

$$\mathbf{J}_1 \in \mathbb{R}^{3n_{\text{atoms}}, n_{\text{feat}}}$$

$$\mathbf{J}_1 = \begin{bmatrix} \frac{\partial \langle q_1 | A_1 \rangle}{\partial \mathbf{r}_{11}} & \cdots & \frac{\partial \langle q_{n_{\text{feat}}} | A_1 \rangle}{\partial \mathbf{r}_{11}} \\ \frac{\partial \langle q_1 | A_1 \rangle}{\partial \mathbf{r}_{21}} & \cdots & \frac{\partial \langle q_{n_{\text{feat}}} | A_1 \rangle}{\partial \mathbf{r}_{21}} \\ \frac{\partial \langle q_1 | A_1 \rangle}{\partial \mathbf{r}_{31}} & \cdots & \frac{\partial \langle q_{n_{\text{feat}}} | A_1 \rangle}{\partial \mathbf{r}_{31}} \end{bmatrix}$$

