{L}(\mathbb{R}^3)$ thus consists of the functions $\Psi^{(\lambda)l}(\boldsymbol{r})$ satisfying

$$D(\ell)\Psi_t^{(\lambda)l}(\boldsymbol{r}) \stackrel{\text{def}}{=} \Psi_t^{(\lambda)l}(\ell^{-1}\boldsymbol{r}) = \sum_{l'=1}^{|\lambda|} D_{l'l}^{(\lambda)}(\ell)\Psi_t^{(\lambda)l'}(\boldsymbol{r}), \qquad t = 1, \ldots, f, \qquad l = 1, \ldots, |\lambda|. \tag{2}$$

Index t distinguishes between f multiplets formed by covariants counted by the row index l (with λ and t fixed).

In particular, invariants or harmonics are the functions $\Psi_t^{(0)1}(\boldsymbol{r})$ corresponding to the identity representation $D^{(\lambda=0)}(\ell) = 1$, and they form the basis of the f-dimensional subspace $\mathcal{L}_0(\mathbb{R}^3)$; this subspace contains all the fixed points of the group action (1). Generally, to each irreducible representation we associate the subspace $\mathcal{L}^{(\lambda)}(\mathbb{R}^3) = \oplus_l \mathcal{L}^{(\lambda)l}(\mathbb{R}^3)$ of $\mathcal{L}(\mathbb{R}^3)$, where the f-dimensional subspaces $\mathcal{L}^{(\lambda)l}(\mathbb{R}^3)$ are spanned by the covariants $\Psi_t^{(\lambda)l}(\boldsymbol{r})$ for $t = 1, \ldots, f$. This allows the generalization of the Bloch theorem: the subspaces $\mathcal{L}^{(\lambda)l}(\mathbb{R}^3)$ can be obtained multiplying $\mathcal{L}^{(0)}(\mathbb{R}^3)$ by suitably chosen representative functions $\Psi_{00}^{(\lambda)l}(\boldsymbol{r})$, which are independent of t.

The aim of this paper is to present the representative functions for each irreducible representation of all line groups.

It is convenient to use cylindrical coordinates, as the line group transformations do not affect the radial coordinate ρ. This means that SAB functions are factorized in the form $R(\rho)\Phi^{(\lambda)l}(\varphi, z)$. Here, only the functions $\Phi^{(\lambda)l}(\varphi, z)$, defined on the cylinder, determine the transformation rules of the total function. Consequently, the symmetry adapted basis in the space of the functions over cylinder is to be found, and then the symmetry adapted basis in the total space $\mathcal{L}(\mathbb{R}^3)$ is obtained by multiplying this by any basis of radial functions. Altogether, the generalized Bloch form of the symmetry adapted basis in the total space is

$$\Psi_{IKM}^{(\lambda)l}(\boldsymbol{r}) = R_{IK}^{M}(\rho)\Phi_{00}^{(\lambda)l}(\varphi, z)H_K^M(\varphi, z), \tag{3}$$

where $\Phi_{00}^{(\lambda)l}(\varphi, z)$ are representative functions looked for, while $H_K^M(\varphi, z)$ and $R_{IK}^M(\rho)$ are harmonics and radial basis. The indices M and K together count the different appearances of $D^{(\lambda)}(\boldsymbol{L})$ in the space of the functions over cylinder, i.e. they take the role of t in this space (of course, the frequency number in this space is again the same for all the irreducible representations, $f_C^{\lambda} = f_C$). Further, index I, for fixed M and K counts a basis of the functions $R_{IK}^M(\rho)$ in the space of the functions over ρ. Note that the representative functions $\Phi_{00}^{(\lambda)l}(\varphi, z)$ for fixed λ form themselves a multiplet corresponding to $D^{(\lambda)}(\boldsymbol{L})$.

A basis of the cylindrical invariants has explicitly been found recently [13]. Covariant functions, i.e. the functions transforming according to the nonsymmetric irreducible representations, will be tabulated here.

The first family line groups are Abelian having thus only one-dimensional irreducible representations [9] which are classified by *helical* ($\tilde{k}$ and $\tilde{m}$) quasi-momenta:

$$_{\tilde{k}}A_{\tilde{m}}\big((C_q^r|f)^t C_n^s\big) = \mathrm{e}^{\mathrm{i}(\tilde{k}ft+\tilde{m}\frac{2\pi}{n}s)}, \qquad \tilde{k} \in \left(-\frac{\pi}{f}, \frac{\pi}{f}\right], \qquad \tilde{m} \in \left(-\frac{n}{2}, \frac{n}{2}\right]. \tag{4}$$

Only for commensurate groups (when $Q = q/r$, [13]) *linear* momenta (k and m) can be used to get another classification:

$$_{k}A_{m}\big((C_q^r|f)^t C_n^s\big) = \mathrm{e}^{\mathrm{i}(kft+m\frac{2\pi}{Q}tm\frac{2\pi}{n}s)}, \qquad k \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right], \qquad m \in \left(-\frac{q}{2}, \frac{q}{2}\right]. \tag{5}$$

With helical quantum numbers (for the linear ones the procedure is quite analogous), the condition (2) reduces to the system of the eigenequations (for each generator one independent), with eigenvalues being matrix elements of the irreducible representations:

$$D\big(C_q^r|f\big)\Phi_{00}^{(\tilde{k}\tilde{m})}(\varphi, z) = \mathrm{e}^{\mathrm{i}\tilde{k}f}\Phi_{00}^{(\tilde{k}\tilde{m})}(\varphi, z) \quad D(C_n)\Phi_{00}^{(\tilde{k}\tilde{m})}(\varphi, z) = \mathrm{e}^{\mathrm{i}2\pi\frac{\tilde{m}}{n}}\Phi_{00}^{(\tilde{k}\tilde{m})}(\varphi, z). \tag{6}$$

This way the subspace of the covariants with fixed quasi-momenta is completely determined, and the representative functions may be taken in the form:

$$\Phi_{00}^{(\tilde{k}\tilde{m})}(\varphi, z) = \mathrm{e}^{-\mathrm{i}\tilde{m}\varphi+\mathrm{i}(\frac{2\pi\tilde{m}}{Qf}-\tilde{k})z}, \qquad \Phi_{00}^{(km)}(\varphi, z) = \mathrm{e}^{-\mathrm{i}(m\varphi+kz)}. \tag{7}$$

Multiplying representative functions by harmonics one gets complete SAB $\Phi_{KM}^{(km)}(\varphi, z) = \Phi_{00}^{(km)}(\varphi, z)H_M^K(\varphi, z)$, where $H_M^K(\varphi, z)$ is the first family harmonic. Note that each $\Phi_{KM}^{(km)}$ is itself a representative function and $\Phi_{00}^{(km)}$ is taken by convention.

All other line group families, as non-Abelian, have two- and/or four-dimensional irreducible representations as well. The corresponding representative functions are constructed from the first family ones, with then the help of the inductive procedure. Namely, the first family line groups are the halving subgroup for the families 2–8, while the later are the halving subgroups for the families 9–13. Therefore, conditions (6) are to be complemented by one (for the families 2–8) or two (families 9–13) equations. The results are listed in table 1, and here we only briefly discuss the procedure used in the calculations.

Note that according to definition (2), the exact form of covariants depends on irreducible representations. Hence, it is important that we use the representations derived by induction from the first family line groups [10, 11]. This means that all the covariants satisfy conditions (6), with the additional one (2) for the additional generators.

These additional conditions, depending on the irreducible representation considered, reduce to one of the two general forms, related to the inductive construction [14] of the irreducible representations $D^{(\lambda)}(\boldsymbol{L})$ of $\boldsymbol{L}$ from the irreducible representations $\Delta^{(\mu)}(\boldsymbol{L}')$ of $\boldsymbol{L}'$. In fact the representations of $\boldsymbol{L}'$ (and $\boldsymbol{L}$) belong to one of the two disjoint types. In the first one, there are $\Delta^{(\mu)}(\boldsymbol{L}')$ which give two representations $D^{(\mu\pm)}(\boldsymbol{L})$ of the same dimension as $\Delta^{(\mu)}(\boldsymbol{L}')$, both of them having the same restriction $D^{(\mu\pm)}(\boldsymbol{L}') = \Delta^{(\mu)}(\boldsymbol{L}')$ on the subgroup:

$$D^{(\mu\pm)}(\ell') = \Delta^{(\mu)}(\ell'), \qquad D^{(\mu\pm)}(g) = \pm Z(\forall\, \ell' \in \boldsymbol{L}'), \tag{8}$$

where Z is a matrix satisfying $Z^{-1}\Delta^{(\mu)}(\ell')Z = \Delta^{(\mu)}(g^{-1}\ell' g)$ and $Z^2 = \Delta^{(\mu)}(g^2)$. For the representations of the second type, a pair of $\Delta^{(\mu)}(\boldsymbol{L}')$ and $\Delta^{(\mu')}(\boldsymbol{L}')$ (satisfying $\Delta^{(\mu')}(\ell') = \Delta^{(\mu)}(g^{-1}\ell' g)$), gives a single irreducible representation $D^{(\mu)}(\boldsymbol{L})$ of $\boldsymbol{L}$ with the doubled dimension, with restriction on $\boldsymbol{L}'$ being sum $D^{(\mu)}(\boldsymbol{L}') = \Delta^{(\mu)}(\boldsymbol{L}') \oplus \Delta^{(\mu')}(\boldsymbol{L}')$:

$$D^{(\mu)}(\ell') = \begin{pmatrix} \Delta^{(\mu)}(\ell') & 0 \\ 0 & \Delta^{(\mu')}(\ell') \end{pmatrix}, \qquad D^{(\mu)}(g) = \begin{pmatrix} 0 & \Delta^{(\mu)}(g\ell' g) \\ \Delta^{(\mu)}(\ell') & 0 \end{pmatrix} (\ell' \in \boldsymbol{L}'). \tag{9}$$

Quantum number $\pm$ is related to the additional generator g. We call it parity quantum number Π_g and by convention for the representations of the second type Π_g is set to zero.

Table 1. Representative covariant functions of the line groups. For each family $\boldsymbol{L}^{(F)}$ its irreducible representations are listed in the first column, and the corresponding representative function in the second one.

IR	Representative function
1	$\boldsymbol{T}_Q(f)\otimes\boldsymbol{C}_n$
${}_kA_m$	$\mathrm{e}^{-\mathrm{i}(m\varphi+kz)}$
${}_{\tilde{k}}A_{\tilde{m}}$	$\mathrm{e}^{-\mathrm{i}\tilde{m}\varphi+\mathrm{i}(\frac{2\pi\tilde{m}}{Qf}-\tilde{k})z}$
2	$\boldsymbol{T}(a)\boldsymbol{S}_{2n}$
${}_kA_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{-\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{2\pi}{a}-k)z}+\Pi_U\,\mathrm{e}^{-\mathrm{i}(\frac{2\pi}{a}-k)z}\right)$
${}_kE_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}\frac{m\pi}{n}}\,\mathrm{e}^{-\mathrm{i}m\varphi+\mathrm{i}kz}$
3	$\boldsymbol{T}(a)\boldsymbol{C}_{n\mathrm{h}}$
${}_kA_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{-\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{2\pi}{a}-k)z}+\Pi_\mathrm{h}\,\mathrm{e}^{-\mathrm{i}(\frac{2\pi}{a}-k)z}\right)$
${}_kE_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{-\mathrm{i}m\varphi+\mathrm{i}kz}$
4	$\boldsymbol{T}^1_{2n}\left(\frac{a}{2}\right)\boldsymbol{C}_{n\mathrm{h}}$
${}_0A_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{-\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{4\pi}{a}-k)z}+\Pi_\mathrm{h}\,\mathrm{e}^{-\mathrm{i}(\frac{4\pi}{a}-k)z}\right)$
${}_kE_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{-\mathrm{i}m\varphi+\mathrm{i}kz}$
5	$\boldsymbol{T}_Q(f)\boldsymbol{D}_n$
${}_kA_m^{\Pi_U}$	$\mathrm{e}^{\mathrm{i}(n-m)\varphi-\mathrm{i}(\frac{2\pi n}{Qf}+k)z}+\Pi_U\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi+\mathrm{i}(\frac{2\pi n}{Qf}+k)z}$
${}_kE_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi+\mathrm{i}kz}$
${}_{\tilde{k}}A_{\tilde{m}}^{\Pi_U}$	$\mathrm{e}^{\mathrm{i}(n-\tilde{m})\varphi-\mathrm{i}(\frac{2\pi(n-\tilde{m})}{Qf}+\tilde{k})z}+\Pi_U\,\mathrm{e}^{-\mathrm{i}(n-\tilde{m})\varphi+\mathrm{i}(\frac{2\pi(n-\tilde{m})}{Qf}+\tilde{k})z}$
${}_{\tilde{k}}E_{\tilde{m}}$	$\mathrm{e}^{-\mathrm{i}\tilde{m}\varphi-\mathrm{i}(-\frac{2\pi\tilde{m}}{Qf}+\tilde{k})z}$ $\mathrm{e}^{\mathrm{i}\tilde{m}\varphi+\mathrm{i}(-\frac{2\pi\tilde{m}}{Qf}+\tilde{k})z}$
6	$\boldsymbol{T}(a)\boldsymbol{C}_{n\mathrm{v}}$
${}_kA/B_m$	$\mathrm{e}^{-\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(n-m)\varphi}+\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi})$
${}_kE_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi-\mathrm{i}kz}$
7	$\boldsymbol{T}'\left(\frac{a}{2}\right)\boldsymbol{C}_n$
${}_kA/B_m$	$\mathrm{e}^{-\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(n-m)\varphi}+\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi})$
${}_kE_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi-\mathrm{i}kz}$
8	$\boldsymbol{T}^1_{2n}\left(\frac{a}{2}\right)\boldsymbol{C}_{n\mathrm{v}}$
${}_kA/B_m$	$\mathrm{e}^{-\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(2n-m)\varphi}+\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(2n-m)\varphi})$
${}_kE_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi-\mathrm{i}kz}$
${}_{\tilde{k}}A/B_0$	$\mathrm{e}^{\mathrm{i}(\tilde{k}-\frac{2\pi}{a})z}(\mathrm{e}^{\mathrm{i}n\varphi}+\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}n\varphi})$

Table 1. (continued).

IR	Representative function
$_{\tilde{k}}E_{\tilde{m}}$	$\mathrm{e}^{-\mathrm{i}\tilde{m}\varphi+\mathrm{i}(\frac{2\pi\tilde{m}}{na}-\tilde{k})z}$ $\mathrm{e}^{\mathrm{i}\tilde{m}\varphi-\mathrm{i}(\frac{2\pi\tilde{m}}{na}-\tilde{k})z}$
9	$\boldsymbol{T}(a)\boldsymbol{D}_{n\mathrm{d}}$
$_kA/B_0^{\Pi_U}$	$\mathrm{e}^{\mathrm{i}n\varphi+\mathrm{i}(\frac{2\pi}{a}-k)z}+\Pi_U\,\mathrm{e}^{-\mathrm{i}n\varphi-\mathrm{i}(\frac{2\pi}{a}-k)z}$ $+\,\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}n\varphi+\mathrm{i}(\frac{2\pi}{a}-k)z}+\Pi_U\Pi_\mathrm{v}\,\mathrm{e}^{\mathrm{i}n\varphi-\mathrm{i}(\frac{2\pi}{a}-k)z}$
$_kE_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{-\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{2\pi}{a}-k)z}+\Pi_\mathrm{h}\,\mathrm{e}^{-\mathrm{i}(\frac{2\pi}{a}-k)z}\right)$ $\mathrm{e}^{\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{2\pi}{a}-k)z}+\Pi_\mathrm{h}\,\mathrm{e}^{-\mathrm{i}(\frac{2\pi}{a}-k)z}\right)$
$_kE_{\frac{n}{2}}$	$\cos m\varphi\,\mathrm{e}^{-\mathrm{i}kz}$ $\sin m\varphi\,\mathrm{e}^{-\mathrm{i}kz}$
$_kE_m^{\Pi_\mathrm{v}}$	$\mathrm{e}^{-\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(n-m)\varphi}+(-1)^{\Pi_\mathrm{v}}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi})$ $\mathrm{e}^{\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(n-m)\varphi}+\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi})$
$_kG_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi+\mathrm{i}kz}$ $\mathrm{e}^{-\mathrm{i}m\varphi+\mathrm{i}kz}$
10	$\boldsymbol{T}'\left(\frac{a}{2}\right)\boldsymbol{S}_{2n}$
$_kA/B_m^{\Pi_U}$	$\mathrm{e}^{\mathrm{i}(n-m)\varphi+\mathrm{i}(\frac{2\pi}{a}-k)z}-\Pi_U\Pi_\mathrm{v}\,\mathrm{e}^{\mathrm{i}\frac{\pi m}{n}+\mathrm{i}\frac{ka}{2}}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi+\mathrm{i}(\frac{2\pi}{a}-k)z}$ $+\,\Pi_U\,\mathrm{e}^{\mathrm{i}\frac{\pi m}{n}}\,\mathrm{e}^{\mathrm{i}(n-m)\varphi-\mathrm{i}(\frac{2\pi}{a}-k)z}-\Pi_\mathrm{v}\,\mathrm{e}^{\mathrm{i}\frac{ka}{2}}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi-\mathrm{i}(\frac{2\pi}{a}-k)z}$
$_0E_m$	$\cos m\varphi$ $\sin m\varphi$
$_\pi E_m$	$\mathrm{e}^{-\mathrm{i}\frac{\pi}{a}z}$ $\mathrm{e}^{\mathrm{i}\frac{\pi}{a}z}$
$_kE_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{-\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{4\pi}{a}-k)z}+\Pi_\mathrm{h}\mathrm{e}^{\mathrm{i}\frac{ka}{2}}\,\mathrm{e}^{-\mathrm{i}(\frac{4\pi}{a}-k)z}\right)$ $\mathrm{e}^{\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{4\pi}{a}-k)z}+\Pi_\mathrm{h}\mathrm{e}^{\mathrm{i}\frac{ka}{2}}\,\mathrm{e}^{-\mathrm{i}(\frac{4\pi}{a}-k)z}\right)$
$_kE_m^{\Pi_\mathrm{v}}$	$\mathrm{e}^{-\mathrm{i}kz}\left(\mathrm{e}^{\mathrm{i}(n-m)\varphi}+\Pi_\mathrm{v}\,\mathrm{e}^{\mathrm{i}\frac{2\pi m}{n}}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi}\right)$ $\mathrm{e}^{\mathrm{i}kz}\left(\mathrm{e}^{\mathrm{i}(n-m)\varphi}+\Pi_\mathrm{v}\,\mathrm{e}^{\mathrm{i}\frac{2\pi m}{n}}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi}\right)$
$_kG_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{-\mathrm{i}m\varphi+\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi+\mathrm{i}kz}$
11	$\boldsymbol{T}(a)\boldsymbol{D}_{n\mathrm{h}}$
$_kA/B_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{\mathrm{i}(n-m)\varphi+\mathrm{i}(\frac{2\pi}{a}-k)z}+\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi+\mathrm{i}(\frac{2\pi}{a}-k)z}$ $+\,\Pi_\mathrm{h}\,\mathrm{e}^{\mathrm{i}(n-m)\varphi-\mathrm{i}(\frac{2\pi}{a}-k)z}+\Pi_\mathrm{h}\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi-\mathrm{i}(\frac{2\pi}{a}-k)z}$
$_kE_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{-\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{2\pi}{a}-k)z}+\Pi_\mathrm{h}\,\mathrm{e}^{-\mathrm{i}(\frac{2\pi}{a}-k)z}\right)$ $\mathrm{e}^{\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{2\pi}{a}-k)z}+\Pi_\mathrm{h}\,\mathrm{e}^{-\mathrm{i}(\frac{2\pi}{a}-k)z}\right)$
$_kE_m^{\Pi_\mathrm{v}}$	$\mathrm{e}^{-\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(n-m)\varphi}+\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi})$ $\mathrm{e}^{\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(n-m)\varphi}+\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi})$

Table 1. (continued).

IR	Representative function
${}_kG_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{-\mathrm{i}m\varphi+\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi+\mathrm{i}kz}$
12	$\boldsymbol{T}'\left(\frac{a}{2}\right)\boldsymbol{C}_{n\mathrm{h}}$
${}_0A/B_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{\mathrm{i}(n-m)\varphi+\mathrm{i}\frac{4\pi}{a}z}+\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi+\mathrm{i}\frac{4\pi}{a}z}+$ $+\,\Pi_\mathrm{h}\,\mathrm{e}^{\mathrm{i}(n-m)\varphi-\mathrm{i}\frac{4\pi}{a}z}+\Pi_\mathrm{h}\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi-\mathrm{i}\frac{4\pi}{a}z}$
${}_kE_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{-\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{4\pi}{a}-k)z}+\Pi_\mathrm{h}\,\mathrm{e}^{-\mathrm{i}(\frac{4\pi}{a}-k)z}\right)$ $\mathrm{e}^{\mathrm{i}m\varphi}\left(\mathrm{e}^{\mathrm{i}(\frac{4\pi}{a}-k)z}+\Pi_\mathrm{h}\,\mathrm{e}^{-\mathrm{i}(\frac{4\pi}{a}-k)z}\right)$
${}_kE_m^{\Pi_\mathrm{v}}$	$\mathrm{e}^{-\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(n-m)\varphi}+\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(n-m)\varphi})$ $\mathrm{e}^{\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(n-m)\varphi}+\Pi_\mathrm{v}\mathrm{e}^{-\mathrm{i}(n-m)\varphi})$
${}_\pi E_m$	$\mathrm{e}^{-\mathrm{i}kz}\cos(n-m)\varphi$ $\mathrm{e}^{\mathrm{i}kz}\cos(n-m)\varphi$
${}_kG_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{-\mathrm{i}m\varphi+\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi+\mathrm{i}kz}$
13	$\boldsymbol{T}^1_{2n}\left(\frac{a}{2}\right)\boldsymbol{D}_{n\mathrm{h}}$
${}_0A/B_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{\mathrm{i}(2n-m)\varphi+\mathrm{i}\frac{4\pi}{a}z}+\Pi_U\,\mathrm{e}^{-\mathrm{i}(2n-m)\varphi-\mathrm{i}\frac{4\pi}{a}z}$ $+\,\Pi_\mathrm{v}\,\mathrm{e}^{-\mathrm{i}(2n-m)\varphi+\mathrm{i}\frac{4\pi}{a}z}+\Pi_U\Pi_\mathrm{v}\,\mathrm{e}^{\mathrm{i}(2n-m)\varphi-\mathrm{i}\frac{4\pi}{a}z}$
${}_0E_m^{\Pi_\mathrm{h}}$	$\mathrm{e}^{-\mathrm{i}m\varphi}(\mathrm{e}^{\mathrm{i}\frac{4\pi}{a}z}+\Pi_\mathrm{h}\mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}z})$ $\mathrm{e}^{\mathrm{i}m\varphi}(\mathrm{e}^{\mathrm{i}\frac{4\pi}{a}z}+\Pi_\mathrm{h}\mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}z})$
${}_kE_m^{A/B}$	$\mathrm{e}^{-\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(2n-m)\varphi}+\Pi_\mathrm{v}\mathrm{e}^{-\mathrm{i}(2n-m)\varphi})$ $\mathrm{e}^{\mathrm{i}kz}(\mathrm{e}^{\mathrm{i}(2n-m)\varphi}+\Pi_\mathrm{v}\mathrm{e}^{-\mathrm{i}(2n-m)\varphi})$
${}_\pi E_{n/2}^{\Pi_U}$	$\mathrm{e}^{\mathrm{i}m\varphi+\mathrm{i}kz}+\Pi_U\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{-\mathrm{i}m\varphi+\mathrm{i}kz}+\Pi_U\mathrm{e}^{\mathrm{i}m\varphi-\mathrm{i}kz}$
${}_kG_m$	$\mathrm{e}^{-\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi-\mathrm{i}kz}$ $\mathrm{e}^{-\mathrm{i}m\varphi+\mathrm{i}kz}$ $\mathrm{e}^{\mathrm{i}m\varphi+\mathrm{i}kz}$

For simplicity, we first analyze groups of the families 2–8, when the halving subgroup is of the first family, then the representation label μ corresponds to the pair of momenta $\tilde{k}$ and $\tilde{m}$, and the whole space $\mathcal{L}$ is decomposed as $\mathcal{L}=\oplus_{\tilde{k}\tilde{m}}\mathcal{L}^{(\tilde{k}\tilde{m})}$ onto covariant subspaces of $\boldsymbol{L}'=\boldsymbol{L}^{(1)}$.

When $D^{(\tilde{k}\tilde{m})}(\boldsymbol{L}')$ is of the first type, then $\mathcal{L}^{(\tilde{k}\tilde{m})}$ is obviously invariant under the additional generator g, meaning that $\mathcal{L}^{(\tilde{k}\tilde{m})}=\mathcal{L}^{(\tilde{k}\tilde{m}+)}\oplus\mathcal{L}^{(\tilde{k}\tilde{m}-)}$. Therefore, the role of the additional generator is to separate these subspaces, i.e. to determine SAB (of the whole group) in $\mathcal{L}^{(\tilde{k}\tilde{m})}$. This is performed with the group projector [8]: $P^{(\tilde{k}\tilde{m}\pm)}=X\sum_{\ell\in\boldsymbol{L}}D^{(\tilde{k}\tilde{m}\pm)^*}(\ell)D(\ell)$, which is reduced in the space $\mathcal{L}^{(\tilde{k}\tilde{m})}$ to $P^{(\tilde{k}\tilde{m}\pm)}=Y(1\pm Z)$ (as the covariants are to be normalized at the end, the constants X and Y are not important). Thus, the representative functions have the form

$$\Phi^{(\tilde{k}\tilde{m}\pm)}=\Phi_t^{(\tilde{k}\tilde{m})}\pm Z\Phi_t^{(\tilde{k}\tilde{m})}. \tag{10}$$

Note that when $Z = 1$ the simplest choice $\Phi_t^{(\tilde{k}\tilde{m})} = \Phi_{00}^{(\tilde{k}\tilde{m})}$ has vanishing projection by $P^{(\tilde{k}\tilde{m}\pm)}$. Therefore, for uniqueness of notation and compact presentation, we usually use $\Phi_{01}^{(\tilde{k}\tilde{m})}$ or $\Phi_{10}^{(\tilde{k}\tilde{m})}$ for building the supergroup invariants.

When $D^{(\tilde{k}\tilde{m})}(\boldsymbol{L}')$ is of the second type, then $D(g)$ maps $\mathcal{L}^{(\tilde{k}\tilde{m})}$ into another space $\mathcal{L}^{(\tilde{k}'\tilde{m}')}$, which gives rise to doubling of the dimension of the resulting irreducible representation $D^{(\mu)}(\boldsymbol{L})$ of $\boldsymbol{L}$. While the projector

$$X\sum_{\ell\in\boldsymbol{L}} D_{11}^{(\mu)^*}(\ell) = X\begin{pmatrix}\sum_{\ell'\in\boldsymbol{L}'}\Delta^{(\mu)^*}(\ell') & 0\\ 0 & 0\end{pmatrix}$$

leaves $\Phi_t^{(\tilde{k}\tilde{m})}$ invariant, the transfer operator

$$X\sum_{\ell\in\boldsymbol{L}} D_{21}^{(\mu)^*}(\ell) = X\begin{pmatrix}0 & 0\\ \sum_{\ell'\in\boldsymbol{L}'}\Delta^{(\mu)^*}(\ell') & 0\end{pmatrix}$$

maps $\Phi_t^{(\tilde{k}\tilde{m})}$ into $\Phi_t^{(\tilde{k}'\tilde{m}')} = D(g)\Phi_t^{(\tilde{k}\tilde{m})}$. Thus, it is natural to take the simplest representative doublet $\Phi_{00}^{(\tilde{k}\tilde{m})}$ and $D(g)\Phi_{00}^{(\tilde{k}\tilde{m})}$.

In the case of the groups from the families 9–13, the procedure is completely analogous, except that $\boldsymbol{L}'$ is one of the groups from the families 2–8, having besides $\tilde{k}$ and $\tilde{m}$ also the parity quantum number from the induction of the first step.

The results obtained, listed in table 1, together with the line group invariants [13] complete the task of finding SAB for quasi-one-dimensional systems. Any function $\Psi^{(\lambda)l}(\boldsymbol{r})$ can now be easily and accurately represented as an expansion over the corresponding line group SAB (3):

$$\Psi^{(\lambda)l}(\boldsymbol{r}) = \sum_{IKM}\alpha_{IKM}\Phi_{00}^{(\lambda)l}(\varphi,z)R_{IK}^{M}(\rho)H_{K}^{M}(\varphi,z), \tag{11}$$

where the sum is over all allowed values of I, M and K, while the amplitudes are scalar products: $\alpha_{IKM} = \left(\Psi_{IKM}^{(\lambda)l}, \Psi^{(\lambda)l}\right) = \int \Psi_{IKM}^{(\lambda)l^*}(\rho,\varphi,z)\Psi^{(\lambda)l}(\rho,\varphi,z)\rho\,\mathrm{d}\rho\,\mathrm{d}\varphi\,\mathrm{d}z$ and the harmonics are tabulated within the previous article of the series [13].

Derived functions describe various potentials of the systems with line group symmetry displaced according to a normal mode. Let $\boldsymbol{d}^{(\mu)t_\mu m}$ be the displacement vector of the normal mode corresponding to the irreducible representation $D^{(\mu)}$ (where $t_\mu = 1,\ldots,f_\mu$ and f_μ is a frequency number of $D^{(\mu)}$) in the dynamical representation of the system, i.e. t_μ counts different frequencies of the modes transforming according to $D^{(\mu)}$); this means that the coordinate of the ith atom is $\boldsymbol{r}_i = \boldsymbol{r}_i^0 + \boldsymbol{d}_i^{(\mu)t_\mu m}$ (equilibrium is at $\boldsymbol{r}^0$; $\boldsymbol{d}^{(\mu)t_\mu m}$ is time dependent). Then the potential $V(\boldsymbol{r})$ produced by the system is a function of type (11), i.e. the mth component of the multiplet corresponding to $D^{(\mu)}$. Usually, this potential is the sum over atoms of the atomic potentials v: $V(\boldsymbol{r}) = \sum_i v(|\boldsymbol{r}-\boldsymbol{r}_i|)$.

As an illustration we consider a carbon nanotube (6, 0) with the line group $\boldsymbol{L}^{(13)} = \boldsymbol{T}_{12}^{1}(2.13\text{Å})\boldsymbol{C}_6$ symmetry. Atomic Lenard–Jones potential [15]

$$v(r) = -\frac{18.5426}{|\boldsymbol{r}|^6} + \frac{29000.4}{|\boldsymbol{r}|^{12}} \tag{12}$$

is responsible for the interaction with the outer wall in the double-walled nanotube. The outer wall is approximately of radius $\rho_0 = 2.35$ Å, and we calculate the potential $V(\rho_0,\varphi,z)$ during the vibration of the mode with frequency 763.901 cm^{-1}. This is an alternating twisting mode (each monomer of 12 atoms is circumferentially rotated oppositely to the adjacent monomers, figure 1) corresponding to the representation ${}_0B_6^-$, i.e. its quantum numbers are $k = 0, m = 6$ (or $\tilde{k} = \pi/f, \tilde{m} = 0$), $\Pi_U = 1$, $\Pi_{\mathrm{v}} = \Pi_{\mathrm{h}} = -1$. We calculate numerically expansion of $V(\rho_0,\varphi,z)$ over SAB with representative function $\sin(2\pi z/f)\sin(6\varphi)$ (see table 1). It turns

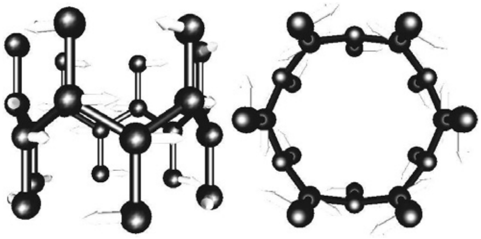

Figure 1. Elementary cell (with two monomers) of carbon nanotube $(6, 0)$. Arrows denote atomic displacements corresponding to the mode ${}_0B_6^-$.

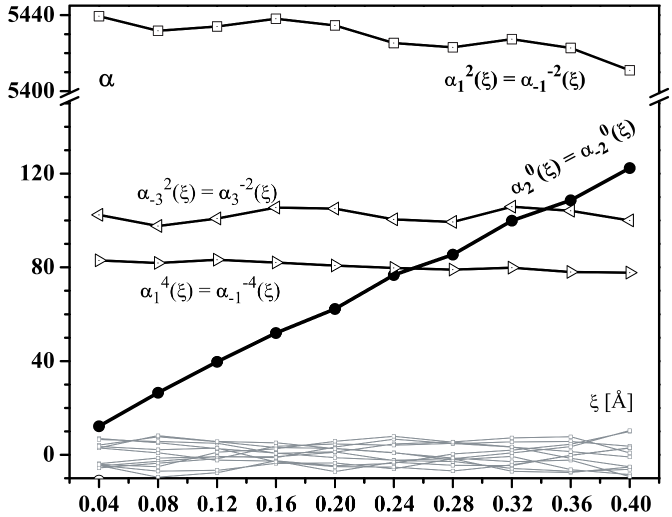

Figure 2. Coefficients α_K^M of the expansion (11) of the potential $V(\rho_0, \varphi, z)$ as a function of the elongation ξ of the mode ${}_0B_6^-$. Besides the several significant coefficients, all the others are with negligible absolute value (gray lines close to $\alpha = 0$ axis). Since $\alpha_1^{-2} = \alpha_{-1}^2 = -\alpha_1^2, \alpha_3^2 = \alpha_{-3}^{-2} = -\alpha_{-3}^2, \alpha_{-4}^1 = \alpha_4^{-1} = -\alpha_4^1$ and $\alpha_0^0 = -\alpha_2^0$, only the positive coefficients are plotted. Also, only positive elongations are presented, as the potential is invariant under reversing the displacement direction, i.e. $\alpha_K^M(\xi) = \alpha_K^M(-\xi)$.

out that only several bases function significantly contributes (figure 2) for all elongations ξ. In fact, the coefficients $\alpha_K^M(\xi)$ of all but the three harmonics are almost constant (independent of the elongation ξ): $\alpha_{\pm1}^{\pm2}$ are in absolute value 50 times greater than $\alpha_{\pm3}^{\pm2}$ and $\alpha_{\pm1}^{\pm4}$, which are further by one or two orders of magnitude greater than the coefficients of the other harmonics. Only the coefficients $\alpha_{\pm0}^0 = -\alpha_0^0$ significantly vary with elongation (for two orders of magnitude). Therefore, only this component of potential is relevant for inter-wall interaction along this degree of freedom. Note also that if Coulomb interaction is taken for v, this type of calculation can significantly facilitate the calculation of electron–phonon matrix elements.

To summarize, we showed that a covariant function of a line group can be factorized to the product of a representative function determining the transformation properties and an invariant function. Besides, representative functions determined by the symmetry solely, can be tabulated *a priori*. Such a generalization of the Bloch theorem to the full line group symmetry can straightforwardly be extended to the more dimensional crystals. Further, as the bases of invariants, i.e. harmonics, have been found for the all line groups [13] it is easy now to compose the total symmetry adapted basis in the quantum mechanical state space of any (commensurate or incommensurate) quasi-1D crystal (e.g., stereo-regular polymers or nanotubes) from the representative functions and harmonics. Such a basis significantly improves quality and efficiency of the density functional calculations as the basis set of functions used is optimal.

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