1 Full matrix-vector derivation

Using (10) as a look-up table and applying the transformations we used to derive (23) from the main body of the paper it can be shown that

$$\begin{aligned}
[\mathbf{H}_1 \triangle \mathbf{p}]_{5(i-1)+1} &= \Sigma^{xx}_{5(i-1)+1} + \Sigma^{xy}_{5(i-1)+1} \\
&+ \Sigma^{xz}_{5(i-1)+1} + \Sigma^{xB}_{5(i-1)+1} + \Sigma^{xO}_{5(i-1)+1} \\
&= \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 h^2 w(\mathbf{s}) \\
&\times \exp[2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{x}_{5(j-1)+1} O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 hkw(\mathbf{s}) \\
&\times \exp[2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{y}_{5(j-1)+2} O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 hlw(\mathbf{s}) \\
&\times \exp[2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{z}_{5(j-1)+3} O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, \pi i h s^2/2w(\mathbf{s}) \\
&\times \exp[2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{B}_{5(j-1)+4} O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 2\pi i h w(\mathbf{s}) \\
&\times \exp[2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{O}_{5j} g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s}\mathbf{r}_j]. \qquad (1)
\end{aligned}$$

Summation for all other sets of rows gives the following result:

$$
\begin{aligned}
[\mathbf{H}_1 \triangle \mathbf{p}]_{5(i-1)+2} = {} & \Sigma^{yx}_{5(i-1)+2} + \Sigma^{yy}_{5(i-1)+2} \\
& + \Sigma^{yz}_{5(i-1)+2} + \Sigma^{yB}_{5(i-1)+2} + \Sigma^{yO}_{5(i-1)+2} \\
& = \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 hkw(\mathbf{s}) \\
& \times \exp[2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{x}_{5(j-1)+1} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& + \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 k^2 w(\mathbf{s}) \\
& \times \exp[2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{y}_{5(j-1)+2} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& + \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 klw(\mathbf{s}) \\
& \times \exp[2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{z}_{5(j-1)+3} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& - \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, \pi i k s^2/2w(\mathbf{s}) \\
& \times \exp[2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{B}_{5(j-1)+4} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& + \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 2\pi i k w(\mathbf{s}) \\
& \times \exp[2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{O}_{5j} g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j], \qquad (2)
\end{aligned}
$$

$$
\begin{aligned}
\left[\mathbf{H}_1 \triangle \mathbf{p}\right]_{5(i-1)+3} = {} & \Sigma^{zx}_{5(i-1)+3} + \Sigma^{zy}_{5(i-1)+3} \\
& + \Sigma^{zz}_{5(i-1)+3} + \Sigma^{zB}_{5(i-1)+3} + \Sigma^{zO}_{5(i-1)+3} \\
& = \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 hlw\left(\mathbf{s}\right) \\
& \times \exp\left[2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^{x}_{5(j-1)+1} O_j g_j\left(\mathbf{s}\right) \\
& \times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
& + \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 klw\left(\mathbf{s}\right) \\
& \times \exp\left[2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^{y}_{5(j-1)+2} O_j g_j\left(\mathbf{s}\right) \\
& \times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
& + \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 l^2 w\left(\mathbf{s}\right) \\
& \times \exp\left[2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^{z}_{5(j-1)+3} O_j g_j\left(\mathbf{s}\right) \\
& \times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
& - \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) \pi i l s^2/2w\left(\mathbf{s}\right) \\
& \times \exp\left[2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^{z}_{5(j-1)+4} O_j g_j\left(\mathbf{s}\right) \\
& \times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
& + \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 2\pi i lw\left(\mathbf{s}\right) \\
& \times \exp\left[2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^{O}_{5j} g_j\left(\mathbf{s}\right) \\
& \times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right], \qquad (3)
\end{aligned}
$$

$$
\begin{aligned}
[\mathbf{H}_1 \triangle \mathbf{p}]_{5(i-1)+4} = {} & \Sigma^{Bx}_{5(i-1)+4} + \Sigma^{By}_{5(i-1)+4} \\
& + \Sigma^{Bz}_{5(i-1)+4} + \Sigma^{BB}_{5(i-1)+4} + \Sigma^{BO}_{5(i-1)+4} \\
& = \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \, \pi i h s^2 / 2w(\mathbf{s}) \\
& \times \exp[2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{x}_{5(j-1)+1} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
& + \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \, \pi i k s^2 / 2w(\mathbf{s}) \\
& \times \exp[2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{y}_{5(j-1)+2} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
& + \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \, \pi i l s^2 / 2w(\mathbf{s}) \\
& \times \exp[2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{z}_{5(j-1)+3} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
& - \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \, s^4 / 16w(\mathbf{s}) \\
& \times \exp[2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{B}_{5(j-1)+4} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
& - \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \, s^2 / 4w(\mathbf{s}) \\
& \times \exp[2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{O}_{5j} g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s} \mathbf{r}_j],
\end{aligned} \tag{4}
$$

$$
\begin{aligned}
[\mathbf{H}_1 \triangle \mathbf{p}]_{5i} = \Sigma_{5i}^{Ox} + \Sigma_{5i}^{Oy} + \Sigma_{5i}^{Oz} + \Sigma_{5i}^{OB} + \Sigma_{5i}^{OO} = \\
& - \sum_{\mathbf{s}} g_i(\mathbf{s})\, 2\pi i h w(\mathbf{s}) \\
& \times \exp\left[2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^{x}_{5(j-1)+1} O_j g_j(\mathbf{s}) \\
& \times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
& - \sum_{\mathbf{s}} g_i(\mathbf{s})\, 2\pi i k w(\mathbf{s}) \\
& \times \exp\left[2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^{y}_{5(j-1)+2} O_j g_j(\mathbf{s}) \\
& \times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
& - \sum_{\mathbf{s}} g_i(\mathbf{s})\, 2\pi i l w(\mathbf{s}) \\
& \times \exp\left[2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^{z}_{5(j-1)+3} O_j g_j(\mathbf{s}) \\
& \times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
& - \sum_{\mathbf{s}} g_i(\mathbf{s})\, s^2/4 w(\mathbf{s}) \\
& \times \exp\left[2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^{B}_{5(j-1)+4} O_j g_j(\mathbf{s}) \\
& \times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
& + \sum_{\mathbf{s}} g_i(\mathbf{s})\, w(\mathbf{s}) \\
& \times \exp\left[2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^{O}_{5j} g_j(\mathbf{s}) \\
& \times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right]. \qquad (5)
\end{aligned}
$$

The product $\mathbf{H}_1 \triangle \mathbf{p}$ has been calculated. Substituting $\mathbf{H}_2$ instead of $\mathbf{H}_1$ in (16–20) from the main body of the paper and expanding the equations for the H_2 terms we get the following result:

$$
\begin{aligned}
[\mathbf{H}_2 \triangle \mathbf{p}]_{5(i-1)+1} = \Sigma^{xx}_{5(i-1)+1} + \Sigma^{xy}_{5(i-1)+1} \\
+\Sigma^{xz}_{5(i-1)+1} + \Sigma^{xB}_{5(i-1)+1} + \Sigma^{xO}_{5(i-1)+1} = \\
-\sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 h^2 w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
\times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{x}_{5(j-1)+1} O_j g_j(\mathbf{s}) \\
\times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
-\sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 hk w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
\times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{y}_{5(j-1)+2} O_j g_j(\mathbf{s}) \\
\times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
-\sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 hl w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
\times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{z}_{5(j-1)+3} O_j g_j(\mathbf{s}) \\
\times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
+\sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, \pi i h s^2/2 w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
\times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{B}_{5(j-1)+4} O_j g_j(\mathbf{s}) \\
\times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
-\sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 2\pi i h w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
\times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{O}_{5j} g_j(\mathbf{s}) \\
\times \exp[-2\pi i \mathbf{s}\mathbf{r}_j], \qquad (6)
\end{aligned}
$$

$$
\begin{aligned}
\left[\mathbf{H}_2 \triangle \mathbf{p}\right]_{5(i-1)+2} = \Sigma^{yx}_{5(i-1)+2} + \Sigma^{yy}_{5(i-1)+2} \\
+\Sigma^{yz}_{5(i-1)+2} + \Sigma^{yB}_{5(i-1)+2} + \Sigma^{yO}_{5(i-1)+2} = \\
-\sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 hkw\left(\mathbf{s}\right) \exp\left[2i\varphi_c\left(\mathbf{s}\right)\right] \\
\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^x_{5(j-1)+1} O_j g_j\left(\mathbf{s}\right) \\
\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
-\sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 k^2 w\left(\mathbf{s}\right) \exp\left[2i\varphi_c\left(\mathbf{s}\right)\right] \\
\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^y_{5(j-1)+2} O_j g_j\left(\mathbf{s}\right) \\
\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
-\sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 klw\left(\mathbf{s}\right) \exp\left[2i\varphi_c\left(\mathbf{s}\right)\right] \\
\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^z_{5(j-1)+3} O_j g_j\left(\mathbf{s}\right) \\
\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
+\sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) \pi i k s^2/2w\left(\mathbf{s}\right) \exp\left[2i\varphi_c\left(\mathbf{s}\right)\right] \\
\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^B_{5(j-1)+4} O_j g_j\left(\mathbf{s}\right) \\
\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
-\sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 2\pi i k w\left(\mathbf{s}\right) \exp\left[2i\varphi_c\left(\mathbf{s}\right)\right] \\
\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^O_{5j} g_j\left(\mathbf{s}\right) \\
\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right], \qquad (7)
\end{aligned}
$$

$$
\begin{aligned}
[\mathbf{H}_2 \triangle \mathbf{p}]_{5(i-1)+3} = {} & \Sigma^{zx}_{5(i-1)+3} + \Sigma^{zy}_{5(i-1)+3} \\
& + \Sigma^{zz}_{5(i-1)+3} + \Sigma^{zB}_{5(i-1)+3} + \Sigma^{zO}_{5(i-1)+3} = \\
& - \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 hlw(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^x_{5(j-1)+1} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& - \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 klw(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^y_{5(j-1)+2} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& - \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 4\pi^2 l^2 w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^z_{5(j-1)+3} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& + \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, \pi i l s^2/2 w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^B_{5(j-1)+4} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& - \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, 2\pi i l w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^O_{5j} g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j], \qquad (8)
\end{aligned}
$$

$$
\begin{aligned}
[\mathbf{H}_2\triangle\mathbf{p}]_{5(i-1)+4} &= \Sigma^{Bx}_{5(i-1)+4} + \Sigma^{By}_{5(i-1)+4} \\
&+\Sigma^{Bz}_{5(i-1)+4} + \Sigma^{BB}_{5(i-1)+4} + \Sigma^{BO}_{5(i-1)+4} \\
&= \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\,\pi i h s^2/2w(\mathbf{s}) \exp\left[2i\varphi_c(\mathbf{s})\right] \\
&\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^x_{5(j-1)+1} O_j g_j(\mathbf{s}) \\
&\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\,\pi i k s^2/2w(\mathbf{s}) \exp\left[2i\varphi_c(\mathbf{s})\right] \\
&\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^y_{5(j-1)+2} O_j g_j(\mathbf{s}) \\
&\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\,\pi i l s^2/2w(\mathbf{s}) \exp\left[2i\varphi_c(\mathbf{s})\right] \\
&\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^z_{5(j-1)+3} O_j g_j(\mathbf{s}) \\
&\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, s^4/16w(\mathbf{s}) \exp\left[2i\varphi_c(\mathbf{s})\right] \\
&\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^B_{5(j-1)+4} O_j g_j(\mathbf{s}) \\
&\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, s^2/4w(\mathbf{s}) \exp\left[2i\varphi_c(\mathbf{s})\right] \\
&\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_i\right] \sum_{j=1}^{N} \triangle p^O_{5j} g_j(\mathbf{s}) \\
&\times \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right], \qquad (9)
\end{aligned}
$$

$$
\begin{aligned}
[\mathbf{H}_2 \triangle \mathbf{p}]_{5i} = \Sigma_{5i}^{Ox} + \Sigma_{5i}^{Oy} + \Sigma_{5i}^{Oz} + \Sigma_{5i}^{OB} + \Sigma_{5i}^{OO} = \\
& - \sum_{\mathbf{s}} g_i(\mathbf{s})\, 2\pi i h w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{x}_{5(j-1)+1} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& - \sum_{\mathbf{s}} g_i(\mathbf{s})\, 2\pi i k w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{y}_{5(j-1)+2} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& - \sum_{\mathbf{s}} g_i(\mathbf{s})\, 2\pi i l w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{z}_{5(j-1)+3} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& - \sum_{\mathbf{s}} g_i(\mathbf{s})\, s^2/4 w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{B}_{5(j-1)+4} O_j g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j] \\
& + \sum_{\mathbf{s}} g_i(\mathbf{s})\, w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \sum_{j=1}^{N} \triangle p^{O}_{5j} g_j(\mathbf{s}) \\
& \times \exp[-2\pi i \mathbf{s}\mathbf{r}_j]\,. \qquad (10)
\end{aligned}
$$

The equations (1-10) can be simplified using the following simple but crucial assumption. The components of vector $\triangle\mathbf{p} = (\triangle x_1,\triangle y_1,\triangle z_1,\triangle B_1,\triangle O_1,\ldots,\triangle \mathrm{B}_N,\triangle \mathrm{O}_N)^T$ can be viewed simply as (artificial) *occupancies*. To distinguish them from real atomic occupancies we shall call them *quasi-occupancies*. We may write then:

$$\triangle\mathbf{p} \equiv \mathbf{q} = (q_1, q_2, \ldots, q_{5N})^T \qquad (11)$$

and

$$\mathbf{H}\triangle\mathbf{p} = \mathbf{H}\mathbf{q}. \tag{12}$$

Since $\triangle\mathbf{p}$ and $\mathbf{q}$ are mathematically identical by definition (11) we can divide them into the same sets defined by (24) in the main body of the paper. Note that in (1–10) we repeatedly get the same sums along index j. Using (11) , (6) from the main body of the paper and, for instance, the first sum along index j in (1) we immediately obtain the following result:

$$\begin{aligned} F_c^{x*}(\mathbf{s}) &= \sum_{j=1}^{N} q^x_{5(j-1)+1} O_j g_j(\mathbf{s}) \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\ &= \sum_{j=1}^{N} \triangle p^x_{5(j-1)+1} O_j g_j(\mathbf{s}) \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right], \end{aligned} \tag{13}$$

There are five different sums along index j in (1–10). The first one is just given above, the four other sums are given below:

$$\begin{aligned} F_c^{y*}(\mathbf{s}) &= \sum_{j=1}^{N} q^y_{5(j-1)+2} O_j g_j(\mathbf{s}) \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\ &= \sum_{j=1}^{N} \triangle p^y_{5(j-1)+2} O_j g_j(\mathbf{s}) \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right], \end{aligned} \tag{14}$$

$$\begin{aligned} F_c^{z*}(\mathbf{s}) &= \sum_{j=1}^{N} q^z_{5(j-1)+3} O_j g_j(\mathbf{s}) \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\ &= \sum_{j=1}^{N} \triangle p^z_{5(j-1)+3} O_j g_j(\mathbf{s}) \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right], \end{aligned} \tag{15}$$

$$\begin{aligned} F_c^{B*}(\mathbf{s}) &= \sum_{j=1}^{N} q^B_{5(j-1)+4} O_j g_j(\mathbf{s}) \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\ &= \sum_{j=1}^{N} \triangle p^B_{5(j-1)+4} O_j g_j(\mathbf{s}) \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right], \end{aligned} \tag{16}$$

$$\begin{aligned} F_c^{O*}(\mathbf{s}) &= \sum_{j=1}^{N} q_{5j}^{O} g_j(\mathbf{s}) \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right] \\ &= \sum_{j=1}^{N} \triangle p_{5j}^{O} g_j(\mathbf{s}) \exp\left[-2\pi i \mathbf{s}\mathbf{r}_j\right]. \end{aligned} \tag{17}$$

Therefore, the five sets of modified occupancies must be formed to calculate corresponding F_cs:

$$\mathbf{q}^{mod} = \begin{cases} q_{5(j-1)+1}^{x} O_j, \\ q_{5(j-1)+2}^{y} O_j, \\ q_{5(j-1)+3}^{z} O_j, \quad j = 1, 2, \ldots, N \\ q_{5(j-1)+4}^{B} O_j, \\ q_{5j}^{O}. \end{cases} \tag{18}$$

The following definitions may be introduced to simplify the final result:

$$E^{x}(\mathbf{s}) = F_c^{x}(\mathbf{s}) - F_c^{x*}(\mathbf{s}) \exp\left[2i\varphi_c(\mathbf{s})\right] \tag{19}$$

$$E^{y}(\mathbf{s}) = F_c^{y}(\mathbf{s}) - F_c^{y*}(\mathbf{s}) \exp\left[2i\varphi_c(\mathbf{s})\right] \tag{20}$$

$$E^{z}(\mathbf{s}) = F_c^{z}(\mathbf{s}) - F_c^{z*}(\mathbf{s}) \exp\left[2i\varphi_c(\mathbf{s})\right] \tag{21}$$

$$E^{B}(\mathbf{s}) = F_c^{B}(\mathbf{s}) + F_c^{B*}(\mathbf{s}) \exp\left[2i\varphi_c(\mathbf{s})\right] \tag{22}$$

$$E^{O}(\mathbf{s}) = F_c^{O}(\mathbf{s}) + F_c^{O*}(\mathbf{s}) \exp\left[2i\varphi_c(\mathbf{s})\right] \tag{23}$$

Substituting (13–17) in (1–10) and summing up equivalent rows in $\mathbf{H}_1$ and $\mathbf{H}_2$ matrices using (20) from the main body of the paper we obtain:

$$
\begin{aligned}
[\mathbf{H}\triangle\mathbf{p}]_{5(i-1)+1} = &\sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 h^2 w\left(\mathbf{s}\right) E^x\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+ \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 hkw\left(\mathbf{s}\right) E^y\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+ \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 hlw\left(\mathbf{s}\right) E^z\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+ \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) \pi i h s^2/2w\left(\mathbf{s}\right) E^B\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&- \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 2\pi i h w\left(\mathbf{s}\right) E^O\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i],
\end{aligned} \tag{24}
$$

$$
\begin{aligned}
[\mathbf{H}\triangle\mathbf{p}]_{5(i-1)+2} = &\sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 hkw\left(\mathbf{s}\right) E^x\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+ \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 k^2 w\left(\mathbf{s}\right) E^y\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+ \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 klw\left(\mathbf{s}\right) E^z\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+ \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) \pi i k s^2/2w\left(\mathbf{s}\right) E^B\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&- \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 2\pi i k w\left(\mathbf{s}\right) E^O\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i],
\end{aligned} \tag{25}
$$

$$
\begin{aligned}
[\mathbf{H}\triangle\mathbf{p}]_{5(i-1)+3} = &\sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 hlw\left(\mathbf{s}\right) E^x\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+ \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 klw\left(\mathbf{s}\right) E^y\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+ \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 4\pi^2 l^2 w\left(\mathbf{s}\right) E^z\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+ \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) \pi i l s^2/2w\left(\mathbf{s}\right) E^B\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&- \sum_{\mathbf{s}} O_i g_i\left(\mathbf{s}\right) 2\pi i l w\left(\mathbf{s}\right) E^O\left(\mathbf{s}\right) \exp[-2\pi i \mathbf{s}\mathbf{r}_i],
\end{aligned} \tag{26}
$$

$$
\begin{aligned}
[\mathbf{H}\triangle\mathbf{p}]_{5(i-1)+4} = &-\sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, \pi i h s^2/2w(\mathbf{s})\, E^x(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&-\sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, \pi i k s^2/2w(\mathbf{s})\, E^y(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&-\sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, \pi i l s^2/2w(\mathbf{s})\, E^z(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+\sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, s^4/16w(\mathbf{s})\, E^B(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&-\sum_{\mathbf{s}} O_i g_i(\mathbf{s})\, s^2/4w(\mathbf{s})\, E^O(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i], \qquad (27)
\end{aligned}
$$

$$
\begin{aligned}
[\mathbf{H}\triangle\mathbf{p}]_{5i} = &\sum_{\mathbf{s}} g_i(\mathbf{s})\, 2\pi i h w(\mathbf{s})\, E^x(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+\sum_{\mathbf{s}} g_i(\mathbf{s})\, 2\pi i k w(\mathbf{s})\, E^y(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+\sum_{\mathbf{s}} g_i(\mathbf{s})\, 2\pi i l w(\mathbf{s})\, E^z(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&-\sum_{\mathbf{s}} g_i(\mathbf{s})\, s^2/4w(\mathbf{s})\, E^B(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \\
&+\sum_{\mathbf{s}} g_i(\mathbf{s})\, w(\mathbf{s})\, E^O(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i]. \qquad (28)
\end{aligned}
$$

During the simplification process we assumed that Friedel's law holds and the following two important identities have been used:

$$\sum_{\mathbf{s}} F_c^*(\mathbf{s}) \exp[2\pi i \mathbf{s}\mathbf{r}_i] = \sum_{\mathbf{s}} F_c(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \qquad (29)$$

$$\sum_{\mathbf{s}} i F_c^*(\mathbf{s}) \exp[2\pi i \mathbf{s}\mathbf{r}_i] = -\sum_{\mathbf{s}} i F_c(\mathbf{s}) \exp[-2\pi i \mathbf{s}\mathbf{r}_i] \qquad (30)$$

All single entry vectors $[\mathbf{H}\triangle\mathbf{p}]_{5(i-1)+m}$ can readily be merged into the final $\mathbf{H}\triangle\mathbf{p}$ product:

$$\mathbf{H}\triangle\mathbf{p} = \sum_{m=1}^{5} \sum_{i=1}^{N} [\mathbf{H}\triangle\mathbf{p}]_{5(i-1)+m}\,. \qquad (31)$$

Obviously, vector $\mathbf{H}\triangle\mathbf{p}$ has no empty entries now. The derivation is over.