Chapter 1
Matrix element of $\mathcal{V}$ in a plane-waves basis

In a plane-waves basis, Bloch wavefunctions can be expressed as

$$\phi_{n,\mathbf{k}}(\mathbf{r}) = \frac{e^{i\mathbf{kr}}}{\sqrt{V}} \sum_G c_{n,\mathbf{k}}(\mathbf{G}) e^{i\mathbf{Gr}} \tag{1.1}$$

where V is the volume of the unit-cell.
One wants to compute

$$\langle n,\mathbf{k}|\mathbf{q}\mathcal{V}|n',\mathbf{k}\rangle = \langle n,\mathbf{k}|\frac{\mathcal{C}(z)\mathbf{qv}+\mathbf{qv}\mathcal{C}(z)}{2}|n',\mathbf{k}\rangle \tag{1.2}$$

with $\mathbf{v} = \mathbf{p} + i[V_{nl},\mathbf{r}]$.
One must computes the contributions $\langle n,\mathbf{k}|\frac{\mathcal{C}(z)\mathbf{qp}+\mathbf{qp}\mathcal{C}(z)}{2}|n',\mathbf{k}\rangle$ and $\langle n,\mathbf{k}|\frac{\mathcal{C}(z)[V_{nl},i\mathbf{qr}]+[V_{nl},i\mathbf{qr}]\mathcal{C}(z)}{2}|n',\mathbf{k}\rangle$.

Using Eq. 1.1,

$$\begin{aligned}
\langle n,\mathbf{k}|\frac{\mathcal{C}(z)\mathbf{qp}+\mathbf{qp}\mathcal{C}(z)}{2}|n',\mathbf{k}\rangle &= \frac{-i}{2V}\sum_{\mathbf{G},\mathbf{G}'} c^*_{n,\mathbf{k}}(\mathbf{G})c_{n',\mathbf{k}}(\mathbf{G}') \\
\times \int d^3\mathbf{r}\left[e^{-i(\mathbf{k}+\mathbf{G})\mathbf{r}}\mathcal{C}(z)\nabla_\mathbf{r}(e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}}) - \nabla_\mathbf{r}(e^{-i(\mathbf{k}+\mathbf{G})\mathbf{r}})\mathcal{C}(z)e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}}\right]& \\
= \frac{1}{2}\sum_{\mathbf{G},\mathbf{G}'} c^*_{n,\mathbf{k}}(\mathbf{G})c_{n',\mathbf{k}}(\mathbf{G}')\left[2\mathbf{k}+\mathbf{G}+\mathbf{G}'\right]\frac{1}{V}\int d^3\mathbf{r}e^{-i(\mathbf{G}-\mathbf{G}')\mathbf{r}}\mathcal{C}(z)& \\
= \frac{1}{2}\sum_{\mathbf{G},\mathbf{G}'} c^*_{n,\mathbf{k}}(\mathbf{G})c_{n',\mathbf{k}}(\mathbf{G}')\left[2\mathbf{k}+\mathbf{G}+\mathbf{G}'\right]\delta_{\mathbf{G}_{||}\mathbf{G}'_{||}}F(G_z-G'_z)&
\end{aligned} \tag{1.3}$$

where we have defined $F(G_z) = \frac{1}{2L_z}\int dz e^{-iG_z z}\mathcal{C}(z)$.

In order to compute the term containing the commutator, we introduce the unity operator

$$\langle n,\mathbf{k}|\mathcal{C}(z)[V_{nl},i\mathbf{qr}]|n',\mathbf{k}\rangle = \sum_{\mathbf{G}''}\langle n,\mathbf{k}|\mathcal{C}(z)|\mathbf{k}+\mathbf{G}''\rangle\langle\mathbf{k}+\mathbf{G}''|[V_{nl},i\mathbf{qr}]|n',\mathbf{k}\rangle \tag{1.4}$$

where $\langle\mathbf{r}|\mathbf{k}+\mathbf{G}\rangle = e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}}/\sqrt{V}$.
Using Eq. 1.1,

$$\begin{aligned}
\langle n,\mathbf{k}|\mathcal{C}(z)|\mathbf{k}+\mathbf{G}''\rangle &= \frac{1}{\sqrt{V}}\sum_G c^*_{n,\mathbf{k}}(\mathbf{G})\int d^3\mathbf{r}e^{-i(\mathbf{k}+\mathbf{G})\mathbf{r}}\mathcal{C}(z)e^{i(\mathbf{k}+\mathbf{G}'')\mathbf{r}} \\
&= \frac{1}{\sqrt{V}}\sum_G c^*_{n,\mathbf{k}}(\mathbf{G})\int d^3\mathbf{r}e^{-i(\mathbf{G}-\mathbf{G}'')\mathbf{r}}\mathcal{C}(z)
\end{aligned} \tag{1.5}$$

$$\begin{aligned}
\langle\mathbf{k}+\mathbf{G}''|[V_{nl},i\mathbf{qr}]|n',\mathbf{k}\rangle &= \frac{1}{\sqrt{V}}\sum_{G'} c_{n',\mathbf{k}}(\mathbf{G}')\int d^3\mathbf{r}e^{i(\mathbf{k}+\mathbf{G}'')\mathbf{r}}[V_{nl},i\mathbf{qr}]e^{i(\mathbf{k}+\mathbf{G}')\mathbf{r}} \\
&= \frac{1}{\sqrt{V}}\sum_{G'} c_{n',\mathbf{k}}(\mathbf{G}')\langle\mathbf{k}+\mathbf{G}''|[V_{nl},i\mathbf{qr}]|\mathbf{k}+\mathbf{G}'\rangle
\end{aligned} \tag{1.6}$$

Putting everything together yields

$$\langle n,\mathbf{k}|\mathcal{C}(z)[V_{nl},i\mathbf{q}\mathbf{r}]|n',\mathbf{k}\rangle = \sum_{\mathbf{G},\mathbf{G}',\mathbf{G}''} c^*_{n,\mathbf{k}}(\mathbf{G})c_{n',\mathbf{k}}(\mathbf{G}')\langle\mathbf{k}+\mathbf{G}''|[V_{nl},i\mathbf{q}\mathbf{r}]|\mathbf{k}+\mathbf{G}'\delta_{\mathbf{G}_{||}\mathbf{G}''_{||}}\rangle F(G_z-G''_z) \tag{1.7}$$

So

$$\langle n,\mathbf{k}|\frac{\mathcal{C}(z)[V_{nl},i\mathbf{q}\mathbf{r}]+[V_{nl},i\mathbf{q}\mathbf{r}]\mathcal{C}(z)}{2}|n',\mathbf{k}\rangle = \sum_{\mathbf{G},\mathbf{G}',\mathbf{G}''} c^*_{n,\mathbf{k}}(\mathbf{G})c_{n',\mathbf{k}}(\mathbf{G}')$$

$$\frac{1}{2}\left[\langle\mathbf{k}+\mathbf{G}''|[V_{nl},i\mathbf{q}\mathbf{r}]|\mathbf{k}+\mathbf{G}'\rangle\delta_{\mathbf{G}_{||}\mathbf{G}''_{||}}F(G_z-G''_z)+\langle\mathbf{k}+\mathbf{G}|[V_{nl},i\mathbf{q}\mathbf{r}]|\mathbf{k}+\mathbf{G}''\rangle\delta_{\mathbf{G}'_{||}\mathbf{G}''_{||}}F(G''_z-G'_z)\right] \tag{1.8}$$

We focus now on the special case of the non-local part of the pseudo-potential. We have the relation

$$i\langle\mathbf{K}|[V^{nl},\mathbf{r}]|\mathbf{K}'\rangle = (\nabla_{\mathbf{K}}+\nabla_{\mathbf{K}'})\langle\mathbf{K}|V^{nl}|\mathbf{K}'\rangle \tag{1.9}$$

In case of a Kleinman-Bylander separable form pseudo-potential, we have

$$\langle\mathbf{K}|V^{nl}|\mathbf{K}'\rangle = \sum_s e^{i(\mathbf{K}-\mathbf{K}')\tau_s}\sum_{l=0}^{l_s}\sum_{m=-l}^{l} E_l F^s_{lm}(\mathbf{K})F^{s*}_{lm}(\mathbf{K}') \tag{1.10}$$

So it comes that

$$\begin{aligned}\langle n,\mathbf{k}|[V^{nl},i\mathbf{r}]|n',\mathbf{k}\rangle &= \sum_s\sum_{l=0}^{l_s}\sum_{m=-l}^{l} E_l \sum_{\mathbf{G}\mathbf{G}'} c^*_{n,\mathbf{k}}(\mathbf{G})c_{n',\mathbf{k}}(\mathbf{G}')e^{i(\mathbf{G}-\mathbf{G}')\tau_s} \\ &\qquad (\nabla_{\mathbf{G}}F^s_{lm}(\mathbf{G})F^{s*}_{lm}(\mathbf{G}')+F^s_{lm}(\mathbf{G})\nabla_{\mathbf{G}'}F^{s*}_{lm}(\mathbf{G}')) \\ &= \sum_s\sum_{l=0}^{l_s}\sum_{m=-l}^{l} E_l\left[\left(\sum_{\mathbf{G}} c^*_{n,\mathbf{k}}(\mathbf{G})e^{i(\mathbf{G})\tau_s}\nabla_{\mathbf{G}}F^s_{lm}(\mathbf{G})\right)\left(c_{n',\mathbf{k}}(\mathbf{G}')e^{-i\mathbf{G}'}\tau_s F^{s*}_{lm}(\mathbf{G}')\right)\right. \\ &\qquad \left.+\left(\sum_{\mathbf{G}} c^*_{n,\mathbf{k}}(\mathbf{G})e^{i\mathbf{G}\tau_s}F^s_{lm}(\mathbf{G})\right)\left(c_{n',\mathbf{k}}(\mathbf{G}')e^{-i\mathbf{G}'}\tau_s\nabla_{\mathbf{G}'}F^{s*}_{lm}(\mathbf{G}')\right)\right]\end{aligned} \tag{1.11}$$

$$\langle n,\mathbf{k}|\frac{\mathcal{C}(z)[V_{nl},i\mathbf{q}\mathbf{r}]+[V_{nl},i\mathbf{q}\mathbf{r}]\mathcal{C}(z)}{2}|n',\mathbf{k}\rangle = \sum_{\mathbf{G},\mathbf{G}',\mathbf{G}''} c^*_{n,\mathbf{k}}(\mathbf{G})c_{n',\mathbf{k}}(\mathbf{G}')$$

$$\frac{1}{2}\left[(\nabla_{\mathbf{K}''}+\nabla_{\mathbf{K}'})\langle\mathbf{K}''|V^{nl}|\mathbf{K}'\rangle\delta_{\mathbf{G}_{||}\mathbf{G}''_{||}}F(G_z-G''_z)+(\nabla_{\mathbf{K}}+\nabla_{\mathbf{K}''})\langle\mathbf{K}|V^{nl}|\mathbf{K}''\rangle\delta_{\mathbf{G}'_{||}\mathbf{G}''_{||}}F(G''_z-G'_z)\right] \tag{1.12}$$

Finally, we get

$$
\begin{multline}
\langle n,\mathbf{k}|\frac{\mathcal{C}(z)[V_{nl},i\mathbf{qr}]+[V_{nl},i\mathbf{qr}]\mathcal{C}(z)}{2}|n',\mathbf{k}\rangle = \sum_s \sum_{l=0}^{l_s} \sum_{m=-l}^{l} E_l \\
\frac{1}{2}\Bigg[\left(\sum_{\mathbf{G}''} e^{i\mathbf{G}''\tau_s}\nabla_{\mathbf{G}''}F^s_{lm}(\mathbf{G}'')\sum_{\mathbf{G}} c^*_{n,\mathbf{k}}(\mathbf{G})\delta_{\mathbf{G}_{||}\mathbf{G}''_{||}}F(G_z-G''_z)\right)\left(\sum_{\mathbf{G}'} c_{n',\mathbf{k}}(\mathbf{G}')e^{-i\mathbf{G}'\tau_s}F^{s*}_{lm}(\mathbf{K}')\right) \\
+\left(\sum_{\mathbf{G}''} e^{i\mathbf{G}''\tau_s}F^s_{lm}(\mathbf{G}'')\sum_{\mathbf{G}} c^*_{n,\mathbf{k}}(\mathbf{G})\delta_{\mathbf{G}_{||}\mathbf{G}''_{||}}F(G_z-G''_z)\right)\left(\sum_{\mathbf{G}'} c_{n',\mathbf{k}}(\mathbf{G}')e^{-i\mathbf{G}'\tau_s}\nabla_{\mathbf{K}'}F^{s*}_{lm}(\mathbf{K}')\right) \\
+\left(\sum_{\mathbf{G}} c^*_{n,\mathbf{k}}(\mathbf{G})e^{i\mathbf{G}\tau_s}\nabla_{\mathbf{G}}F^s_{lm}(\mathbf{G})\right)\left(\sum_{\mathbf{G}''} e^{-i\mathbf{G}''\tau_s}F^{s*}_{lm}(\mathbf{G}'')\sum_{\mathbf{G}'} c_{n',\mathbf{k}}(\mathbf{G}')\delta_{\mathbf{G}'_{||}\mathbf{G}''_{||}}F(G''_z-G'_z)\right) \\
+\left(\sum_{\mathbf{G}} c^*_{n,\mathbf{k}}(\mathbf{G})e^{i\mathbf{G}\tau_s}F^s_{lm}(\mathbf{G})\right)\left(\sum_{\mathbf{G}''} e^{-i\mathbf{G}''\tau_s}\nabla_{\mathbf{G}''}F^{s*}_{lm}(\mathbf{G}'')\sum_{\mathbf{G}'} c_{n',\mathbf{k}}(\mathbf{G}')\delta_{\mathbf{G}'_{||}\mathbf{G}''_{||}}F(G''_z-G'_z)\right)\Bigg]
\end{multline}
\tag{1.13}
$$