The matrix elements of the hamiltonian are

$$
\begin{aligned}
< \mathbf{k}+\mathbf{G} \mid H-\epsilon \mid \mathbf{k}+\mathbf{G}' > &= \left(-\frac{\hbar^2}{2m}(\mathbf{k}+\mathbf{G})^2-\epsilon\right)\delta_{\mathbf{G}\mathbf{G}'}+\sum_\mu S_\mu(\mathbf{G}-\mathbf{G}')\left(V_\mu(\mathbf{G}-\mathbf{G}')+\sum_i V_{\mu,i}(\mathbf{k}+\mathbf{G},\mathbf{k}+\mathbf{G}')\right) \\
&+ V_{Hartree}(\mathbf{G}-\mathbf{G}')+V_{xc}(\mathbf{G}-\mathbf{G}').
\end{aligned} \tag{16}
$$

Divergent Terms in the potential

The Hartree term, $V_{Hartree}(\mathbf{G})$, and local potential term, $\sum_\mu S_\mu(\mathbf{G})V_\mu(\mathbf{G})$, are separately divergent at $\mathbf{G}=0$ and must be treated in a special way. Let us consider their sum $\widetilde{V}(\mathbf{r})=V_{loc}(\mathbf{r})+V_{Hartree}(\mathbf{r})$. Its $\mathbf{G}=0$ term is not divergent:

$$
\widetilde{V}(\mathbf{G}=0)=\frac{1}{\Omega}\int d\mathbf{r}\left(\sum_\mu V_\mu(\mathbf{r}-\mathbf{d}_\mu)+\frac{1}{N}e^2\int\frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'\right)=\frac{1}{\Omega}\sum_\mu\int d\mathbf{r}\left(V_\mu(r)+\frac{Z_\mu e^2}{r}\right)=\frac{1}{\Omega}\sum_\mu\alpha_\mu \tag{17}
$$

where we used

$$
V_\mu(r)\sim-\frac{Z_\mu e^2}{r}\quad\text{for large } r,\qquad \frac{1}{N}\int n(\mathbf{r})=\sum_\mu Z_\mu. \tag{18}
$$

The α_μ are parameters depending only on the pseudopotential.