Ewald Force

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实空间：

$$U^R = \frac{1}{2}\sum_{\mathbf{n}}\sum_{i}^{N}\sum_{j}^{N}{}' q_i q_j \frac{erfc(\alpha|\mathbf{r}_i - \mathbf{r}_j + \mathbf{n}|)}{|\mathbf{r}_i - \mathbf{r}_j + \mathbf{n}|}$$

所以对于 j 粒子：

$$U_j^R = q_j \sum_{i \neq j} q_i \frac{erfc(\alpha|\mathbf{r}_i - \mathbf{r}_j|)}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$\begin{aligned}
\mathbf{F}_j^R =& -\nabla U_j^R = -q_j \sum_{i \neq j} q_i \frac{d\frac{erfc(\alpha|\mathbf{r}_i - \mathbf{r}_j|)}{|\mathbf{r}_i - \mathbf{r}_j|}}{d\mathbf{r}_j} \\
=& -q_j \sum_{i\ nej} q_i \frac{\frac{2}{\sqrt{\pi}}(-\alpha)e^{-\alpha^2|\mathbf{r}_i - \mathbf{r}_j|^2}\frac{d|\mathbf{r}_i - \mathbf{r}_j|}{d\mathbf{r}_j}|\mathbf{r}_i - \mathbf{r}_j| - erfc(\alpha|\mathbf{r}_i - \mathbf{r}_j|)\frac{d|\mathbf{r}_i - \mathbf{r}_j|}{d\mathbf{r}_j}}{|\mathbf{r}_i - \mathbf{r}_j|^2} \\
=& -q_j \sum_{i \neq j} q_i \frac{\frac{2\alpha}{\sqrt{\pi}}e^{-\alpha^2|\mathbf{r}_i - \mathbf{r}_j|^2}(\mathbf{r}_i - \mathbf{r}_j) + erfc(\alpha|\mathbf{r}_i - \mathbf{r}_j|)\frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r_i} - \mathbf{r}_j|}}{|\mathbf{r}_i - \mathbf{r_j}|^2} \\
=& -q_j \sum_{i \neq j} q_i [\frac{2\alpha}{\sqrt{\pi}}e^{-\alpha^2|\mathbf{r}_i - \mathbf{r}_j|^2} + \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}erfc(\alpha|\mathbf{r}_i - \mathbf{r}_j|)]\frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^2}
\end{aligned} \tag{1}$$

其中：

$$|\mathbf{r}_i - \mathbf{r}_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

$$\begin{aligned}
\frac{d|\mathbf{r}_i - \mathbf{r}_j|}{d\mathbf{r}_j} =& (\frac{\partial|\mathbf{r}_i - \mathbf{r}_j|}{\partial x_j}, \frac{\partial|\mathbf{r}_i - \mathbf{r}_j|}{\partial y_j}, \frac{\partial|\mathbf{r}_i - \mathbf{r}_j|}{\partial z_j}) \\
=& (-\frac{x_i - x_j}{|\mathbf{r}_i - \mathbf{r}_j|}, -\frac{y_i - y_j}{|\mathbf{r}_i - \mathbf{r}_j|}, -\frac{z_i - z_j}{|\mathbf{r}_i - \mathbf{r}_j|}) \\
=& -\frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|}
\end{aligned} \tag{2}$$

k 空间：

$$U^k = \frac{2\pi}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{1}{k^2} e^{-\dfrac{k^2}{4\alpha^2}} \sum_i^N \sum_j^N q_i q_j e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)}$$

对于 j 粒子：

$$U_j^k = q_j \frac{2\pi}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{1}{k^2} e^{-\dfrac{k^2}{4\alpha^2}} \sum_i^N q_i e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)}$$

$$\begin{aligned}
\mathbf{F}_j^k =& -\nabla U_j^k = -q_j \frac{2\pi}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{1}{k^2} e^{-\dfrac{k^2}{4\alpha^2}} \sum_i^N q_i \frac{e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)}}{d\mathbf{r}_j} \\
=& -q_j \frac{2\pi}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{1}{k^2} e^{-\dfrac{k^2}{4\alpha^2}} \sum_i^N q_i (-i\mathbf{k}) e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} \\
=& -q_j \frac{2\pi}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{1}{k^2} e^{-\dfrac{k^2}{4\alpha^2}} \sum_i^N q_i (-i\mathbf{k}) \{\cos[\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)] + i\sin[\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)]\} \\
=& -q_j \frac{2\pi}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{\mathbf{k}}{k^2} e^{-\dfrac{k^2}{4\alpha^2}} \sum_i^N q_i \sin[\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)] \\
&+ iq_j \frac{2\pi}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{\mathbf{k}}{k^2} e^{-\dfrac{k^2}{4\alpha^2}} \sum_i^N q_i \cos[\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)]
\end{aligned} \tag{3}$$

当 $\mathbf{k} \in [-\mathbf{kmax}, \mathbf{kmax}]$ 时，cos 是偶函数，此时虚部为 0，则:

$$\mathbf{F}_j = -q_j \frac{2\pi}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \frac{\mathbf{k}}{k^2} e^{-\dfrac{k^2}{4\alpha^2}} \sum_i^N q_i \sin[\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)]$$