

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

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

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

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

$$\begin{aligned}
[\mathbf{H}_1 \Delta \mathbf{p}]_{5(i-1)+3} &= \Sigma_{5(i-1)+3}^{zx} + \Sigma_{5(i-1)+3}^{zy} \\
&+ \Sigma_{5(i-1)+3}^{zz} + \Sigma_{5(i-1)+3}^{zB} + \Sigma_{5(i-1)+3}^{zO} \\
&= \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 4\pi^2 h l w(\mathbf{s}) \\
&\times \exp[2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+1}^x O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 4\pi^2 k l w(\mathbf{s}) \\
&\times \exp[2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+2}^y O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 4\pi^2 l^2 w(\mathbf{s}) \\
&\times \exp[2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+3}^z O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \pi i l s^2 / 2w(\mathbf{s}) \\
&\times \exp[2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+4}^z O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 2\pi i l w(\mathbf{s}) \\
&\times \exp[2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5j}^O g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j], \tag{3}
\end{aligned}$$

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

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

The product $\mathbf{H}_1 \Delta \mathbf{p}$ 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:

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

$$\begin{aligned}
[\mathbf{H}_2 \Delta \mathbf{p}]_{5(i-1)+2} &= \Sigma_{5(i-1)+2}^{yx} + \Sigma_{5(i-1)+2}^{yy} \\
&+ \Sigma_{5(i-1)+2}^{yz} + \Sigma_{5(i-1)+2}^{yB} + \Sigma_{5(i-1)+2}^{yO} = \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 4\pi^2 h k w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+1}^x O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 4\pi^2 k^2 w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+2}^y O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 4\pi^2 k l w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+3}^z O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \pi i k s^2 / 2 w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+4}^B O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 2\pi i k w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5j}^O g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j], \tag{7}
\end{aligned}$$

$$\begin{aligned}
[\mathbf{H}_2 \Delta \mathbf{p}]_{5(i-1)+3} &= \Sigma_{5(i-1)+3}^{zx} + \Sigma_{5(i-1)+3}^{zy} \\
&+ \Sigma_{5(i-1)+3}^{zz} + \Sigma_{5(i-1)+3}^{zB} + \Sigma_{5(i-1)+3}^{zO} = \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 4\pi^2 h l w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+1}^x O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 4\pi^2 k l w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+2}^y O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 4\pi^2 l^2 w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+3}^z O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \pi i l s^2 / 2w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+4}^B O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) 2\pi i l w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5j}^O g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j], \tag{8}
\end{aligned}$$

$$\begin{aligned}
[\mathbf{H}_2 \Delta \mathbf{p}]_{5(i-1)+4} &= \Sigma_{5(i-1)+4}^{Bx} + \Sigma_{5(i-1)+4}^{By} \\
&+ \Sigma_{5(i-1)+4}^{Bz} + \Sigma_{5(i-1)+4}^{BB} + \Sigma_{5(i-1)+4}^{BO} \\
&= \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \pi i h s^2 / 2w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+1}^x O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \pi i k s^2 / 2w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+2}^y O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) \pi i l s^2 / 2w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+3}^z O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&+ \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) s^4 / 16w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5(j-1)+4}^B O_j g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\
&- \sum_{\mathbf{s}} O_i g_i(\mathbf{s}) s^2 / 4w(\mathbf{s}) \exp[2i\varphi_c(\mathbf{s})] \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_i] \sum_{j=1}^N \Delta p_{5j}^O g_j(\mathbf{s}) \\
&\times \exp[-2\pi i \mathbf{s} \mathbf{r}_j], \tag{9}
\end{aligned}$$

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

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

$$\Delta \mathbf{p} \equiv \mathbf{q} = (q_1, q_2, \dots, q_{5N})^T \tag{11}$$

and

$$\mathbf{H}\Delta\mathbf{p} = \mathbf{H}\mathbf{q}. \quad (12)$$

Since $\Delta\mathbf{p}$ 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:

$$\begin{aligned} F_c^{x*}(\mathbf{s}) &= \sum_{j=1}^N q_{5(j-1)+1}^x O_j g_j(\mathbf{s}) \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\ &= \sum_{j=1}^N \Delta p_{5(j-1)+1}^x O_j g_j(\mathbf{s}) \exp[-2\pi i \mathbf{s} \mathbf{r}_j], \end{aligned} \quad (13)$$

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:

$$\begin{aligned} F_c^{y*}(\mathbf{s}) &= \sum_{j=1}^N q_{5(j-1)+2}^y O_j g_j(\mathbf{s}) \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\ &= \sum_{j=1}^N \Delta p_{5(j-1)+2}^y O_j g_j(\mathbf{s}) \exp[-2\pi i \mathbf{s} \mathbf{r}_j], \end{aligned} \quad (14)$$

$$\begin{aligned} F_c^{z*}(\mathbf{s}) &= \sum_{j=1}^N q_{5(j-1)+3}^z O_j g_j(\mathbf{s}) \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\ &= \sum_{j=1}^N \Delta p_{5(j-1)+3}^z O_j g_j(\mathbf{s}) \exp[-2\pi i \mathbf{s} \mathbf{r}_j], \end{aligned} \quad (15)$$

$$\begin{aligned} F_c^{B*}(\mathbf{s}) &= \sum_{j=1}^N q_{5(j-1)+4}^B O_j g_j(\mathbf{s}) \exp[-2\pi i \mathbf{s} \mathbf{r}_j] \\ &= \sum_{j=1}^N \Delta p_{5(j-1)+4}^B O_j g_j(\mathbf{s}) \exp[-2\pi i \mathbf{s} \mathbf{r}_j], \end{aligned} \quad (16)$$

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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

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

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

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

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

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