Orbital angular momentum

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1 Theory of the orbital angular momentum

For a solid state system, let a Bloch-type wave function for a wave vector k be, in general,

$$\begin{aligned}
|\Psi_{\mathbf{k}}> &= \mathbf{1}.|\Psi_{\mathbf{k}}> \\
&= \sum_{nlm} |\phi_{nlm}><\phi_{nlm}|\Psi_{\mathbf{k}}> \\
&= \sum_{nlm} |\phi_{nlm}> C_{nlm}
\end{aligned}$$

Where ϕ_{nlm} are the all atomic orbitals, which forms the basis set. The projected wavefunction onto the i-th atomic site, $\psi_{\mathbf{k},i}$, is given by

$$\begin{aligned}
|\psi_{\mathbf{k},i}> &= \mathbf{1}.|\psi_{\mathbf{k},i}> \\
&= \sum_{nlm} |\phi(r-r_i)_{nlm}><\phi(r-r_i)_{nlm}|\psi_{\mathbf{k},i}> \\
&= \sum_{nlm} |\phi(r-r_i)_{nlm}> C_{nlm,i}
\end{aligned}$$

Therefore, the angular momentum vector around the i-th atomic site is

$$\vec{L}_i = <\psi_{\mathbf{k},i}|\hat{L}_{i,x}|\psi_{\mathbf{k},i}> \hat{x} + <\psi_{\mathbf{k},i}|\hat{L}_{i,y}|\psi_{\mathbf{k},i}> \hat{y} + <\psi_{\mathbf{k},i}|\hat{L}_{i,z}|\psi_{\mathbf{k},i}> \hat{z}$$

Here, $\hat{L}_{i,x}$, $\hat{L}_{i,y}$, $\hat{L}_{i,z}$, are operators for x-, y-, and z-components of the OAM around the i-th atomic site, respectively.

$$\begin{aligned}
<\psi_{\mathbf{k},i}|\hat{L}_{i,z}|\psi_{\mathbf{k},i}> &= <\sum_{nlm} \phi(r-r_i)_{nlm} C_{nlm,i}|\hat{L}_{i,z}|\sum_{n'l'm'} \phi(r-r_i)_{n'l'm'} C_{n'l'm',i}> \\
&= \sum_{nlm}\sum_{n'l'm'} <C_{nlm,i}\phi(r-r_i)_{nlm}|\hat{L}_{i,z}|C_{n'l'm',i}\phi(r-r_i)_{n'l'm'}> \\
&= \sum_{nlm}\sum_{n'l'm'} C^*_{nlm,i} C_{n'l'm',i} <\phi(r-r_i)_{nlm}|\hat{L}_{i,z}|\phi(r-r_i)_{n'l'm'}> \\
&= \sum_{nlm}\sum_{n'l'm'} C^*_{nlm,i} C_{n'l'm',i} <R_{nl} Y_l^m|\hat{L}_{i,z}|R_{n'l'} Y_{l'}^{m'}> \\
&= \sum_{nlm}\sum_{n'l'm'} C^*_{nlm,i} C_{n'l'm',i} <Y_l^m|\hat{L}_{i,z}|Y_{l'}^{m'}> \text{(Radial part wavefunction } \mathrm{R_{nl}} \text{ is normalized)}
\end{aligned}$$

VASP use the atomic orbital basis (AOB) instead of spherical harmonic basis (SHB). The transformation from SHB to AOB was made by the following formulas:

$$
\begin{aligned}
|s> &= |Y_0^0> \\
|p_y> &= \frac{i}{\sqrt{2}}(|Y_1^{-1}> + |Y_1^1>) \\
|p_z> &= |Y_1^0> \\
|p_x> &= \frac{1}{\sqrt{2}}(|Y_1^{-1}> - |Y_1^1>) \\
|d_{xy}> &= \frac{i}{\sqrt{2}}(|Y_2^{-2}> - |Y_2^2>) \\
|d_{yz}> &= \frac{i}{\sqrt{2}}(|Y_2^{-1}> + |Y_2^1>) \\
|d_{z^2}> &= |Y_2^0> \\
|d_{xz}> &= \frac{1}{\sqrt{2}}(|Y_2^{-1}> - |Y_2^1>) \\
|d_{x^2-y^2}> &= \frac{1}{\sqrt{2}}(|Y_2^{-2}> + |Y_2^2>)
\end{aligned}
$$

In the matrix form, it will be

$$
\begin{bmatrix} |s> \\ |p_y> \\ |p_z> \\ |p_x> \\ |d_{xy}> \\ |d_{yz}> \\ |d_{z^2}> \\ |d_{xz}> \\ |d_{x^2-y^2}> \end{bmatrix}
=
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{i}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{i}{\sqrt{2}} & 0 & 0 & 0 & -\frac{i}{\sqrt{2}} \\
0 & 0 & 0 & 0 & 0 & \frac{i}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}}
\end{bmatrix}
\begin{bmatrix} |Y_0^0> \\ |Y_1^{-1}> \\ |Y_1^0> \\ |Y_1^1> \\ |Y_2^{-2}> \\ |Y_2^{-1}> \\ |Y_2^0> \\ |Y_2^1> \\ |Y_2^2> \end{bmatrix}
$$

Let

$$
X=\begin{bmatrix} |s> \\ |p_y> \\ |p_z> \\ |p_x> \\ |d_{xy}> \\ |d_{yz}> \\ |d_{z^2}> \\ |d_{xz}> \\ |d_{x^2-y^2}> \end{bmatrix}
U=\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{i}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{i}{\sqrt{2}} & 0 & 0 & 0 & -\frac{i}{\sqrt{2}} \\
0 & 0 & 0 & 0 & 0 & \frac{i}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}}
\end{bmatrix}
Y=\begin{bmatrix} |Y_0^0> \\ |Y_1^{-1}> \\ |Y_1^0> \\ |Y_1^1> \\ |Y_2^{-2}> \\ |Y_2^{-1}> \\ |Y_2^0> \\ |Y_2^1> \\ |Y_2^2> \end{bmatrix}
$$

$$
<L_z>_{AOB}=X^*\hat{L}_zX^T=\begin{bmatrix} <s| \\ <p_y| \\ <p_z| \\ <p_x| \\ <d_{xy}| \\ <d_{yz}| \\ <d_{z^2}| \\ <d_{xz}| \\ <d_{x^2-y^2}| \end{bmatrix}\hat{L}_z\Big[|s>|p_y>|p_z>|p_x>|d_{xy}>|d_{yz}>|d_{z^2}>|d_{xz}>|d_{x^2-y^2}>\Big]=
$$

$$
\begin{bmatrix}
<s|\hat{L}_z|s> & <s|\hat{L}_z|p_y> & <s|\hat{L}_z|p_z> & <s|\hat{L}_z|p_x> & <s|\hat{L}_z|d_{xy}> & <s|\hat{L}_z|d_{yz}> & <s|\hat{L}_z|d_{z^2}> & <s|\hat{L}_z|d_{xz}> & <s|\hat{L}_z|d_{x^2-y^2}> \\
<P_y|\hat{L}_z|s> & <P_y|\hat{L}_z|p_y> & <P_y|\hat{L}_z|p_z> & <P_y|\hat{L}_z|p_x> & <P_y|\hat{L}_z|d_{xy}> & <P_y|\hat{L}_z|d_{yz}> & <P_y|\hat{L}_z|d_{z^2}> & <P_y|\hat{L}_z|d_{xz}> & <P_y|\hat{L}_z|d_{x^2-y^2}> \\
<p_z|\hat{L}_z|s> & <p_z|\hat{L}_z|p_y> & <p_z|\hat{L}_z|p_z> & <p_z|\hat{L}_z|p_x> & <p_z|\hat{L}_z|d_{xy}> & <p_z|\hat{L}_z|d_{yz}> & <p_z|\hat{L}_z|d_{z^2}> & <p_z|\hat{L}_z|d_{xz}> & <p_z|\hat{L}_z|d_{x^2-y^2}> \\
<p_x|\hat{L}_z|s> & <p_x|\hat{L}_z|p_y> & <p_x|\hat{L}_z|p_z> & <p_x|\hat{L}_z|p_x> & <p_x|\hat{L}_z|d_{xy}> & <p_x|\hat{L}_z|d_{yz}> & <p_x|\hat{L}_z|d_{z^2}> & <p_x|\hat{L}_z|d_{xz}> & <p_x|\hat{L}_z|d_{x^2-y^2}> \\
<d_{xy}|\hat{L}_z|s> & <d_{xy}|\hat{L}_z|p_y> & <d_{xy}|\hat{L}_z|p_z> & <d_{xy}|\hat{L}_z|p_x> & <d_{xy}|\hat{L}_z|d_{xy}> & <d_{xy}|\hat{L}_z|d_{yz}> & <d_{xy}|\hat{L}_z|d_{z^2}> & <d_{xy}|\hat{L}_z|d_{xz}> & <d_{xy}|\hat{L}_z|d_{x^2-y^2}> \\
<d_{yz}|\hat{L}_z|s> & <d_{yz}|\hat{L}_z|p_y> & <d_{yz}|\hat{L}_z|p_z> & <d_{yz}|\hat{L}_z|p_x> & <d_{yz}|\hat{L}_z|d_{xy}> & <d_{yz}|\hat{L}_z|d_{yz}> & <d_{yz}|\hat{L}_z|d_{z^2}> & <d_{yz}|\hat{L}_z|d_{xz}> & <d_{yz}|\hat{L}_z|d_{x^2-y^2}> \\
<d_{z^2}|\hat{L}_z|s> & <d_{z^2}|\hat{L}_z|p_y> & <d_{z^2}|\hat{L}_z|p_z> & <d_{z^2}|\hat{L}_z|p_x> & <d_{z^2}|\hat{L}_z|d_{xy}> & <d_{z^2}|\hat{L}_z|d_{yz}> & <d_{z^2}|\hat{L}_z|d_{z^2}> & <d_{z^2}|\hat{L}_z|d_{xz}> & <d_{z^2}|\hat{L}_z|d_{x^2-y^2}> \\
<d_{xz}|\hat{L}_z|s> & <d_{xz}|\hat{L}_z|p_y> & <d_{xz}|\hat{L}_z|p_z> & <d_{xz}|\hat{L}_z|p_x> & <d_{xz}|\hat{L}_z|d_{xy}> & <d_{xz}|\hat{L}_z|d_{yz}> & <d_{xz}|\hat{L}_z|d_{z^2}> & <d_{xz}|\hat{L}_z|d_{xz}> & <d_{xz}|\hat{L}_z|d_{x^2-y^2}> \\
<d_{x^2-y^2}|\hat{L}_z|s> & <d_{x^2-y^2}|\hat{L}_z|p_y> & <d_{x^2-y^2}|\hat{L}_z|p_z> & <d_{x^2-y^2}|\hat{L}_z|p_x> & <d_{x^2-y^2}|\hat{L}_z|d_{xy}> & <d_{x^2-y^2}|\hat{L}_z|d_{yz}> & <d_{x^2-y^2}|\hat{L}_z|d_{z^2}> & <d_{x^2-y^2}|\hat{L}_z|d_{xz}> & <d_{x^2-y^2}|\hat{L}_z|d_{x^2-y^2}>
\end{bmatrix}
$$

$$
\begin{aligned}
&=U^*Y^*\hat{L}_zY^TU^T \\
&=U^*(Y^*\hat{L}_zY^T)U^T \\
&=U^*<L_z>_{SHB}U^T
\end{aligned}
$$

$$< L_z >_{SHB} = Y^* \hat{L}_z Y^T$$

$$= \begin{bmatrix}
< Y_0^0|\hat{L}_z|Y_0^0 > & < Y_0^0|\hat{L}_z|Y_1^{-1} > & < Y_0^0|\hat{L}_z|Y_1^0 > & < Y_0^0|\hat{L}_z|Y_1^1 > & < Y_0^0|\hat{L}_z|Y_2^{-2} > & < Y_0^0|\hat{L}_z|Y_2^{-1} > & < Y_0^0|\hat{L}_z|Y_2^0 > & < Y_0^0|\hat{L}_z|Y_2^1 > & < Y_0^0|\hat{L}_z|Y_2^2 > \\
< Y_1^{-1}|\hat{L}_z|Y_0^0 > & < Y_1^{-1}|\hat{L}_z|Y_1^{-1} > & < Y_1^{-1}|\hat{L}_z|Y_1^0 > & < Y_1^{-1}|\hat{L}_z|Y_1^1 > & < Y_1^{-1}|\hat{L}_z|Y_2^{-2} > & < Y_1^{-1}|\hat{L}_z|Y_2^{-1} > & < Y_1^{-1}|\hat{L}_z|Y_2^0 > & < Y_1^{-1}|\hat{L}_z|Y_2^1 > & < Y_1^{-1}|\hat{L}_z|Y_2^2 > \\
< Y_1^0|\hat{L}_z|Y_0^0 > & < Y_1^0|\hat{L}_z|Y_1^{-1} > & < Y_1^0|\hat{L}_z|Y_1^0 > & < Y_1^0|\hat{L}_z|Y_1^1 > & < Y_1^0|\hat{L}_z|Y_2^{-2} > & < Y_1^0|\hat{L}_z|Y_2^{-1} > & < Y_1^0|\hat{L}_z|Y_2^0 > & < Y_1^0|\hat{L}_z|Y_2^1 > & < Y_1^0|\hat{L}_z|Y_2^2 > \\
< Y_1^1|\hat{L}_z|Y_0^0 > & < Y_1^1|\hat{L}_z|Y_1^{-1} > & < Y_1^1|\hat{L}_z|Y_1^0 > & < Y_1^1|\hat{L}_z|Y_1^1 > & < Y_1^1|\hat{L}_z|Y_2^{-2} > & < Y_1^1|\hat{L}_z|Y_2^{-1} > & < Y_1^1|\hat{L}_z|Y_2^0 > & < Y_1^1|\hat{L}_z|Y_2^1 > & < Y_1^1|\hat{L}_z|Y_2^2 > \\
< Y_2^{-2}|\hat{L}_z|Y_0^0 > & < Y_2^{-2}|\hat{L}_z|Y_1^{-1} > & < Y_2^{-2}|\hat{L}_z|Y_1^0 > & < Y_2^{-2}|\hat{L}_z|Y_1^1 > & < Y_2^{-2}|\hat{L}_z|Y_2^{-2} > & < Y_2^{-2}|\hat{L}_z|Y_2^{-1} > & < Y_2^{-2}|\hat{L}_z|Y_2^0 > & < Y_2^{-2}|\hat{L}_z|Y_2^1 > & < Y_2^{-2}|\hat{L}_z|Y_2^2 > \\
< Y_2^{-1}|\hat{L}_z|Y_0^0 > & < Y_2^{-1}|\hat{L}_z|Y_1^{-1} > & < Y_2^{-1}|\hat{L}_z|Y_1^0 > & < Y_2^{-1}|\hat{L}_z|Y_1^1 > & < Y_2^{-1}|\hat{L}_z|Y_2^{-2} > & < Y_2^{-1}|\hat{L}_z|Y_2^{-1} > & < Y_2^{-1}|\hat{L}_z|Y_2^0 > & < Y_2^{-1}|\hat{L}_z|Y_2^1 > & < Y_2^{-1}|\hat{L}_z|Y_2^2 > \\
< Y_2^0|\hat{L}_z|Y_0^0 > & < Y_2^0|\hat{L}_z|Y_1^{-1} > & < Y_2^0|\hat{L}_z|Y_1^0 > & < Y_2^0|\hat{L}_z|Y_1^1 > & < Y_2^0|\hat{L}_z|Y_2^{-2} > & < Y_2^0|\hat{L}_z|Y_2^{-1} > & < Y_2^0|\hat{L}_z|Y_2^0 > & < Y_2^0|\hat{L}_z|Y_2^1 > & < Y_2^0|\hat{L}_z|Y_2^2 > \\
< Y_2^1|\hat{L}_z|Y_0^0 > & < Y_2^1|\hat{L}_z|Y_1^{-1} > & < Y_2^1|\hat{L}_z|Y_1^0 > & < Y_2^1|\hat{L}_z|Y_1^1 > & < Y_2^1|\hat{L}_z|Y_2^{-2} > & < Y_2^1|\hat{L}_z|Y_2^{-1} > & < Y_2^1|\hat{L}_z|Y_2^0 > & < Y_2^1|\hat{L}_z|Y_2^1 > & < Y_2^1|\hat{L}_z|Y_2^2 > \\
< Y_2^2|\hat{L}_z|Y_0^0 > & < Y_2^2|\hat{L}_z|Y_1^{-1} > & < Y_2^2|\hat{L}_z|Y_1^0 > & < Y_2^2|\hat{L}_z|Y_1^1 > & < Y_2^2|\hat{L}_z|Y_2^{-2} > & < Y_2^2|\hat{L}_z|Y_2^{-1} > & < Y_2^2|\hat{L}_z|Y_2^0 > & < Y_2^2|\hat{L}_z|Y_2^1 > & < Y_2^2|\hat{L}_z|Y_2^2 >
\end{bmatrix}$$

$$= \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2
\end{bmatrix}$$

$$< L_z >_{AOB} = U^* < L_z >_{SHB} U^T$$

$$= \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\frac{i}{\sqrt{2}} & 0 & 0 & 0 & \frac{i}{\sqrt{2}} \\
0 & 0 & 0 & 0 & 0 & -\frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}}
\end{bmatrix}
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2
\end{bmatrix}
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{i}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{i}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{i}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \\
0 & 0 & 0 & 0 & 0 & \frac{i}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{i}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 0 & -\frac{i}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}}
\end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2i \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2i & 0 & 0 & 0 & 0 \end{bmatrix}$$

To obtain the $< \hat{L}_x >$ and $< \hat{L}_y >$, it needs ladder operators:

$$\begin{aligned} \hat{L}^+|Y_l^m> &= \hbar\sqrt{l(l+1)-m(m+1)}|Y_l^{m+1}>, \\ \hat{L}^-|Y_l^m> &= \hbar\sqrt{l(l+1)-m(m-1)}|Y_l^{m-1}>, \\ \hat{L}_x &= \frac{1}{2}(\hat{L}^+ + \hat{L}^-), \\ \hat{L}_y &= \frac{1}{2i}(\hat{L}^+ - \hat{L}^-), \end{aligned}$$