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Wigner–Eckart theorem in the inductive spaces and applications to optical transitions in nanotubes

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Abstract

The analytical form of the optical transitions probabilities in carbon nanotubes is found. The derived general form of the Wigner–Eckart theorem for inductive spaces is relevant for any crystal tight-binding model. Within the previously developed modified group projector technique the symmetry based procedure of the matrix elements calculations is obtained.

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1. Introduction

The properties of quantum mechanical systems are related (usually through the perturbative approach and transition probabilities) to the matrix elements of the suitably chosen operators between the Hamiltonian eigenstates. It is well known that the symmetry of the system is a powerful tool in such calculations: using symmetry adapted eigenbasis (SAB) and irreducible tensor operators (ITO) one may apply the Wigner–Eckart theorem [1]. Besides the tremendous reduction of the calculations, the Clebsch–Gordan coefficients give the selection rules sublimating all the conservation laws.

The one-particle approximation simplifies the structure of the state space of a complex system, retaining only its part induced by the atomic states. Such a framework is particularly convenient for symmetry treatment. In solid state physics the eigenproblem is reduced to the elementary cell, and recently even to the symcell [2], being the contents of the asymmetric unit, i.e. the minimal set of atoms that restore the whole crystal when mapped by the symmetry operations. Less attention has been paid to implement symmetry in the matrix elements calculations for such systems, despite conceptual and efficiency importance. Here we fill in this gap, which is particularly valuable in nanotube physics, due to the high symmetry of nanotubes. At first, we use the modified group projector technique (outlined in section 2) to obtain in section 3 a general expression for the matrix elements of the tensors within the tight-binding model of crystals. It is applied in section 4 to obtain optical transitions

matrix elements for nanotubes [3]. Finally, in the following two sections we give a quite general interpretation of the Wigner–Eckart theorem for the crystal tight-binding model; the readers interested in applications only, may skip these more mathematically difficult parts. The rest of the introduction is a necessary reminder of the Wigner–Eckart theorem.

Let $\mathcal{S}$ be the state space of a quantum system with the symmetry group $\boldsymbol{G}$. The group acts in $\mathcal{S}$ by its representation $D = \oplus_\mu a^\mu D^{(\mu)}$: it reduces in the subspaces $\mathcal{S}^{(\mu t_\mu)}$ ($t_\mu = 1, \ldots, a^\mu$; a^μ is the frequency number) onto the $|\mu|$-dimensional irreducible components $D^{(\mu)}$. A SAB is built of the $\mathcal{S}^{(\mu t_\mu)}$ bases $|\mu t_\mu m\rangle$ satisfying

$$D(g)|\mu t_\mu m\rangle = \sum_{m'=1}^{|\mu|} D^{(\mu)}_{m'm}(g)|\mu t_\mu m'\rangle \qquad m = 1, \ldots, |\mu|. \tag{1}$$

The corresponding group action $D(g)AD^{-1}(g)$ on the operator A defines the ITO components $A^{\mu m}$ by the analogous requirement:

$$D(g)A^{\mu m}D^{-1}(g) = \sum_{m'=1}^{|\mu|} D^{(\mu)}_{m'm}(g)A^{\mu m'} \qquad m = 1, \ldots, |\mu|. \tag{2}$$

Consequently, expanding vectors in SAB and operators in ITO components, any matrix element $\langle x|A|y\rangle$ completely reduces to a sum of the SAB–ITO ones. It is here that the Wigner–Eckart theorem comes in: if the frequency of the irreducible component μ in $D^{(\nu)} \otimes D^{(\lambda)}$ is $a^{\mu\nu\lambda} = 1$, the SAB–ITO matrix element is proportional to the corresponding Clebsch–Gordan coefficient:

$$\langle \mu t_\mu m|A^{\nu n}|\lambda t_\lambda l\rangle = \langle \mu m \mid \nu n; \lambda l\rangle (\mu t_\mu \| A^\nu \| \lambda t_\lambda). \tag{3}$$

The mnl-independent factor is called the reduced matrix element [4].

2. Reminder of modified group projector technique

The modified group projector technique (MGPT) formally develops a very intuitive concept: two objects transforming mutually oppositely under some transformation will be overall invariant under the same transformation. In the present context, the subspaces $\mathcal{S}^{(\mu t_\mu)}$ are defined through the transformation properties (1) of their symmetry adapted subbases $|\mu t_\mu m\rangle$. Thus, $\mathcal{S}$ is multiplied by the dual irreducible space $\mathcal{H}^{(\mu)^*}$, with basis $\{\langle \mu m|m = 1, \ldots, |\mu|\}$ transforming counter-gradient, i.e. oppositely to $|\mu t_\mu m\rangle$. In the auxiliary space $\mathcal{S}^{\mu^*} = \mathcal{S} \otimes \mathcal{H}^{(\mu)^*}$ acts as the representation $\Gamma^{\mu^*}(g) \stackrel{\text{def}}{=} D(g) \otimes D^{(\mu)^*}(g)$, leaving invariant [5] the vectors from the subspace $\mathcal{F}^{\mu^*}$ spanned by

$$|\mu t_\mu\rangle = Y^\mu_{t_\mu} = \sum_m |\mu t_\mu m\rangle \otimes \langle \mu m| \qquad t_\mu = 1, \ldots, a^\mu. \tag{4a}$$

Notation $Y^\mu_{t_\mu}$ emphasizes that the vectors from $\mathcal{S}^{\mu^*}$ are also linear maps $Y : \mathcal{H}^{(\mu)} \to \mathcal{S}$ defined by the partial scalar product: $Y|\mu m\rangle = \langle \mu^* m \mid Y\rangle$.

The subspace $\mathcal{F}^{\mu^*}$ of the invariant vectors for Γ^{μ^*} may be easily selected as a range of the modified Wigner's projector $\boldsymbol{G}(\Gamma^{\mu^*}) = \sum_{g\in\boldsymbol{G}} \Gamma^{\mu^*}(g)$. Alternatively, this fixed points subspace can be found as the common eigenspace for the eigenvalue 1 of the group generators; this way summation over infinite groups (as in crystal physics) is avoided. Finally, any basis in $\mathcal{F}^{\mu^*}$ can be used as $Y^\mu_{t_\mu}$, and from (4*a*) immediately follows that the corresponding μth part ($t_\mu = 1, \ldots, a^\mu$; $m = 1, \ldots |\mu|$) of SAB (1) is obtained as

$$|\mu t_\mu m\rangle = Y^\mu_{t_\mu}|\mu m\rangle = \langle \mu^* m \mid \mu t_\mu\rangle. \tag{4b}$$

Of course, the choice of the basis $Y^{\mu}_{t_\mu}$ is essentially non-unique if $a^{\mu} > 1$, as well as the final SAB. This non-uniqueness is reduced if a SAB which is also the eigenbasis of some observable is looked for.

A particularly important application of this technique is in the induced spaces, which necessarily appear in crystal physics when phonons or electrons (within the tight-binding approximation) are studied. Structural properties of modified projectors enable us to define a sort of inverted induction, and using this 'pull-down' procedure [6] the problem is exactly reduced [2] from the infinite-dimensional total space $\mathcal{S}$ to the finite-dimensional one corresponding to the symcell only. In this sense, using the full symmetry group MGPT generalizes the Bloch theorem, which takes into account the translational subgroup; note that the elementary cell in nanotubes may contain hundreds of atoms, in contrast to the symcell with a single atom. The crystal groups are within MGPT considered infinite, and Born–von Karman conditions are not relevant in further considerations.

3. Tight-binding matrix elements

We start by the direct calculation of the SAB–ITO matrix elements within the solid state electron tight-binding model. For simplicity and further application to nanotubes, a crystal with a single atom in a symcell is considered. This means that the set of the atoms generated by symmetry transformations from any arbitrary chosen initial atom (i.e. orbit of this atom) is exactly the whole crystal. The site-symmetry group (stabilizer) of this atom $\boldsymbol{S}$ contains the elements s of $\boldsymbol{G}$ for which the initial atom is a fixed point. Thus, the whole crystal is really generated only by the transversal $\boldsymbol{Z}$, which is the set of the coset representatives z_p ($p = 0, \ldots, |\boldsymbol{Z}| - 1$) of the decomposition of $\boldsymbol{G}$ with respect to $\boldsymbol{S}$, and the atoms may be generated by these coset representatives. We assume that $\boldsymbol{Z}$ is an infinite subgroup of the full symmetry group $\boldsymbol{G}$; this can be straightforwardly generalized, as well as the restriction to the monoatomic symcell.

Each atom p ($p = 0, 1, \ldots$) contributes to the electronic state space $\mathcal{S}$ by the atomic orbitals $|p; \psi\rangle$ ($\psi = 1, \ldots, |\delta|$). All these orbitals form a basis in $\mathcal{S}$. Due to symmetry, all the atoms have the same types of orbitals. The p-atom orbitals $|p; \psi\rangle$ span the interior space $\mathcal{S}_{p\delta}$, i.e. $\mathcal{S} = \oplus_p \mathcal{S}_{p\delta}$. The site symmetry group acts in $\mathcal{S}_\delta = \mathcal{S}_{0\delta}$ by the interior representation $\delta(\boldsymbol{S})$, while for any other element $g = z_p s$ the action is $D(g)|0; \psi\rangle = D(z_p)(\delta(s)|0; \psi\rangle) = \sum_{\phi=1}^{|\delta|} \delta_{\phi\psi}(s)|p; \phi\rangle$: this induced representation $D(\boldsymbol{G}) = \delta(\boldsymbol{S} \uparrow \boldsymbol{G})$ manifests the state space inductive structure. In particular, for the transversal elements $D(z_p)|0; \psi\rangle = |p; \psi\rangle$.

In the obtained state space, MGPT relates the auxiliary representation Γ^{μ^*} of $\boldsymbol{G}$ to the representation $\gamma^{\mu^*} = \delta \otimes D^{(\mu)^*}$ of $\boldsymbol{S}$ in $\mathcal{S}_{\gamma^{\mu^*}} = \mathcal{S}_\delta \otimes \mathcal{H}^{(\mu)^*}$ ($D^{(\mu)^*}$ is here restricted to $\boldsymbol{S}$). The modified projector onto the fixed points space $\mathcal{F}^{\mu^*}$ is 'pulled-down' to the subgroup projector $\boldsymbol{S}(\gamma^{\mu^*}) = \sum_{s\in\boldsymbol{S}} \gamma^{\mu^*}(g)$:

$$E^0_0 \otimes \boldsymbol{S}(\gamma^{\mu^*}) = B^{\mu\dagger}\boldsymbol{G}(\Gamma^{\mu^*})B^{\mu} \qquad B^{\mu} = \frac{1}{\sqrt{|\boldsymbol{Z}|}} \sum_p E^p_0 \otimes I_\delta \otimes D^{(\mu)^*}(z_p). \tag{5}$$

(I_δ is the identity map in $\mathcal{S}_\delta$, and E^p_q is the matrix with elements $\left(E^p_q\right)_{st} = \delta_{ps}\delta_{qt}$.) The terms $E^p_0 \otimes I_\delta \otimes D^{(\mu)^*}(z_p)$ are mappings from $\mathcal{S}_{\gamma^{\mu^*}}$ to the subspaces $\mathcal{S}_{p\gamma^{\mu^*}} = \mathcal{S}_{p\delta} \otimes \mathcal{H}^{(\mu)^*}$, such that $B^{\mu} : \mathcal{S}_{\gamma^{\mu^*}} \to \mathcal{S}_{\Gamma^{\mu^*}}$ is partial isometry. Hence, $\boldsymbol{G}(\Gamma^{\mu^*})$ and $\boldsymbol{S}(\gamma^{\mu^*})$ are essentially equivalent and any basis $|\mu t_\mu{}^{\downarrow}\rangle$ in the range of $\boldsymbol{S}(\gamma^{\mu^*})$ determines uniquely the $\mathcal{F}^{\mu^*}$ basis $|\mu t_\mu\rangle = B^{\mu}|\mu t_\mu{}^{\downarrow}\rangle$, yielding the μth part of SAB (4*b*):

$$|\mu t_\mu m\rangle = \langle \mu^* m|(B^{\mu}|\mu t_\mu{}^{\downarrow}\rangle). \tag{6}$$

The MGPT results on the tight-binding eigenproblem are eigenenergies $\epsilon_{\mu t_\mu}$ and the pulled-down eigenstates $|\mu t_\mu{}^{\downarrow}\rangle$ in the initial auxiliary space $\mathcal{S}_{\gamma^{\mu^*}}$. Since in the atomic orbitals basis $|\mu t_\mu{}^{\downarrow}\rangle = \sum_{m\psi} c_\psi^{(\mu t_\mu m)} |0;\psi\rangle\langle\mu m|$, the coefficients $c_\psi^{(\mu t_\mu m)}$ are immediately given. From (6) and (5) follows that the pth atom component $|p;\mu t_\mu m\rangle \in \mathcal{S}_{p\delta}$ of the eigenorbital $|\mu t_\mu m\rangle$ is

$$|p;\mu t_\mu m\rangle = \langle\mu^* m|\left(\frac{E_0^p \otimes I_\delta \otimes D^{(\mu)^*}(z_p)}{\sqrt{|\boldsymbol{Z}|}}|\mu t_\mu{}^{\downarrow}\rangle\right) = \sum_{m'\psi} c_\psi^{(\mu t_\mu m')} \frac{D^{(\mu)^*}_{mm'}(z_p)}{\sqrt{|\boldsymbol{Z}|}}|p;\psi\rangle. \tag{7}$$

With $\left(A^{\nu n}_{pq}\right)^{\psi}_{\phi} = \langle p;\psi|A^{\nu n}|q;\phi\rangle$, the transformation properties (2) may be used to show that the pqth block $A^{\nu n}_{pq} = \sum_{\psi\phi} |p;\psi\rangle\left(A^{\nu n}_{pq}\right)^{\psi}_{\phi}\langle q;\phi|$ of $A^{\nu n}$ satisfies

$$A^{\nu n}_{pq} = \sum_{n'} D^{(\nu)}_{n'n}\left(z_q^{-1}\right)\delta(s(z_q,z_p))A^{\nu n'}_{p_q 0} \tag{8}$$

where z_p and z_q determine p_q and s_{qp} by $z_q z_{p_q} = z_p s_{qp}$. When $\boldsymbol{Z}$ is a subgroup, this simplifies to $s_{qp} = e$ and $z_{p_q} = z_q^{-1} z_p$.

With the help of (7) and (8) for $p = 0$, and using the tensor $[\mu|\nu^*|\lambda^*] = \frac{1}{|\boldsymbol{Z}|}\sum_q D^{(\mu)}(z_q)\otimes D^{(\nu)^*}(z_q)\otimes D^{(\lambda)^*}(z_q)$ the explicit form of SAB–ITO matrix elements is directly found:

$$\begin{aligned}\langle\mu t_\mu m|A^{\nu n}|\lambda t_\lambda l\rangle &= \sum_{m'l'n'}[\mu|\nu^*|\lambda^*]^{mnl}_{m'n'l'}\sum_{m''p} D^{(\mu)}_{m'm''}(z_p)\langle 0;\mu t_\mu m''|A^{\nu n'}_{p0}|0;\lambda t_\lambda l'\rangle \\ &= \sum_{m'l'n'}[\mu|\nu^*|\lambda^*]^{mnl}_{m'n'l'}\sum_{m''\psi\phi} c_\psi^{(\mu t_\mu m'')^*} c_\phi^{(\lambda t_\lambda l')}\sum_p D^{(\mu)}_{m'm''}(z_p)\left(A^{\nu n'}_{p0}\right)^{\psi}_{\phi}.\end{aligned} \tag{9}$$

The discussion of this result is postponed to section 6, after we demonstrate its applicability and introduce the modified formalism of the Wigner–Eckart theorem.

4. Optical transition in nanotube physics

We look for the matrix elements of the linear momenta in the tight-binding electron SAB of a single wall carbon nanotube (SWNT). As the optical transition probabilities are expressed through these matrix elements, they completely determine SWNT optical properties [7].

The symmetry group of the chiral ($\mathcal{C}$) and zig-zag ($\mathcal{Z}$) or armchair ($\mathcal{A}$) SWNT (n_1, n_2) is the rod (line) group [8]:

$$\boldsymbol{L}_{\mathcal{C}} = \boldsymbol{T}^r_q(a)\boldsymbol{D}_n = \boldsymbol{L}q_p 22 \qquad \boldsymbol{L}_{\mathcal{ZA}} = \boldsymbol{T}^1_{2n}\boldsymbol{D}_{nh} = \boldsymbol{L}2n_n/mcm. \tag{10}$$

Here, the factorized form is followed by the international symbol (usually 75 rod groups constrained by the crystallographic principal axes 1, 2, 3, 4 or 6 are denoted [9] by the letter $\boldsymbol{p}$ instead of $\boldsymbol{L}$ which we use here). The translational period a and the integers q, r and n are functions of n_1 and n_2. The elements of these groups are $\left(C^r_q\left|\frac{na}{q}\right.\right)^t C^s_n U^u \sigma^v_x$ ($t = 0, \pm1, \ldots$; $s = 0, \ldots, n-1$; $u = 0, 1$; $v = 0$ for $\mathcal{C}$ and $v = 0, 1$ for $\mathcal{Z}$ and $\mathcal{A}$). SWNT is a mono-orbit system: its atom C_{tsu} is obtained by the action of $\left(C^r_q\left|\frac{na}{q}\right.\right)^t C^s_n U^u$ onto the initial one C_{000}. Therefore, the transversal is $\boldsymbol{Z} = \boldsymbol{L}_{\mathcal{C}}$, while the site-symmetry group, depending on the SWNT type is $\boldsymbol{S}_{\mathcal{C}} = \{e\}$, $\boldsymbol{S}_{\mathcal{Z}} = \{e, C_n\sigma_x\}$ and $\boldsymbol{S}_{\mathcal{A}} = \{e, \sigma_h = U\sigma_x\}$. When *sp*-hybridization is neglected [10], the relevant electronic tight-binding space $\mathcal{S}$ is built up of the p-orbitals pointing outwards from the tube. Thus, the atomic, i.e. transversal, indices enumerate basis $|p;\psi\rangle = |tsu\rangle$. This orbital is invariant under the site symmetries in all cases, and the interior representation is trivial, $\delta = 1$. The resulting electron bands are assigned [2, 11] by the symmetry based quantum numbers of the corresponding irreducible representations. Here

we use the z-components of the quasilinear momentum $k \in [0, \pi/a]$ and the quasiangular momentum m. Also, there is U-axis parity $\Pi^U = \pm 1$ at the edge points $k = 0, \pi/a$, and only for the achiral tubes are there horizontal (at $k = 0, \pi/a$) and vertical mirror parities $\Pi^h = \pm 1$ and $\Pi^v = A/B$.

The irreducible components of the momentum observables $\boldsymbol{p}$ are $P^0 = P^{\nu 1} = p_z$, corresponding to the one-dimensional representation $\nu = {}_0A_0^-$ for all the tubes, and $P^{\pm 1} = p_x \mp \mathrm{i}p_y$ ($P^1 = P^{\nu 1}$, $P^{-1} = P^{\nu 2}$), spanning the two-dimensional irreducible representation $\nu = {}_0E_1$ in the chiral and $\nu = {}_0E_1^+$ in the achiral cases.

Only the transitions for $k \in (0, \pi/a)$ will be considered. In fact, in the optical properties calculations the integration in k is performed, and the particular values of matrix elements in $k = 0, \pi/a$ are irrelevant, although they can be easily calculated analogously (some comments will be given in section 7). Accordingly, for the $\mathcal{C}$ tubes within $k \in (0, \pi/a)$, the bands are assigned by integer $m \in (-q/2, q/2]$. For each k and m there is an irreducible representation ${}_kE_m$ given by ${}_kE_m(t, s, 0) = \mathrm{diag}\big[\mathrm{e}^{\mathrm{i}\psi_m^k(t,s)}, \mathrm{e}^{-\mathrm{i}\psi_m^k(t,s)}\big]$ and ${}_kE_m(t, s, 1) = {}_kE_m(t, s, 0)\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, where $\psi_m^k(t, s) = \frac{kan + 2\pi mr}{q}t + \frac{2\pi m}{n}s$. As ${}_kE_m$ is two dimensional, the bands are double degenerate. For the achiral tubes there are either four-fold or double degenerate bands corresponding respectively to the representations ${}_kG_m$ ($m = 1, \ldots, n-1$) and ${}_kE_m^{\Pi^v}$ ($m = 0, n$). To get the matrix elements in the compact form with transparent selection rules, the vectors $|\mu t_\mu m\rangle$ of SAB will be denoted by $|km\tilde{\Pi}; T\rangle$. Here, $\tilde{\Pi} = -1$ for the σ_v-odd states, while $\tilde{\Pi} = 1$ otherwise (σ_v-even states and the states without sharp σ_v-parity; e.g. all $\mathcal{C}$ tube bands and all the four-fold degenerate bands). The representation label μ is the set of the quantum numbers $(km\tilde{\Pi})$, with k and m within the given intervals, while the momenta k and m in the corresponding SAB vector $|km\tilde{\Pi}; T\rangle$ may have also the opposite sign; as their actual values automatically distinguish between the vectors, the counter m in $|\mu t_\mu m\rangle$ is redundant. For the two-dimensional representations ${}_kE_m^{\tilde{\Pi}}$ (this includes both the chiral ${}_kE_m$ and the achiral ${}_kE_m^{\Pi^v}$) $|(km\tilde{\Pi})T1\rangle = |km\tilde{\Pi}; T\rangle$ and $|(km\tilde{\Pi})T2\rangle = |-k, -m, \tilde{\Pi}; T\rangle$; also, the part of the SAB corresponding to ${}_kG_m$ is $|(km1)T1\rangle = |km1; T\rangle$, $|(km1)T2\rangle = |k, -m, 1; T\rangle$, $|(km1)T3\rangle = |-k, m, 1; T\rangle$ and $|(km1)T4\rangle = |-k, -m, 1; T\rangle$. Since the interior space is one dimensional, (7) reduces to $|0; km\tilde{\Pi}; T\rangle = c^{(km\tilde{\Pi};T)}|000\rangle$, and the coefficients are easily found.

All together, the optical transition probability amplitudes are determined by $\langle k'm'\tilde{\Pi}'; T'|P^M|km\tilde{\Pi}; T\rangle$. The nonvanishing tensors $[\mu|\nu^*|\lambda^*]$ are given in table 1. Applying this to (9), one directly obtains the matrix elements:

$$\begin{aligned}\langle k'm'\tilde{\Pi}'; T'|P^M|km\tilde{\Pi}; T\rangle = \delta_k^{k'}\delta_{m+M}^{m'}\big(1 - \delta_0^M + \delta_0^M\delta_{\tilde{\Pi}}^{\tilde{\Pi}'}\big) \\ \times \sum_{ts}\Big\{\mathrm{e}^{\mathrm{i}\psi_{m'}^k(t,s)}c^{(km\tilde{\Pi};T)}\left(c^{(km'\tilde{\Pi}';T')^*}P_{ts0}^M + \tilde{\Pi}'c^{(-k,-m',\tilde{\Pi}';T')^*}P_{ts1}^M\right) \\ + \Theta\,\mathrm{e}^{-\mathrm{i}\psi_{m'}^k(t,s)}c^{(-k,-m,\tilde{\Pi};T)}\left(c^{(-k,-m',\tilde{\Pi}';T')^*}P_{ts0}^{-M} + \tilde{\Pi}'c^{(km'\tilde{\Pi}';T')^*}P_{ts1}^{-M}\right)\Big\}. \quad (11)\end{aligned}$$

Here, Kronecker delta $\delta_{m+M}^{m'}$ is 1 if $m + M = m' \bmod(q)$, $P_{tsu}^M = \langle tsu|P^M|000\rangle$, while $\Theta = 1$ if simultaneously $M \neq 0$ and $\tilde{\Pi} = \tilde{\Pi}'$, and $\Theta = -1$ otherwise. Substituting k and m by $-k$ and $-m$ one finds

$$\langle k'm'\tilde{\Pi}'; T'|P^M|km\tilde{\Pi}; T\rangle = \Theta\langle -k', -m'\tilde{\Pi}'; T'|P^{-M}|-k, -m\tilde{\Pi}; T\rangle. \quad (12)$$

These results clearly manifest the selection rules: $\Delta k = k' - k = 0$ (the transitions are vertical); $\Delta m = m' - m = M$ ($M = 0, 1, -1$ correspond to the linear, right and left circular polarized fields with respect to the tube axis). Only P^0 has sharp σ_v parity (even), and obviously this parity is conserved in P^0 transitions. Note that the elements P_{tsu}^M rapidly decrease with the interatomic distance, enabling us to reduce the summation to several neighbouring atoms only.

Table 1. Nonvanishing tensors for the optical transitions in achiral SWNTs. Their nonzero elements $[\mu|\nu^*|\lambda^*]^{mnl}_{m'n'l'}$ are specified by the indices (columns 3 and 5) and the corresponding values in columns 4 and 6.

	$[\mu\|\nu^*\|\lambda^*]$	$[\mu\|\nu^*\|\lambda^*]^{mnl}_{m'n'l'}$		$[\mu\|\nu^*\|\lambda^*]^{mnl}_{m'n'l'}$	
$\mathcal{CZA}$	$[{}_kE^{\tilde\Pi'}_m\|{}_0A^-_0\|{}_kE^{\tilde\Pi^*}_m]$	111 212 111 212	1	111 212 212 111	$-\tilde\Pi'\tilde\Pi$
$\mathcal{ZA}$	$[{}_kG_m\|{}_0A^-_0\|{}_kG^*_m]$	111 212 313 414 111 212 313 414	1	111 212 313 414 414 313 212 111	-1
$\mathcal{C}$	$[{}_kE_{m+1}\|{}_0E^*_1\|{}_kE^*_m]$	111 222 111 222	1	111 222 222 111	1
	$[{}_kE_{m-1}\|{}_0E^*_1\|{}_kE^*_m]$	121 212 121 212	1	121 212 212 121	1
$\mathcal{ZA}$	$[{}_kG_{m+1}\|{}_0E^{+^*}_1\|{}_kG^*_m]$	111 222 313 424 111 222 313 424	1	111 222 313 424 424 313 222 111	1
	$[{}_kG_{m-1}\|{}_0E^{+^*}_1\|{}_kG^*_m]$	121 212 323 414 121 212 323 414	1	121 212 323 414 414 323 212 121	1
	$[{}_kG_1\|{}_0E^{+^*}_1\|{}_kE^{\Pi^*}_0]$	111 221 312 422 111 221 312 422	1	111 221 312 422 422 312 221 111	Π
	$[{}_kE^{\Pi}_0\|{}_0E^{+^*}_1\|{}_kG^*_1]$	112 121 214 223 112 121 214 223	1	112 121 214 223 223 214 121 112	Π
	$[{}_kG_{n-1}\|{}_0E^{+^*}_1\|{}_kE^{\Pi^*}_n]$	121 211 322 412 121 211 322 412	1	121 211 322 412 412 322 211 121	Π
	$[{}_kE^{\Pi}_n\|{}_0E^{+^*}_1\|{}_kG^*_{n-1}]$	111 122 213 224 111 122 213 224	1	111 122 213 224 224 213 122 111	Π

Within the model considered, for each pair k, m there are two eigenenergies $\epsilon^-_m(k)$ and $\epsilon^+_m(k)$, below and above the Fermi level, respectively (the frequency numbers of ${}_kE_m$ and ${}_kG_m$ are 2; those of ${}_kE^A_m$ and ${}_kE^B_m$ are 2 and 0 for $\mathcal{Z}$, and 1 for $\mathcal{A}$ tubes). In the simplest approximation the atomic orbitals are assumed to be orthogonal and only the zero temperature transitions from the valence to the conducting bands (i.e. from $\epsilon^-_m(k)$ to $\epsilon^+_{m'}(k)$) are considered. Further, with the atomic π orbitals all the matrix elements $\langle tsu|p_i|000\rangle$ are pure imaginary, implying $P^M_{tsu} = -P^{M^*}_{tsu}$, as well as $P^M_{000} = 0$. Since (11) involves only the pairs $c^{(km\tilde\Pi;T)} = c^{(km\tilde\Pi;\pm)}$ and $c^{(-k,-m,\tilde\Pi;\pm)}$ their phases can be suitably chosen in the form $c^{(km\tilde\Pi;\pm)} = \mathrm{e}^{-\mathrm{i}\alpha^k_m/2}$ and $c^{(-k,-m,\tilde\Pi;\pm)} = \pm c^{(km\tilde\Pi;\pm)^*}$. Therefore, when the three nearest neighbours $\mathrm{C}_{t_is_i1}$ of C_{000} are included (11) obtains the analytical form:

$$\langle km\tilde\Pi;+|P^M|km\tilde\Pi;-\rangle = 2\mathrm{i}^{\frac{1-\Theta}{2}}\tilde\Pi'\delta^{k'}_k\delta^{m'}_{m+M}\left(1-\delta^M_0+\delta^M_0\delta^{\tilde\Pi'}_{\tilde\Pi}\right)$$
$$\times\sum_{i=1}^{3}\left|P^M_{ts1}\right|\cos\left[\psi^k_{m'}(t_i,s_i)-\frac{\alpha^k_m+\alpha^k_{m'}}{2}+\mathrm{Arg}\left(P^M_{t_is_i1}\right)-\delta^\Theta_{-1}\frac{\pi}{2}\right]. \tag{13}$$

In particular, $\alpha^k_m = \mathrm{Arg}\left[V\sum_i \mathrm{e}^{\mathrm{i}\psi^k_m(t_i,s_i)}\right]$ for the first vector in the SAB (the quantum numbers $k > 0$ and m are equal to those in the irreducible representation label [2]).

5. Modified formalism of Wigner–Eckart theorem

Here we reconsider the Wigner–Eckart theorem within the context of MGPT in order to clarify the notion of the reduced matrix element and the structure of (9) in the induced space case.

To this end in the space $\mathcal{S}^{\mu\lambda^*} = \mathrm{Hom}(\mathcal{H}^{(\lambda)}, \mathcal{H}^{(\mu)}) = \mathcal{H}^{(\mu)} \otimes \mathcal{H}^{(\lambda)^*}$ (of the operators mapping from the irreducible space $\mathcal{H}^{(\lambda)}$ to $\mathcal{H}^{(\mu)}$), we use MGPT to select the subspace $\mathrm{Hom}^{\nu n}(\mathcal{H}^{(\lambda)}, \mathcal{H}^{(\mu)})$ of the ITO components $A^{\nu n}$. The auxiliary space $\mathcal{S}^{\mu\nu^*\lambda^*} = \mathcal{H}^{(\mu)} \otimes \mathcal{H}^{(\nu)^*} \otimes \mathcal{H}^{(\lambda)^*}$ carries the representation $\Gamma^{\mu\nu^*\lambda^*}$ (for convenience, the representation ν is in the middle). A basis of the subspace $\mathcal{F}^{\mu\nu^*\lambda^*}$ comprises the operators $Y_t^{\mu\nu^*\lambda^*} : \mathcal{H}^{(\nu)} \to \mathcal{H}^{(\mu)} \otimes \mathcal{H}^{(\lambda)^*}$. Their tensor structure in the initial bases $|\mu m\rangle$, $\langle \nu n|$ and $\langle \lambda l|$ of the factor spaces $\mathcal{H}^{(\mu)}$, $\mathcal{H}^{(\nu)^*}$ and $\mathcal{H}^{(\lambda)^*}$ is

$$Y_t^{\mu\nu^*\lambda^*} = \sum_{mnl} Y_{mnl;t}^{\mu\nu^*\lambda^*} |\mu m\rangle \otimes \langle \nu n| \otimes \langle \lambda l|. \tag{14}$$

According to (4*a*) the operators $Y_t^{\mu\nu^*\lambda^*}|\nu n\rangle$ are the basis in $\mathrm{Hom}^{\nu n}(\mathcal{H}^{(\lambda)}, \mathcal{H}^{(\mu)})$. The same auxiliary space $\mathcal{S}^{\mu\nu^*\lambda^*}$ and the tensors $Y_t^{\mu\nu^*\lambda^*}$ appear when the μ^*th part of SAB is to be found in the space $\mathcal{H}^{(\nu)^*} \otimes \mathcal{H}^{(\lambda)^*}$. Therefore $t = 1, \ldots, a^{\mu\nu\lambda}$; note that $a^{\mu^*\nu^*\lambda^*} = a^{\mu\nu\lambda}$. Obviously the resulting SAB vector $\langle \mu t m| = \langle \mu m|Y_t^{\mu\nu^*\lambda^*}$ is expanded in the basis $\langle \nu n; \lambda l| = \langle \nu n| \otimes \langle \lambda l|$ of $\mathcal{S}^{\mu\lambda^*}$ with the coefficients

$$\langle \mu t m \mid \nu n; \lambda l\rangle = Y_{mnl;t}^{\mu\nu^*\lambda^*}. \tag{15}$$

So, when $a^{\mu\nu\lambda} = 1$ as in the Wigner–Eckart theorem, $Y_{mnl;t=1}^{\mu\nu^*\lambda^*} = Y_{mnl}^{\mu\nu^*\lambda^*}$ are the Clebsch–Gordan coefficients. Generally, $a^{\mu\nu\lambda} = \dim\mathcal{F}^{\mu\nu^*\lambda^*} = \dim\mathrm{Hom}^{\nu n}(\mathcal{H}^{(\lambda)}, \mathcal{H}^{(\mu)})$ is the number of ITO prototypes $Y_t^{\mu\nu^*\lambda^*}|\nu n\rangle$.

Let the general state space $\mathcal{S}$ decompose onto the irreducible subspaces $\mathcal{S}^{(\mu t_\mu)}$. The matrix elements $\langle \mu t_\mu m|A^{\nu n}|\lambda t_\lambda l\rangle$ of (3) for all m and l form the sub-matrix of $A^{\nu n}$ mapping $\mathcal{S}^{(\lambda t_\lambda)}$ into $\mathcal{S}^{(\mu t_\mu)}$. Therefore, this sub-matrix is from $\mathrm{Hom}^{\nu n}(\mathcal{S}^{(\lambda t_\lambda)}, \mathcal{S}^{(\mu t_\mu)})$, and it must be a linear combination $\sum_t C_{t_\mu t_\lambda t}^{\nu} \tilde{Y}_t^{\mu\nu^*\lambda^*}|\nu n\rangle$ of the operators analogous to (14) but involving SAB of $\mathcal{S}$:

$$\tilde{Y}_t^{\mu\nu^*\lambda^*} = \sum_{mnl} Y_{mnl;t}^{\mu\nu^*\lambda^*} |\mu t_\mu m\rangle \otimes \langle \nu n| \otimes \langle \lambda t_\lambda l|. \tag{16}$$

This reveals the general form of the operators belonging to $\mathrm{Hom}^{\nu n}(\mathcal{S}, \mathcal{S})$:

$$A^{\nu n} = \sum_{\mu t_\mu m} \sum_{\lambda t_\lambda l} \sum_t C_{t_\mu t_\lambda t}^{\mu^*\nu\lambda} Y_{mnl;t}^{\mu\nu^*\lambda^*} |\mu t_\mu m\rangle\langle \lambda t_\lambda l|. \tag{17}$$

Finally, assume $a^{\mu\nu\lambda} = 1$. The Wigner–Eckart theorem directly follows: there is no sum over t, so that the matrix element (3) reduces to $C_{t_\mu t_\lambda}^{\mu^*\nu\lambda} Y_{mnl}^{\mu\nu^*\lambda^*}$. In view of (15), the reduced matrix element is just the coefficient $C_{t_\mu t_\lambda}^{\mu^*\nu\lambda}$. More profound insight is obtained if proceeded further along the MGPT concept of invariants. Firstly, note that the SABs $|\nu n\rangle$ and $\langle \nu n|$ of $\mathcal{H}^{(\nu)}$ and $\mathcal{H}^{(\nu)^*}$ are dual: $\langle \nu n \mid \nu n'\rangle = \delta_{n'}^n$. The adjoint operators $Y^{\mu\nu^*\lambda^*}$ and $Y^{\mu^*\nu\lambda}$, respectively, map them into the dual spaces $\mathcal{H}^{(\mu)} \otimes \mathcal{H}^{(\lambda)^*}$ and $\mathcal{H}^{(\mu)^*} \otimes \mathcal{H}^{(\lambda)}$, giving thus the mutually dual SABs $|\nu, t = 1, n\rangle = Y^{\mu\nu^*\lambda^*}|\nu n\rangle$ and $\langle \nu 1n| = \langle \nu n|Y^{\mu^*\nu\lambda}$:

$$\delta_{n'}^n = \langle \nu 1n \mid \nu 1n'\rangle = \mathrm{Tr}\big[\big(\langle \nu n|Y^{\mu^*\nu\lambda}\big)\big(Y^{\mu\nu^*\lambda^*}|\nu n'\rangle\big)\big] = \sum_{ml} Y_{mnl}^{\mu^*\nu\lambda} Y_{mn'l}^{\mu\nu^*\lambda^*}. \tag{18}$$

(In the case of the unitary representations this points to the unitarity of the Clebsch–Gordan coefficient matrix.) Secondly, the operator

$$A^{\nu} = \sum_n A^{\nu n} \otimes (\langle \nu n|Y^{\mu^*\nu\lambda}) \tag{19}$$

is manifestly G-invariant map from the MGPT auxiliary space $\mathcal{S} \otimes \mathcal{H}^{(\lambda)^*}$ to another one $\mathcal{S} \otimes \mathcal{H}^{(\mu)^*}$. Therefore, it particularly interrelates the relevant fixed point subspaces: $A^{\nu} : \mathcal{F}^{\lambda^*} \to \mathcal{F}^{\mu^*}$. With the help of (4), (17) and (18) one obtains,

$$(\mu t_\mu \| A^\nu \| \lambda t_\lambda) = C^\nu_{t_\mu t_\lambda} = \frac{1}{|\nu|}\langle \mu t_\mu | A^\nu | \lambda t_\lambda \rangle \tag{20}$$

establishing the MGPT form of the Wigner–Eckart theorem

$$\langle \mu t_\mu m | A^{\nu n} | \lambda t_\lambda l \rangle = Y^{\mu\nu^*\lambda^*}_{mnl} \frac{1}{|\nu|}\langle \mu t_\mu | A^\nu | \lambda t_\lambda \rangle. \tag{21}$$

According to (18) this can be given an inverse form:

$$\langle \mu t_\mu | A^\nu | \lambda t_\lambda \rangle = \sum_{mnl} Y^{\mu^*\nu\lambda}_{mnl} \langle \mu t_\mu m | A^{\nu n} | \lambda t_\lambda l \rangle. \tag{22}$$

6. Wigner–Eckart theorem for tight-binding spaces

Here we apply the results of section 5 to the inductive state spaces, e.g. phonon or electron state space of a crystal within the tight-binding model. Being G-invariants in the corresponding auxiliary spaces, all the ingredients of the reduced matrix element $\langle \mu t_\mu | A^\nu | \lambda t_\lambda \rangle$ can be pulled down to the low-dimensional auxiliary interior spaces: $\mathcal{S}_{\gamma^{\mu^*}}$, $\mathcal{S}_{\gamma^{\lambda^*}}$ and $\mathrm{Hom}(\mathcal{S}_{\gamma^{\lambda^*}}, \mathcal{S}_{\gamma^{\mu^*}})$. Since B^μ is partial isometry, $B^{\mu\dagger}B^\mu$ is the identity in $S_{\gamma^{\mu^*}}$. Using (5) and the pulled-down operator $A^{\nu\downarrow} = B^{\mu\dagger}A^\nu B^\lambda$, the matrix element becomes $\langle \mu t_\mu | A^\nu | \lambda t_\lambda \rangle = \langle \mu t_\mu{}^\downarrow | A^{\nu\downarrow} | \lambda t_\lambda{}^\downarrow \rangle$. Finally, the Wigner–Eckart theorem in the inductive space is formulated in terms of the pulled-down invariants only:

$$\langle \mu t_\mu m | A^{\nu n} | \lambda t_\lambda l \rangle = Y^{\mu\nu^*\lambda^*}_{mnl} \frac{1}{|\nu|}\langle \mu t_\mu{}^\downarrow | A^{\nu\downarrow} | \lambda t_\lambda{}^\downarrow \rangle. \tag{23}$$

The pulled down operator $A^{\nu\downarrow}$ is straightforwardly found from its definition:

$$A^{\nu\downarrow} = \sum_{\substack{mnl \\ m'l'n'}} Y^{\mu^*\nu\lambda}_{mnl} [\mu|\nu^*|\lambda^*]^{mnl}_{m'n'l'} \sum_{m''p} D^{(\mu)}_{m'm''}(z_p) A^{\nu n'}_{t0} (|\mu^* m''\rangle \otimes \langle \lambda^* l'|) \tag{24}$$

giving the (reduced) matrix element

$$\langle \mu t_\mu{}^\downarrow | A^{\nu\downarrow} | \lambda t_\lambda{}^\downarrow \rangle = \sum_{\substack{mm'l \\ nn'l'}} Y^{\mu^*\nu\lambda}_{mnl} [\mu|\nu^*|\lambda^*]^{mnl}_{m'n'l'} \sum_{m''p} D^{(\mu)}_{m'm''}(z_p) \langle 0;\, \mu t_\mu m'' | A^{\nu n'}_{p0} | 0;\, \lambda t_\lambda l' \rangle.$$

Note that this is (9) inverted in the sense of (22).

7. Discussion

The profound meaning of the Wigner–Eckart theorem is emphasized by its MGPT form (21). The observable A is the quantum mechanical description of some physical quantity. Its physical content is accessible only in the measurements the results of which are within the formalism described through the matrix elements of A. Hence, the matrix elements reveal all the physical properties of the corresponding quantity. In particular, the transformation properties of A are comprised in Clebsch–Gordan coefficients. All the others are sublimated in the reduced matrix elements: its ingredients are the invariants only, thus with the transformation rules independent of the symmetry group (as the trivial group was encountered). This is reflected also in the inverted form (22), giving the reduced matrix elements as the total contraction of two tensors with dual (thus mutually opposite) transformation properties. In the inductive state spaces (discussed within the familiar tight-binding framework), the invariance of the reduced matrix element ingredients allows us to pull them down to the interior spaces where they are determined on the site-symmetry group level.

The obtained results are neither restricted to the unitary representations nor to the compact groups, since no scalar product, but the duality is used. The $a^{\mu\nu\lambda} = 1$ condition is necessary for the derivation of the Wigner–Eckart theorem in its closed form. Otherwise, some extra condition, necessary to provide the unique choice of the ITO prototypes $Y_t^{\mu\nu^*\lambda^*}$, would yield a slightly more complicated form, with the linear combination over t in (19) and (21). The MGPT fixed point space $\mathcal{F}^{\mu\nu^*\lambda^*}$ appears in section 5 within the context of decompositions of both $\mathrm{Hom}(\mathcal{H}^{(\lambda)}, \mathcal{H}^{(\mu)})$ and $\mathcal{H}^{(\nu^*)} \otimes \mathcal{H}^{(\lambda^*)}$, but the same space gives also the λ part of SAB in $\mathcal{H}^{\mu} \otimes \mathcal{H}^{\nu^*}$, etc. This fact immediately yields the well-known theorems relating various Clebsch–Gordan- or $3J$-coefficients.

The tensor $[\mu|\nu^*|\lambda^*]$ appearing in inductive space considerations, is obviously the transversal projector of the representation $\Gamma^{\mu\nu^*\lambda}$: $[\mu|\nu^*|\lambda^*] = \boldsymbol{Z}(\Gamma^{\mu\nu^*\lambda})$ (recall that $\boldsymbol{Z}$ is a subgroup; otherwise $\boldsymbol{Z}(\Gamma^{\mu\nu^*\lambda})$ is not idempotent, but the comments below are still valid). The fixed points of the corresponding group projector $\boldsymbol{G}(\Gamma^{\mu\nu^*\lambda^*}) = \frac{1}{|G|}\sum_{g\in G}\Gamma^{\mu\nu^*\lambda}(g)$ are exactly the Clebsch–Gordan coefficients tensor (15). Therefore, $[\mu|\nu^*|\lambda^*]$ does not include all the restrictions imposed by the whole group, and it is the super-projector with respect to $\boldsymbol{G}(\Gamma^{\mu\nu^*\lambda^*}) = \boldsymbol{Z}(\Gamma^{\mu\nu^*\lambda^*})\boldsymbol{S}(\Gamma^{\mu\nu^*\lambda^*})$. This has several consequences. Firstly, it follows that $[\mu|\nu^*|\lambda^*]Y_t^{\mu\nu^*\lambda^*} = Y_t^{\mu\nu^*\lambda^*}$, and the dual relation $\sum_{mnl} Y_{mnl}^{\mu^*\nu\lambda}[\mu|\nu^*|\lambda^*]_{m'n'l'}^{mnl} = Y_{m'n'l'}^{\mu^*\nu\lambda}$ additionally reduces (24) and (6). Further, all the corresponding matrix elements (9) may vanish even when $[\mu|\nu^*|\lambda^*]$ does not (the transversal selection rules are less stringent). Clearly, when the transversal is the whole group, as for the $\mathcal{C}$ tubes, the selection rules are completely given by $[\mu|\nu^*|\lambda^*]$. On the other hand, the achiral tubes offer a counterexample: $\left[{}_kE_m^{-\Pi}\middle|{}_0A_0^-\middle|{}_kE_m^{\Pi^*}\right]$ is not zero, although the ${}_kE_m^{\Pi} \to {}_kE_m^{-\Pi}$ transitions are forbidden (i.e. all the Clebsch–Gordan coefficients and the matrix elements vanish).

The matrix elements necessary to derive SWNT optical properties are found. They have the tube independent general form (11), where the tube characterization comes through the values of the parameters. The main difference stems from the selection rules caused by the symmetry based quantum numbers assigned to the bands. The above counterexample shows that in the armchair tubes the P^0-transitions between the $m = 0, n$ bands (with the opposite σ_v parity) are forbidden, while the corresponding transitions in the chiral and zig-zag tubes are allowed. This is due to the nontrivial site-symmetry group projector $\boldsymbol{S}(\Gamma^{\mu\nu^*\lambda^*})$ in the cases when all the representations have sharp parity introduced through a site symmetry.

The coefficients $c^{(km\Pi;T)}$, as well as the momenta matrix elements P_{tsu}^M appearing in the results of section 4, depend on the form of the atomic π-orbital radial function. It is usually found numerically by Hartree–Fock or DFT algorithms [12]. In the simplest case of the hydrogen-like orbitals, the matrix elements are two-centre integrals which are exactly calculated [13]. As an example we consider armchair tube. Note that the neighbours C_{-111} and C_{101} are at the same distance above and below the horizontal plane of C_{000}, while the third one C_{011} is in this plane. Therefore $P_{101}^0 = -P_{-111}^0 = \mathrm{i}P$ ($P > 0$) and $P_{011}^0 = 0$, and (13) gives

$$\langle km\tilde{\Pi};\ +|P^0|km\tilde{\Pi}\rangle = -4\mathrm{i}P\tilde{\Pi}\sin\left(\frac{m\pi}{n} - \alpha_m^k\right)\sin\frac{ka}{2}.$$

Obviously, in the limit $k = 0$ the transitions are forbidden. Indeed, at $k = 0$ the states are even with respect to σ_h, while P^0 is odd. Therefore, P^0-transitions are forbidden by the selection rules. This example shows alternatively that the matrix elements continuity in k enables us to neglect the Brillouin zone edge points, since they are implicitly included. The validity of the above expression (and equation (13)) is restricted to thick nanotubes (diameter greater than 7Å), as the involved approximations of the nearest neighbours and p-orbitals are plausible for

them only. Nevertheless, the described method is quite general, and can be applied to narrow tubes [14] without the mentioned approximations.

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