Ewald Summation in Variable Shape MD (I)

Basics

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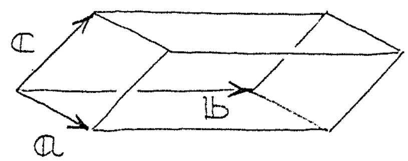
§. Coordinate System



$$\mathbf{r}_i = \xi_i \mathbf{a} + \eta_i \mathbf{b} + \zeta_i \mathbf{c}$$

i.e.,

$$\begin{bmatrix} x_i \\ y_i \\ z_i \end{bmatrix} = \begin{bmatrix} \xi_i a_x + \eta_i b_x + \zeta_i c_x \\ \xi_i a_y + \eta_i b_y + \zeta_i c_y \\ \xi_i a_z + \eta_i b_z + \zeta_i c_z \end{bmatrix} = \begin{bmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{bmatrix} \begin{bmatrix} \xi_i \\ \eta_i \\ \zeta_i \end{bmatrix}$$

$$\mathbf{r}_i = \mathbf{h}\, \mathbf{s}_i \tag{1}$$

where

$$\mathbf{h} = (\mathbf{a} \quad \mathbf{b} \quad \mathbf{c}) \tag{2}$$

$$\mathbf{r}_i = \begin{bmatrix} x_i \\ y_i \\ z_i \end{bmatrix}, \qquad \mathbf{s}_i = \begin{bmatrix} \xi_i \\ \eta_i \\ \zeta_i \end{bmatrix} \qquad (0 \le \xi_i, \eta_i, \zeta_i \le 1)$$

(Volume)

$$\det \mathbf{h} = a_x \underbrace{\begin{vmatrix} b_y & c_y \\ b_z & c_z \end{vmatrix}}_{(\mathbf{b}\times\mathbf{c})_x} - a_y \underbrace{\begin{vmatrix} b_x & c_x \\ b_z & c_z \end{vmatrix}}_{-(\mathbf{b}\times\mathbf{c})_y} + a_z \underbrace{\begin{vmatrix} b_x & c_x \\ b_y & c_y \end{vmatrix}}_{(\mathbf{b}\times\mathbf{c})_z}$$

$$= \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \Omega$$

$$\Omega = \det \mathbf{h} = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = \mathbf{b}\cdot(\mathbf{c}\times\mathbf{a}) = \mathbf{c}\cdot(\mathbf{a}\times\mathbf{b}) \tag{3}$$

§. Fourier Transform

(Basis Set)

$$\boxed{\left\{ b_{\mathbb{k}}(\mathbb{r}) = \frac{1}{\sqrt{\Omega}} \exp(i\mathbb{k}\cdot\mathbb{r}) \;\middle|\; \mathbb{k} = \frac{2\pi}{\Omega}\left[n_x(\mathbb{b}\times\mathbb{c}) + n_y(\mathbb{c}\times\mathbb{a}) + n_z(\mathbb{a}\times\mathbb{b})\right],\; n_x, n_y, n_z = 0, \pm 1, \pm 2, \ldots \right\} \qquad (4)}$$

(Orthonormality)

$$\boxed{\int_\Omega d\mathbb{r}\; b^*_{\mathbb{k}}(\mathbb{r})\, b_{\mathbb{q}}(\mathbb{r}) = \delta_{\mathbb{k},\mathbb{q}} \qquad (5)}$$

(∵) $(\text{lhs}) = \displaystyle\int_0^1 d\mathbb{s} \underbrace{\left|\frac{\partial \mathbb{r}}{\partial \mathbb{s}}\right|}_{\det \mathbb{h} = \cancel{\Omega}} \frac{1}{\cancel{\Omega}} \exp\left[i(\mathbb{q}-\mathbb{k})\cdot\mathbb{r}\right]$

$$= \int_0^1 d\mathbb{s}\, \exp\left\{ i\frac{2\pi}{\Omega}\left[\delta n_x(\mathbb{b}\times\mathbb{c}) + \delta n_y(\mathbb{c}\times\mathbb{a}) + \delta n_z(\mathbb{a}\times\mathbb{b})\right](\xi\mathbb{a} + \eta\mathbb{b} + \zeta\mathbb{c}) \right\}$$

$$= \int_0^1 d\mathbb{s}\, \exp\left[i\frac{2\pi}{\cancel{\Omega}} \cancel{\Omega}\, (\delta n_x \xi + \delta n_y \eta + \delta n_z \zeta) \right]$$

$$= \underbrace{\int_0^1 d\xi\, e^{i2\pi\delta n_x \xi}}_{\left\{\begin{array}{ll} \left[\dfrac{e^{i2\pi\delta n_x\xi}}{i2\pi\delta n_x}\right]_0^1 = 0 & (\delta n_x \neq 0) \\ 1 & (\delta n_x = 0) \end{array}\right.} \int_0^1 d\eta\, e^{i2\pi\delta n_y \eta} \int_0^1 d\zeta\, e^{i2\pi\delta n_z \zeta}$$

$$= \delta_{\mathbb{k},\mathbb{q}} \quad //$$

(Completeness)

Any periodic function, $f(\mathbb{r})$, with a unit cell formed by $\mathbb{a}, \mathbb{b}, \mathbb{c}$ can be expanded with the basis set

$$f(\mathbb{r}) = \sum_{\mathbb{k}} b_{\mathbb{k}}(\mathbb{r}) \int_{\Omega} d\mathbb{r}' \, \mathbb{b}_{\mathbb{k}}^{*}(\mathbb{r}) f(\mathbb{r}) \tag{6}$$

(Fourier Transform)

$$\begin{cases} f(\mathbb{r}) = \dfrac{1}{\Omega} \sum_{\mathbb{k}} \tilde{f}(\mathbb{k}) \, e^{i\mathbb{k}\cdot\mathbb{r}} & (7) \\ \tilde{f}(\mathbb{k}) = \int_{\Omega} d\mathbb{r} \, f(\mathbb{r}) \, e^{-i\mathbb{k}\cdot\mathbb{r}} & (8) \end{cases}$$

§. Periodic Coulomb Potential

(Coulomb Potential)

Suppose there is a unit charge at the origin in the infinite space. Electrostatic potential, $\phi(\mathbb{r})$, satisfies the Poisson equation,

$$\nabla^2 \phi(\mathbb{r}) = -4\pi\delta(\mathbb{r}) \tag{9}$$

Using the Fourier transform in infinite space, Eq. (9) is rewritten as

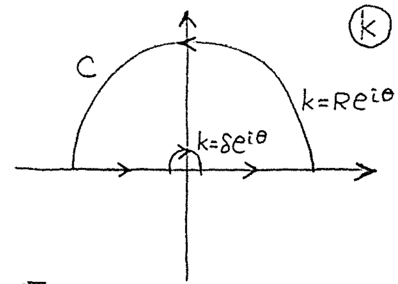
$$\int \frac{d\mathbb{k}}{(2\pi)^3}\left[-k^2\tilde{\phi}(\mathbb{k})\right]e^{i\mathbb{k}\cdot\mathbb{r}} = \int \frac{d\mathbb{k}}{(2\pi)^3}\left[-4\pi\right]e^{i\mathbb{k}\cdot\mathbb{r}}$$

$$\therefore\ \tilde{\phi}(\mathbb{k}) = \frac{4\pi}{k^2} \qquad (\mathbb{k} \neq 0) \tag{10}$$

Then,

$$\begin{aligned}
\phi(\mathbb{r}) &= \int \frac{d\mathbb{k}}{(2\pi)^3}\frac{4\pi}{k^2}e^{i\mathbb{k}\cdot\mathbb{r}} \\
&= \int_0^\infty \frac{2\pi \cancel{k^2}}{(2\pi)^3}dk\,\frac{4\pi}{\cancel{k^2}}\underbrace{\int_{-1}^{1}dx\,e^{ikrx}}_{\left[\frac{e^{ikrx}}{ikr}\right]_{-1}^{1}} \\
&= \frac{1}{i\pi r}\int_0^\infty \frac{dk}{k}\left(e^{ikr} - \underbrace{e^{-ikr}}_{k\leftrightarrow -k}\right) \\
&= \frac{1}{i\pi r}\lim_{\delta\to 0}\left(\int_{-\infty}^{-\delta} + \int_{\delta}^{\infty}\right)\frac{dk}{k}e^{ikr}
\end{aligned}$$

Here,



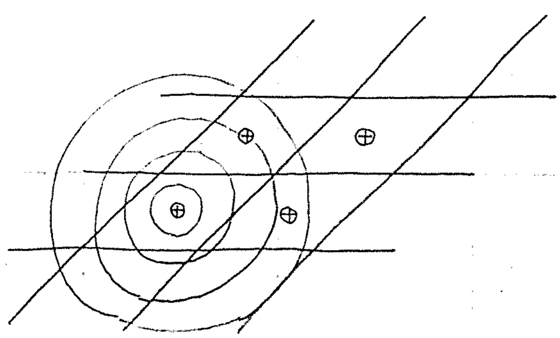
$$0 = \int_C \frac{dk}{k} e^{ikr}$$

$$= \left(\int_{-\infty}^{-\delta} + \int_{\delta}^{\infty}\right)\frac{dk}{k} e^{ikr} + \underbrace{\int_{\pi}^{0} \frac{\cancel{\delta e^{i\theta}}\, i d\theta}{\cancel{\delta e^{i\theta}}} \underbrace{e^{i\delta e^{i\theta} r}}_{1}}_{-i\pi} + \int_{0}^{\pi} \frac{\cancel{Re^{i\theta}}\, i d\theta}{\cancel{Re^{i\theta}}} \underbrace{e^{iRe^{i\theta} r}}_{e^{iRr\cos\theta - Rr\sin\theta} \to 0 \, (R\to\infty}$$

$$\therefore \left(\int_{-\infty}^{-\delta} + \int_{\delta}^{\infty}\right)\frac{dk}{k} e^{ikr} = i\pi \qquad (11)$$

$$\therefore \phi(\mathbf{r}) = \frac{1}{r} \qquad (12)$$

(Periodically Repeated Coulomb Potential)



$$\nabla^2 \phi(\mathbf{r}) = -4\pi \sum_{\nu} \delta(\mathbf{r} - \nu) \qquad (13)$$

The solution of the Poisson equation, Eq. (13), is simply a superposition of Eq. (12),

$$\phi(\mathbf{r}) = \sum_{\nu} \frac{1}{|\mathbf{r} - \nu|} \qquad (14)$$

In the Fourier space, using the basis (4),

$$\frac{1}{\Omega}\sum_{\mathbb{k}}\left[-k^2\tilde{\Phi}(\mathbb{k})\right]e^{i\mathbb{k}\cdot\mathbb{r}} = \frac{1}{\Omega}\sum_{\mathbb{k}}\left[-4\pi\right]e^{i\mathbb{k}\cdot\mathbb{r}} \tag{15}$$

(∵ Whatever the repetion is, the Fourier components are obtained by integration in a unit cell,

$$\int_\Omega d\mathbb{r}\sum_{\nu}\delta(\mathbb{r}-\nu) = \int_\Omega d\mathbb{r}\,\delta(\mathbb{r}) = 1 \quad //$$
)

※ Note

$$\boxed{\sum_{\nu}\delta(\mathbb{r}-\nu) = \frac{1}{\Omega}\sum_{\mathbb{k}}e^{i\mathbb{k}\cdot\mathbb{r}}} \tag{16}$$

From Eq. (15), we get the Fourier transform of Eq. (14) as

$$\tilde{\Phi}(\mathbb{k}) = \frac{4\pi}{k^2} \qquad (\mathbb{k}\neq 0) \tag{17}$$

8. Potential Energy of a Periodic System

Potential energy per unit cell is calculated as

$$V = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} {\sum_{\nu}}' \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j - \nu|} \tag{18}$$

where Σ' means the omission of $\nu = 0$ when $i = j$.

(Periodic Charge Distribution)

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} \sum_{\nu} q_i \, \delta(\mathbf{r} - \mathbf{r}_i - \nu) \tag{19}$$

Here, we consider a charge-neutral system such that

$$\sum_{i=1}^{N} q_i = 0 \tag{20}$$

The Fourier transform of the charge density is calculated as

$$\tilde{\rho}(\mathbf{k}) = \int_{\Omega} d\mathbf{r} \left[\sum_{i=1}^{N} \cancel{\sum_{\nu}} q_i \delta(\mathbf{r} - \mathbf{r}_i \cancel{- \nu}) \right] e^{-i\mathbf{k}\cdot\mathbf{r}} = \sum_{i=1}^{N} q_i e^{-i\mathbf{k}\cdot\mathbf{r}_i} \tag{21}$$

From charge neutrality,

$$\tilde{\rho}(\mathbf{k}=0) = \sum_{i=1}^{N} q_i = 0 \tag{22}$$

(Periodic Electrostatic Potential)

$$\nabla^2 \phi(\mathbf{r}) = -4\pi \rho(\mathbf{r}) \tag{23}$$

or

$$\frac{1}{\Omega}\sum_{\mathbf{k}} \left[-k^2 \tilde{\phi}(\mathbf{k})\right] e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{1}{\Omega}\sum_{\mathbf{k}} \left[-4\pi \tilde{\rho}(\mathbf{k})\right] e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\therefore \tilde{\phi}(\mathbf{k}) = \frac{4\pi}{k^2}\tilde{\rho}(\mathbf{k}) = \frac{4\pi}{k^2}\sum_{i=1}^{N} q_i e^{-i\mathbf{k}\cdot\mathbf{r}_i} \qquad (\mathbf{k} \neq 0) \tag{24}$$

(Momentum-Space Representation)

We can rewrite Eq. (18), after correcting the self interaction, as

$$V = \frac{1}{2}\int_\Omega d\mathbf{r}\, \rho(\mathbf{r})\phi(\mathbf{r}) - \frac{1}{2}\sum_{i=1}^{N}\int_\Omega d\mathbf{r}\, \underbrace{q_i\delta(\mathbf{r}-\mathbf{r}_i)}_{\rho_i(\mathbf{r})} \underbrace{\frac{q_i}{|\mathbf{r}-\mathbf{r}_i|}}_{\phi_i(\mathbf{r})}$$

$$= \underbrace{\frac{1}{2}\int_\Omega d\mathbf{r}\, \frac{1}{\Omega}\sum_{\mathbf{k}}\tilde{\rho}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}\frac{1}{\Omega}\sum_{\mathbf{q}}\tilde{\phi}(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}}_{\frac{1}{2\Omega^2}\sum_{\mathbf{k}}\sum_{\mathbf{q}}\tilde{\rho}(\mathbf{k})\tilde{\phi}(\mathbf{q})\underbrace{\int_\Omega d\mathbf{r}\, e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}}}_{\Omega\delta_{\mathbf{k},-\mathbf{q}}}} - \frac{1}{2}\sum_{i=1}^{N} q_i^2 \int_\Omega d\mathbf{r}\, \frac{\delta(\mathbf{r})}{r}$$

$$= \frac{1}{2\Omega}\sum_{\mathbf{k}} \underbrace{\tilde{\rho}(\mathbf{k})}_{\sum_{j=1}^{N} e^{-i\mathbf{k}\cdot\mathbf{r}_j}} \underbrace{\tilde{\phi}(-\mathbf{k})}_{\frac{4\pi}{k^2}\sum_{i=1}^{N} e^{i\mathbf{k}\cdot\mathbf{r}_i}} - \frac{1}{2}\sum_{i=1}^{N} q_i^2 \int_\Omega d\mathbf{r}\, \frac{\delta(\mathbf{r})}{r}$$

Noting the charge neutrality, $\tilde{\rho}(\mathbf{k}=0) = \sum_{i=1}^{N} q_i = 0$, and the Poisson equation, $k^2\tilde{\phi}(\mathbf{k}) = 4\pi\tilde{\rho}(\mathbf{k})$, $\tilde{\rho}(\mathbf{k}=0)\tilde{\phi}(\mathbf{k}=0)$ has no contribution.

$$\therefore\ V = \frac{1}{2\Omega}\sum_{\mathbf{k}}{}' \sum_{i,j=1}^{N} \frac{4\pi}{k^2} e^{i\mathbf{k}\cdot\mathbf{r}_{ij}} - \frac{1}{2}\sum_{i=1}^{N} q_i^2 \int_\Omega d\mathbf{r}\, \frac{\delta(\mathbf{r})}{r} \tag{25}$$

Here, $\sum_{\mathbf{k}}'$ means the omission of $\mathbf{k}=0$; this omission is a consequence of the charge neutrality. $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$.

$$V = \frac{1}{2\Omega}\sum_{\mathbf{k}}{}' \sum_{i\neq j} \frac{4\pi q_i q_j}{k^2} e^{i\mathbf{k}\cdot\mathbf{r}_{ij}} + \underbrace{\frac{1}{2\Omega}\sum_{\mathbf{k}}{}'\sum_i \frac{4\pi q_i^2}{k^2} - \frac{1}{2}\sum_i q_i^2 \int_\Omega d\mathbf{r}\,\frac{\delta(\mathbf{r})}{r}}_{\frac{1}{2}\sum_i q_i^2 \left[\frac{1}{\Omega}\sum_{\mathbf{k}}'\frac{4\pi}{k^2} - \int_\Omega d\mathbf{r}\,\frac{\delta(\mathbf{r})}{r}\right]}$$

Let's define a periodic pseudo Coulomb function, $\psi(r)$, as

$$\boxed{\psi(r) = \frac{1}{\Omega}\sum_{\mathbf{k}}{}' \frac{4\pi}{k^2} e^{i\mathbf{k}\cdot\mathbf{r}} \quad (\text{Periodic, } \tilde{\psi}(\mathbf{k}=0) = 0\ )} \tag{26}$$

Then,

$$V = \frac{1}{2}\sum_{i\neq j} q_i q_j\, \psi(r_{ij}) + \frac{1}{2}\sum_i q_i^2 \lim_{r\to 0}\left[\psi(r) - \frac{1}{r}\right] \tag{27}$$

Here, from charge neutrality,

$$0 = \left(\sum_{i=1}^{N} q_i\right)^2 = \sum_{i\neq j} q_i q_j + \sum_i q_i^2 \tag{28}$$

Using Eq. (28) in (27),

$$\boxed{V = \frac{1}{2}\sum_{i\neq j} q_i q_j \left\{ \psi(r_{ij}) - \lim_{r\to 0}\left[\psi(r) - \frac{1}{r}\right] \right\}} \tag{29}$$

§. Ewald Method

Ewald method introduces a convergence factor, $e^{-\gamma^2 k^2}$, in a momentum-space summation, Eq. (26).

$$\psi(\mathbf{r}) = \frac{1}{\Omega}\sum_{\mathbf{k}}{}' \frac{4\pi}{k^2} e^{-\gamma^2 k^2} e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{1}{\Omega}\sum_{\mathbf{k}}{}' \frac{4\pi}{k^2}(1-e^{-\gamma^2 k^2}) e^{i\mathbf{k}\cdot\mathbf{r}} \tag{30}$$

(Lemma)

(1) $$\sum_{\nu} \frac{1}{|\mathbf{r}-\nu|}\,\mathrm{erf}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right) = \frac{1}{\Omega}\sum_{\mathbf{k}} \frac{4\pi}{k^2} e^{-\gamma^2 k^2} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{31}$$

(2) $$\sum_{\nu} \frac{1}{|\mathbf{r}-\nu|}\,\mathrm{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right) = \frac{1}{\Omega}\sum_{\mathbf{k}} \frac{4\pi}{k^2}(1-e^{-\gamma^2 k^2}) e^{i\mathbf{k}\cdot\mathbf{r}} \tag{32}$$

where

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z dt\, e^{-t^2} \tag{33}$$

$$\mathrm{erfc}(z) = 1 - \mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_z^\infty dt\, e^{-t^2} \tag{34}$$

☺ For $\gamma \ll \Omega^{1/3}$, we can forget the periodicity.

$$\frac{1}{r}\mathrm{erf}\left(\frac{r}{2\gamma}\right) = \frac{2}{\sqrt{\pi}\,r}\int_{-\infty}^{\frac{r}{2\gamma}} dt\, e^{-t^2} - \frac{2}{\sqrt{\pi}\,r}\int_{-\infty}^{0} dt\, e^{-t^2}$$

$$= \frac{2}{\sqrt{\pi}\,r}\int_{-\infty}^{\infty} dt\, e^{-t^2}\underbrace{\Theta\left(\frac{r}{2\gamma}-t\right)}_{-\int \frac{du}{2\pi i}\frac{e^{-iu(\frac{r}{2\gamma}-t)}}{u+i0}} - \frac{1}{r}$$

$$= -\frac{2}{\sqrt{\pi}\,r}\int_{-\infty}^{\infty}\frac{du}{2\pi i}\,\frac{e^{-iur/2\gamma}}{u+i0}\int_{-\infty}^{\infty} dt\, e^{-t^2+iut} - \frac{1}{r}$$

$u \leftrightarrow -2\gamma k$

$$= - \frac{\cancel{2}}{\cancel{\sqrt{\pi}}\, r}\int_{-\infty}^{\infty}\frac{2\gamma\, dk}{\cancel{2}\pi i}\,\frac{e^{ikr}}{-2\gamma k+i0}\,\underbrace{\int_{-\infty}^{\infty} dt\, e^{-t^2+i2\gamma k t}}_{\int_{-\infty}^{\infty} dt\, e^{-(t-i\gamma k)^2}e^{-\gamma^2k^2} \,=\, \cancel{\sqrt{\pi}}\, e^{-\gamma^2k^2}} - \frac{1}{r}$$

$$= \frac{1}{r}\int_{-\infty}^{\infty}\frac{dk}{\pi i}\,\underbrace{\frac{1}{k-i0}}_{\frac{P}{k}+i\pi\delta(k)}\; e^{-\gamma^2k^2+ikr} - \frac{1}{r}$$

$$= \frac{1}{i\pi r}P\int_{-\infty}^{\infty}\frac{dk}{k}\,e^{-\gamma^2k^2+ikr} + \cancel{\frac{1}{r}} - \cancel{\frac{1}{r}}$$

On the other hand,

$$\frac{1}{\Omega}\sum_{\mathbf{k}}\frac{4\pi}{k^2}\,e^{-\gamma^2k^2}\,e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\xrightarrow[\gamma\ll\Omega^{1/3}]{} \int_0^{\infty}\frac{2\pi \cancel{k^2}\, dk}{(2\pi)^3}\,\frac{4\pi}{\cancel{k^2}}\,e^{-\gamma^2k^2}\,\underbrace{\int_{-1}^{1}dx\, e^{ikrx}}_{\frac{e^{ikr}-e^{-ikr}}{ikr}}$$

$$= \frac{1}{i\pi r}\int_0^{\infty}\frac{dk}{k}\,e^{-\gamma^2k^2}\left(e^{ikr}-\underbrace{e^{-ikr}}_{k\leftrightarrow -k}\right)$$

$$= \frac{1}{i\pi r}\lim_{\delta\to 0}\left(\int_{-\infty}^{-\delta}+\int_{\delta}^{\infty}\right)\frac{dk}{k}\,e^{-\gamma^2k^2}e^{ikr}$$

$$= \frac{1}{i\pi r}P\int_{-\infty}^{\infty}\frac{dk}{k}\,e^{-\gamma^2k^2}e^{ikr}$$

Thus, Eq. (31) is proven. Eq. (32) is obtained by subtracting Eq. (31) from the Fourier expansion of $1/r$ (see Eqs. (14) & (17)) //

From Eq. (32),

$$\sum_{\nu}\frac{1}{|\mathbf{r}-\nu|}\,\mathrm{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right)=\frac{1}{\Omega}\sum_{\mathbf{k}}{}'\,\frac{4\pi}{k^2}\left(1-e^{-\gamma^2k^2}\right)e^{i\mathbf{k}\cdot\mathbf{r}}+\underbrace{\frac{1}{\Omega}\cdot\frac{4\pi}{\cancel{k^2}}\left(\cancel{1}-\cancel{1}+\gamma^2\cancel{k^2}\right)}_{\frac{4\pi\gamma^2}{\Omega}}$$

$$\boxed{\therefore\ \psi(\mathbf{r})=\frac{1}{\Omega}\sum_{\mathbf{k}}{}'\,\frac{4\pi}{k^2}e^{-\gamma^2k^2}e^{i\mathbf{k}\cdot\mathbf{r}}+\sum_{\nu}\frac{1}{|\mathbf{r}-\nu|}\,\mathrm{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right)-\frac{4\pi\gamma^2}{\Omega}\qquad(35)}$$

Here,

$$\lim_{r\to 0}\left[\psi(\mathbf{r})-\frac{1}{r}\right]=\frac{1}{\Omega}\sum_{\mathbf{k}}{}'\,\frac{4\pi}{k^2}e^{-\gamma^2k^2}+\frac{1}{r}\left(\cancel{1}-\frac{\cancel{2}}{\sqrt{\pi}}\frac{r}{\cancel{2}\gamma}\right)+\sum_{\nu}\frac{1}{|\nu|}\,\mathrm{erfc}\left(\frac{|\nu|}{2\gamma}\right)$$
$$-\frac{4\pi\gamma^2}{\Omega}-\cancel{\frac{1}{r}}\qquad(36)$$

$$\therefore\ \psi(\mathbf{r})-\lim_{r\to 0}\left[\psi(\mathbf{r})-\frac{1}{r}\right]$$

$$=\frac{1}{\Omega}\sum_{\mathbf{k}}{}'\,\frac{4\pi}{k^2}e^{-\gamma^2k^2}e^{i\mathbf{k}\cdot\mathbf{r}}+\sum_{\nu}\frac{1}{|\mathbf{r}-\nu|}\,\mathrm{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right)-\cancel{\frac{4\pi\gamma^2}{\Omega}}$$
$$-\frac{1}{\Omega}\sum_{\mathbf{k}}{}'\,\frac{4\pi}{k^2}e^{-\gamma^2k^2}+\cancel{\frac{4\pi\gamma^2}{\Omega}}-\sum_{\nu\neq 0}\frac{1}{|\nu|}\,\mathrm{erfc}\left(\frac{|\nu|}{2\gamma}\right)+\frac{1}{\sqrt{\pi}\gamma}$$

$$=\frac{1}{\Omega}\sum_{\mathbf{k}}{}'\,\frac{4\pi}{k^2}e^{-\gamma^2k^2}\left(e^{i\mathbf{k}\cdot\mathbf{r}}-1\right)+\sum_{\nu}\frac{1}{|\mathbf{r}-\nu|}\,\mathrm{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right)$$
$$-\sum_{\nu\neq 0}\frac{1}{|\nu|}\,\mathrm{erfc}\left(\frac{|\nu|}{2\gamma}\right)+\frac{1}{\sqrt{\pi}\gamma}$$

Substituting Eq. (37) in (29),

$$V = \underbrace{\frac{1}{2}\sum_{i\neq j} q_i q_j \frac{1}{\Omega}{\sum_{\mathbf{k}}}' \frac{4\pi}{k^2} e^{-\gamma^2 k^2}\left(e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}-1\right)}_{\frac{1}{2\Omega}{\sum_{\mathbf{k}}}' \frac{4\pi}{k^2} e^{-\gamma^2 k^2} \underbrace{\sum_{i\neq j} q_i q_j \left(e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}-1\right)}_{\sum_{i\neq j} q_i q_j e^{i\mathbf{k}\cdot\mathbf{r}_{ij}} - \sum_{i\neq j} q_i q_j}} + \frac{1}{2}\sum_{i\neq j}\sum_{\boldsymbol{\nu}} \frac{q_i q_j}{|\mathbf{r}_{ij}-\boldsymbol{\nu}|}\,\mathrm{erfc}\left(\frac{|\mathbf{r}_{ij}-\boldsymbol{\nu}|}{2\gamma}\right)$$

$$+ \frac{1}{2}\underbrace{\left(\sum_{i\neq j} q_i q_j\right)}_{-\sum_i q_i^2}\left[\frac{1}{\pi\gamma} - \sum_{\boldsymbol{\nu}\neq 0}\frac{1}{|\boldsymbol{\nu}|}\,\mathrm{erfc}\left(\frac{|\boldsymbol{\nu}|}{2\gamma}\right)\right]$$

$$= \sum_{i\neq j} q_i q_j e^{i\mathbf{k}\cdot\mathbf{r}_{ij}} + \sum_i q_i^2 \quad (\because \text{Eq. } (28))$$

$$= \sum_{i,j} q_i q_j e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}$$

$$= \left|\sum_i q_i e^{i\mathbf{k}\cdot\mathbf{r}_i}\right|^2$$

$$\therefore\ V = \frac{1}{2\Omega}{\sum_{\mathbf{k}}}'\frac{4\pi}{k^2}e^{-\gamma^2k^2}\left|\sum_{i=1}^{N} q_i e^{i\mathbf{k}\cdot\mathbf{r}_i}\right|^2 + \frac{1}{2}\sum_{i\neq j}\sum_{\boldsymbol{\nu}}\frac{q_iq_j}{|\mathbf{r}_{ij}-\boldsymbol{\nu}|}\,\mathrm{erfc}\left(\frac{|\mathbf{r}_{ij}-\boldsymbol{\nu}|}{2\gamma}\right)$$

$$- \frac{1}{2}\sum_i q_i^2\left[\frac{1}{\sqrt{\pi}\gamma} - \sum_{\boldsymbol{\nu}\neq 0}\frac{1}{|\boldsymbol{\nu}|}\,\mathrm{erfc}\left(\frac{|\boldsymbol{\nu}|}{2\gamma}\right)\right] \qquad (37)$$

For $\gamma \ll \Omega^{1/3}$ and neglecting the constant term,

$$V = \frac{1}{2\Omega}{\sum_{\mathbf{k}}}'\frac{4\pi}{k^2}e^{-\gamma^2k^2}\left|\sum_{i=1}^{N} q_i e^{i\mathbf{k}\cdot\mathbf{r}_i}\right|^2 + \sum_{i<j}\frac{q_iq_j}{r_{ij}}\,\mathrm{erfc}\left(\frac{r_{ij}}{2\gamma}\right) \qquad (38)$$

$$\rightarrow\ -\frac{1}{2\sqrt{\pi}\gamma}\sum_i q_i^2 \qquad \text{(Don't neglect)}$$

§. Calculation of Forces

Let's use $\gamma \ll \Omega^{1/3}$, say $\Omega^{1/3}/5$, and use Eq. (38) instead of Eq. (37), for potential.

$$\mathbb{F}_\ell = -\frac{\partial}{\partial \mathbb{r}_\ell} V$$

$$= -\frac{1}{\cancel{2}\Omega} \sum_{\mathbb{k}}{}' \frac{4\pi}{k^2} e^{-\gamma^2 k^2} \underbrace{\frac{\partial}{\partial \mathbb{r}_\ell} \left(\sum_i q_i e^{i\mathbb{k}\cdot\mathbb{r}_i} \sum_j q_j e^{-i\mathbb{k}\cdot\mathbb{r}_j} \right)}$$

$$q_\ell i\mathbb{k}\, e^{i\mathbb{k}\cdot\mathbb{r}_\ell} \left(\sum_j q_j e^{-i\mathbb{k}\cdot\mathbb{r}_j}\right) + \left(\sum_j q_j e^{i\mathbb{k}\cdot\mathbb{r}_j}\right) q_\ell (-i\mathbb{k}) e^{-i\mathbb{k}\cdot\mathbb{r}_\ell}$$

$$= \cancel{2}\,\mathrm{Re}\, q_\ell (i\mathbb{k}) e^{i\mathbb{k}\cdot\mathbb{r}_\ell} \left(\sum_j q_j e^{-i\mathbb{k}\cdot\mathbb{r}_j}\right)$$

$$- \sum_{i<j} q_i q_j (\delta_{i,\ell} - \delta_{j,\ell}) \frac{\mathbb{r}_{ij}}{r_{ij}} \underbrace{\frac{d}{dr_{ij}} \frac{1}{r_{ij}} \mathrm{erfc}\left(\frac{r_{ij}}{2\gamma}\right)}$$

$$-\frac{1}{r_{ij}^2} \mathrm{erfc}\left(\frac{r_{ij}}{2\gamma}\right) + \frac{1}{r_{ij}} \left(-\frac{2}{\sqrt{\pi}} \cdot \frac{1}{2\gamma}\right) e^{-(r_{ij}/2\gamma)^2}$$

$$= -\frac{1}{r_{ij}^2} \mathrm{erfc}\left(\frac{r_{ij}}{2\gamma}\right) - \frac{1}{\sqrt{\pi}\gamma r_{ij}} e^{-(r_{ij}/2\gamma)^2}$$

$$= -\frac{1}{\Omega} \sum_{\mathbb{k}}{}' \frac{4\pi}{k^2} e^{-\gamma^2 k^2}\, \mathrm{Re}\left[q_\ell (i\mathbb{k}) e^{i\mathbb{k}\cdot\mathbb{r}_\ell} \left(\sum_j q_j e^{-i\mathbb{k}\cdot\mathbb{r}_j} \right)\right]$$

$$+ \sum_{i<j} (\delta_{i\ell} - \delta_{j\ell}) q_i q_j \left[\frac{\mathbb{r}_{ij}}{r_{ij}^3} \mathrm{erfc}\left(\frac{r_{ij}}{2\gamma}\right) + \frac{\mathbb{r}_{ij}}{\sqrt{\pi}\gamma r_{ij}^2} e^{-(r_{ij}/2\gamma)^2} \right]$$

$$\therefore \mathbb{F}_\ell = -\frac{\partial}{\partial \mathbb{r}_\ell} V$$

$$= \frac{1}{\Omega} {\sum_{\mathbb{k}}}' \frac{4\pi}{k^2} e^{-\gamma^2 k^2} \operatorname{Re}\Big[\underbrace{q_\ell(-i\mathbb{k}) e^{i\mathbb{k}\cdot\mathbb{r}_\ell}}_{-i\mathbb{k}\,\tilde{\rho}_\ell(-\mathbb{k})} \underbrace{\Big(\sum_i q_i e^{-i\mathbb{k}\cdot\mathbb{r}_i}\Big)}_{\tilde{\rho}(\mathbb{k})} \Big]$$

$$+ \sum_{i<j} (\delta_{i,\ell} - \delta_{j,\ell}) q_i q_j \left[\frac{\mathbb{r}_{ij}}{r_{ij}^3} \operatorname{erfc}\left(\frac{r_{ij}}{2\gamma}\right) + \frac{\mathbb{r}_{ij}}{\sqrt{\pi}\,\gamma r_{ij}^2} e^{-(r_{ij}/2\gamma)^2} \right] \qquad (39)$$

see p. 18

$$= \frac{1}{\Omega} {\sum_{\mathbb{k}}}' \tilde{v}(k) \cancel{\operatorname{Re}} \left[-i\mathbb{k}\, \tilde{\rho}_\ell(-\mathbb{k})\, \tilde{\rho}(\mathbb{k}) \right]$$

$$+ \sum_{i<j} (\delta_{i,\ell} - \delta_{j,\ell})\, \mathbb{r}_{ij} \left(-\frac{1}{r_{ij}} \frac{du}{dr_{ij}} \right) \qquad (40)$$

where

$$u(r) = \frac{1}{r} \operatorname{erfc}\left(\frac{r}{2\gamma}\right) \qquad (41)$$

$$-\frac{1}{r}\frac{du}{dr} = \frac{1}{r^3} \operatorname{erfc}\left(\frac{r}{2\gamma}\right) + \frac{1}{\sqrt{\pi}\,\gamma r^2} e^{-(r/2\gamma)^2} \qquad (42)$$

$$\tilde{v}(k) = \frac{4\pi}{k^2} e^{-\gamma^2 k^2} \qquad (43)$$

$$\tilde{\rho}_\ell(\mathbb{k}) = q_\ell e^{-i\mathbb{k}\cdot\mathbb{r}_\ell} \qquad (44)$$

$$\tilde{\rho}(\mathbb{k}) = \sum_{i=1}^{N} \rho_i(\mathbb{k}) \qquad (45)$$

8. Second Derivation of Force

Apart from a constant term, potential is written as

$$V = \sum_{i<j} q_i q_j \left[\sum_{\nu} \frac{1}{|\mathbf{r}_{ij} - \nu|} \right]_{c.n.} \tag{46}$$

where charge-neutral, periodic Coulomb potential is given by

$$\left[\sum_{\nu} \frac{1}{|\mathbf{r}-\nu|} \right]_{c.n.} = \psi(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{k}}{}' \frac{4\pi}{k^2} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{47}$$

※ In Eq.(46), no self-image interaction appears. Such interaction, since relative self-image distance doesn't alter, doesn't cause any force.

(Charge-Neutral Force)

$$-\frac{\partial}{\partial \mathbf{r}} \sum_{\nu} \frac{1}{|\mathbf{r}-\nu|} = -\frac{\partial}{\partial \mathbf{r}} \left\{ \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{4\pi}{k^2} e^{-\gamma^2 k^2} e^{i\mathbf{k}\cdot\mathbf{r}} + \sum_{\nu} \frac{1}{|\mathbf{r}-\nu|} \operatorname{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma} \right) \right\}$$

$$= \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{4\pi}{k^2} e^{-\gamma^2 k^2} (-i\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$+ \sum_{\nu} \left\{ \frac{\mathbf{r}-\nu}{|\mathbf{r}-\nu|^3} \operatorname{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma} \right) + \frac{\mathbf{r}-\nu}{\sqrt{\pi}\gamma |\mathbf{r}-\nu|^2} e^{-(|\mathbf{r}-\nu|/2\gamma)^2} \right\} \tag{48}$$

$$\left[-\frac{\partial}{\partial \mathbf{r}} \sum_{\nu} \frac{1}{|\mathbf{r}-\nu|} \right]_{c.n.} = \left[-\frac{\partial}{\partial \mathbf{r}} \sum_{\nu} \frac{1}{|\mathbf{r}-\nu|} \right]_{\mathbf{k}\neq 0}$$

$$= \frac{1}{\Omega} \sum_{\mathbf{k}}{}' \frac{4\pi}{k^2} e^{-\gamma^2 k^2} (-i\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$+ \sum_{\nu} \left\{ \frac{\mathbf{r}-\nu}{|\mathbf{r}-\nu|^3} \operatorname{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma} \right) + \frac{\mathbf{r}-\nu}{\sqrt{\pi}\gamma |\mathbf{r}-\nu|^2} e^{-(|\mathbf{r}-\nu|/2\gamma)^2} \right\}$$

$$- \sum_{\nu} \left\{ \frac{\mathbf{r}-\nu}{|\mathbf{r}-\nu|^3} \operatorname{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma} \right) + \frac{\mathbf{r}-\nu}{\sqrt{\pi}\gamma |\mathbf{r}-\nu|^2} e^{-(|\mathbf{r}-\nu|/2\gamma)^2} \right\}_{\mathbf{k}=0} \tag{49}$$

Here, for $\forall$ periodic function,

$$f(\mathbb{r})\big|_{\mathbb{k}=0} = \frac{1}{\Omega}\tilde{f}(\mathbb{k}=0) = \frac{1}{\Omega}\int_{\Omega} d\mathbb{r}\, f(\mathbb{r}) \tag{50}$$

In particular,

$$\sum_{\nu}\left\{\frac{\mathbb{r}-\nu}{|\mathbb{r}-\nu|^3}\operatorname{erfc}\left(\frac{|\mathbb{r}-\nu|}{2\gamma}\right) + \frac{\mathbb{r}-\nu}{\sqrt{\pi}\gamma|\mathbb{r}-\nu|^2}e^{-(|\mathbb{r}-\nu|/2\gamma)^2}\right\}_{\mathbb{k}=0}$$

$$= \frac{1}{\Omega}\int_{\Omega} d\mathbb{r}\left[\frac{\mathbb{r}}{r^3}\operatorname{erfc}\left(\frac{r}{2\gamma}\right) + \frac{\mathbb{r}}{\sqrt{\pi}\gamma r^2}e^{-(r/2\gamma)^2}\right] = 0 \quad \text{(by symmetry)}$$

$$\boxed{\begin{aligned}\therefore \left[-\frac{\partial}{\partial\mathbb{r}}\sum_{\nu}\frac{1}{|\mathbb{r}-\nu|}\right]_{c.n.} &= \frac{1}{\Omega}\sum_{\mathbb{k}}{}' \frac{4\pi}{k^2}e^{-\gamma^2k^2}(-i\mathbb{k})e^{i\mathbb{k}\cdot\mathbb{r}} \\ &+ \sum_{\nu}\left\{\frac{\mathbb{r}-\nu}{|\mathbb{r}-\nu|^3}\operatorname{erfc}\left(\frac{|\mathbb{r}-\nu|}{2\gamma}\right) + \frac{\mathbb{r}-\nu}{\sqrt{\pi}\gamma|\mathbb{r}-\nu|^2}e^{-(|\mathbb{r}-\nu|/2\gamma)^2}\right\}\end{aligned}} \tag{51}$$

$$\mathbb{F}_{\ell} = -\frac{\partial}{\partial\mathbb{r}_{\ell}}\sum_{i<j} q_i q_j\left[\sum_{\nu}\frac{1}{|\mathbb{r}_{ij}-\nu|}\right]_{c.n.}$$

$$= \sum_{i<j} q_i q_j(\delta_{i,\ell}-\delta_{j,\ell})\left[-\frac{\partial}{\partial\mathbb{r}_{ij}}\sum_{\nu}\frac{1}{|\mathbb{r}_{ij}-\nu|}\right]_{c.n.}$$

$$= \frac{1}{\Omega}\sum_{\mathbb{k}}{}'\overbrace{\frac{4\pi}{k^2}e^{-\gamma^2k^2}}^{\tilde{\upsilon}(k)}(-i\mathbb{k})\underbrace{\sum_{i<j}(\delta_{i,\ell}-\delta_{j,\ell})q_i q_j e^{i\mathbb{k}\cdot\mathbb{r}_{\ell i}}}_{\underbrace{\sum_{\ell<j} q_\ell q_j e^{i\mathbb{k}\cdot\mathbb{r}_{\ell j}} - \sum_{i<\ell} q_\ell q_i e^{-i\mathbb{k}\cdot\mathbb{r}_{\ell i}}}_{(-i\mathbb{k})\sum_{i(\neq\ell)} q_\ell q_i e^{i\mathbb{k}\cdot\mathbb{r}_{\ell i}}}}$$

$\mathbb{k} \leftrightarrow -\mathbb{k}$

$$+ \sum_{i<j}(\delta_{i,\ell}-\delta_{j,\ell})q_i q_j\sum_{\nu}\underbrace{\left\{\frac{\mathbb{r}_{ij}-\nu}{|\mathbb{r}_{ij}-\nu|^3}\operatorname{erfc}\left(\frac{|\mathbb{r}_{ij}-\nu|}{2\gamma}\right) + \frac{\mathbb{r}_{ij}-\nu}{\sqrt{\pi}\gamma|\mathbb{r}_{ij}-\nu|^3}e^{-(|\mathbb{r}_{ij}-\nu|/2\gamma)^2}\right\}}_{(\mathbb{r}_{ij}-\nu)\left(-\frac{1}{r}\frac{du}{dr}\right)_{|\mathbb{r}_{ij}-\nu|}}$$

$$\mathbb{F}_\ell = \frac{1}{\Omega}\sum_{\mathbb{k}}{}' \tilde{v}(k)(-i\mathbb{k})\left(\underbrace{\sum_i q_\ell q_i e^{i\mathbb{k}\cdot(\mathbb{r}_\ell-\mathbb{r}_i)}}_{q_\ell e^{i\mathbb{k}\cdot\mathbb{r}_\ell}\sum_i q_i e^{-i\mathbb{k}\cdot\mathbb{r}_i} = \tilde{\rho}_\ell(-\mathbb{k})\tilde{\rho}(\mathbb{k})} - \overset{\nearrow 0 \text{ from symmetry}}{\cancel{q_\ell^2}}\right)$$

$$+ \sum_{i<j}(\delta_{i\ell}-\delta_{j\ell})q_i q_j \sum_{\nu}(\mathbb{r}_{ij}-\nu)\left(-\frac{1}{r}\frac{du}{dr}\right)_{|\mathbb{r}_{ij}-\nu|}$$

$$\therefore\ \mathbb{F}_\ell = \frac{1}{\Omega}\sum_{\mathbb{k}}{}' \tilde{v}(k)(-i\mathbb{k})\tilde{\rho}_\ell(-\mathbb{k})\rho(\mathbb{k})$$

$$+ \sum_{i<j}(\delta_{i\ell}-\delta_{j\ell})q_i q_j \sum_{\nu}(\mathbb{r}_{ij}-\nu)\left(-\frac{1}{r}\frac{du}{dr}\right)_{|\mathbb{r}_{ij}-\nu|} \tag{52}$$

(Reality of Force ?)

$$\left[\frac{1}{\Omega}\sum_{\mathbb{k}}{}' \tilde{v}(k)(-i\mathbb{k})\tilde{\rho}_\ell(-\mathbb{k})\rho(\mathbb{k})\right]^*$$

$$= \frac{1}{\Omega}\sum_{\mathbb{k}}{}' \tilde{v}(k)(i\mathbb{k})\tilde{\rho}_\ell(\mathbb{k})\rho(-\mathbb{k})$$

$\mathbb{k} \leftrightarrow -\mathbb{k}$

$$= \frac{1}{\Omega}\sum_{\mathbb{k}}{}' \tilde{v}(k)(-i\mathbb{k})\tilde{\rho}_\ell(-\mathbb{k})\rho(\mathbb{k})$$

※ The expression, Eq. (52), is automatically real. Therefore, Eqs. (40) & (52) are identical, and we don't need to take the real part of Eq. (40).

8. Calculation of Stress Tensor

From Eq. (48), we can get

$$\sum_{\nu} \frac{(\mathbf{r}-\nu)_a(\mathbf{r}-\nu)_b}{|\mathbf{r}-\nu|^3} = \frac{1}{\Omega}\sum_{\mathbf{k}} \frac{4\pi}{k^2}e^{-\gamma^2k^2}(-\cancel{i}k_a)\underbrace{r_b\, e^{i\mathbf{k}\cdot\mathbf{r}}}_{\frac{1}{\cancel{i}}\frac{\partial}{\partial k_b}e^{i\mathbf{k}\cdot\mathbf{r}}}$$

$$+\sum_{\nu}(\mathbf{r}-\nu)_a(\mathbf{r}-\nu)_b\left[\frac{1}{|\mathbf{r}-\nu|^3}\,\mathrm{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right)+\frac{1}{\sqrt{\pi}\,\gamma\,|\mathbf{r}-\nu|^2}\,e^{-(|\mathbf{r}-\nu|/2\gamma)^2}\right]$$

$$= \frac{1}{\Omega}\sum_{\mathbf{k}}\underbrace{\frac{\partial}{\partial k_b}\left(k_a\frac{4\pi}{k^2}e^{-\gamma^2k^2}\right)}\,e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\delta_{ab}\frac{4\pi}{k^2}e^{-\gamma^2k^2}+\underbrace{\frac{k_ak_b}{k}\,\underbrace{\frac{d}{dk}\left(\frac{4\pi}{k^2}e^{-\gamma^2k^2}\right)}_{-\frac{8\pi}{k^3}e^{-\gamma^2k^2}-\frac{8\pi\gamma^2}{k}e^{-\gamma^2k^2}}}_{-\frac{8\pi k_ak_b}{k^4}(1+\gamma^2k^2)\,e^{-\gamma^2k^2}}$$

$$+\sum_{\nu}(\mathbf{r}-\nu)_a(\mathbf{r}-\nu)_b\left[\frac{1}{|\mathbf{r}-\nu|^3}\,\mathrm{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right)+\frac{1}{\sqrt{\pi}\,\gamma\,|\mathbf{r}-\nu|^2}\,e^{-(|\mathbf{r}-\nu|/2\gamma)^2}\right]$$

$$\sum_{\nu} \frac{(\mathbf{r}-\nu)_a(\mathbf{r}-\nu)_b}{|\mathbf{r}-\nu|^3} = \delta_{ab}\,\frac{1}{\Omega}\sum_{\mathbf{k}}\frac{4\pi}{k^2}e^{-\gamma^2k^2}e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$-\frac{8\pi}{\Omega}\sum_{\mathbf{k}}\frac{k_ak_b}{k^4}(1+\gamma^2k^2)\,e^{-\gamma^2k^2}e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$+\sum_{\nu}(\mathbf{r}-\nu)_a(\mathbf{r}-\nu)_b\left[\frac{1}{|\mathbf{r}-\nu|^3}\,\mathrm{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right)+\frac{1}{\sqrt{\pi}\,\gamma\,|\mathbf{r}-\nu|^2}\,e^{-(|\mathbf{r}-\nu|/2\gamma)^2}\right] \tag{53}$$

$$\left[\sum_{\nu} \frac{(\mathbf{r}-\nu)_a(\mathbf{r}-\nu)_b}{|\mathbf{r}-\nu|^3}\right]_{c.n.} = \delta_{ab}\frac{1}{\Omega}\sum_{\mathbf{k}}{}' \frac{4\pi}{k^2} e^{-\gamma^2 k^2} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$- \frac{8\pi}{\Omega}\sum_{\mathbf{k}} \frac{k_a k_b}{k^4}(1+\gamma^2 k^2)\, e^{-\gamma^2 k^2} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$+ \sum_{\nu} (\mathbf{r}-\nu)_a(\mathbf{r}-\nu)_b\left[\frac{1}{|\mathbf{r}-\nu|^3}\operatorname{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right) + \frac{1}{\sqrt{\pi}\,\gamma\,|\mathbf{r}-\nu|^2} e^{-(|\mathbf{r}-\nu|/2\gamma)^2}\right]$$

$$- \left\{\sum_{\nu} (\mathbf{r}-\nu)_a(\mathbf{r}-\nu)_b\left[\frac{1}{|\mathbf{r}-\nu|^3}\operatorname{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right) + \frac{1}{\sqrt{\pi}\,\gamma\,|\mathbf{r}-\nu|^2} e^{-(|\mathbf{r}-\nu|/2\gamma)^2}\right]\right\}_{\mathbf{k}=0} \tag{54}$$

Here,

$$\{\ \}_{\mathbf{k}=0} = \frac{1}{\Omega}\int_{\Omega} d\mathbf{r}\; r_a r_b \left[\frac{1}{r^3}\operatorname{erfc}\left(\frac{r}{2\gamma}\right) + \frac{1}{\sqrt{\pi}\,\gamma\, r^2} e^{-(r/2\gamma)^2}\right]$$

from symmetry only diagonal elements are non-zero

$$= \frac{\delta_{ab}}{3\Omega}\int_{\Omega} d\mathbf{r}\; r^2 [\quad]$$

xx, yy, zz

as long as $\gamma \ll \Omega^{1/3}$

$$= \frac{\delta_{ab}}{3\Omega}\int_0^\infty 4\pi r^2 dr\, r^2\, [\quad]$$

$$= \frac{4\pi}{3\Omega}\delta_{ab}\int_0^\infty dr\left[r\operatorname{erfc}\left(\frac{r}{2\gamma}\right) + \frac{r^2}{\sqrt{\pi}\,\gamma} e^{-(r/2\gamma)^2}\right]$$

$$r \leftrightarrow 2\gamma t$$

$$= \frac{4\pi}{3\Omega}\delta_{ab}\int_0^\infty dt\left[4\gamma^2\, t\, \operatorname{erfc}(t) + \frac{8\gamma^2}{\sqrt{\pi}} t^2 e^{-t^2}\right.$$

$$= \frac{\cancel{16}^{\,4}\pi\gamma^2}{\cancel{3}\Omega}\delta_{ab}\left\{\underbrace{\cancel{\left[\frac{t^2}{2}\operatorname{erfc}(t)\right]_0^\infty} - \int_0^\infty dt\,\frac{t^2}{\cancel{2}}\left(-\frac{\cancel{2}}{\sqrt{\pi}}\right)e^{-t^2}}_{\frac{\cancel{3}}{\cancel{\sqrt{\pi}}}\underbrace{\int_0^\infty dt\, t^2 e^{-t^2}}_{\frac{\cancel{\sqrt{\pi}}}{\cancel{4}}}} + \frac{2}{\sqrt{\pi}}\int_0^\infty dt\, t^2 e^{-t^2}\right\}$$

$$= \frac{4\pi\gamma^2}{\Omega}\delta_{ab} \tag{55}$$

$$\therefore \left[\sum_{\nu} \frac{(\mathbf{r}-\nu)_a(\mathbf{r}-\nu)_b}{|\mathbf{r}-\nu|^3}\right]_{\text{c.n.}} = \delta_{ab}\left[-\frac{4\pi\gamma^2}{\Omega} + \frac{1}{\Omega}\sum_{\mathbf{k}}{}' \frac{4\pi}{k^2} e^{-\gamma^2k^2} e^{i\mathbf{k}\cdot\mathbf{r}}\right]$$

$$- \frac{8\pi}{\Omega}\sum_{\mathbf{k}} \frac{k_a k_b}{k^4}(1+\gamma^2k^2)\, e^{-\gamma^2k^2} e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$+ \sum_{\nu} (\mathbf{r}-\nu)_a(\mathbf{r}-\nu)_b \left[\frac{1}{|\mathbf{r}-\nu|^3}\,\mathrm{erfc}\left(\frac{|\mathbf{r}-\nu|}{2\gamma}\right) + \frac{1}{\sqrt{\pi}\gamma|\mathbf{r}-\nu|^2}\, e^{-(|\mathbf{r}-\nu|/2\gamma)^2}\right] \tag{55}$$

(*Stress Tensor*: See 3/16/92)

$$\Omega\Pi = \sum_{i<j} \mathbf{F}_{ij}\,\mathbf{r}_{ij}$$

$$= \sum_{i<j} q_i q_j \left[\sum_{\nu} \frac{(\mathbf{r}_{ij}-\nu)_a(\mathbf{r}_{ij}-\nu)_b}{|\mathbf{r}_{ij}-\nu|^3}\right]_{\text{c.n.}}$$

$$= \delta_{ab}\Big[\underbrace{-\frac{4\pi\gamma^2}{\Omega}\sum_{i<j} q_i q_j}\; + \frac{1}{\Omega}\sum_{\mathbf{k}}{}' \frac{4\pi}{k^2} e^{-\gamma^2k^2} \underbrace{\sum_{i<j} q_i q_j\, e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}}_{\frac{1}{2}\left[\sum_{i,j} q_i q_j e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} - \sum_i q_i^2\right]}$$

$$+ \frac{\overset{2}{\cancel{4}}\pi\gamma^2}{\Omega}\sum_i q_i^2 \quad (\because \text{Eq.}(28))$$

$$\sum_{i<j} q_i q_j - \frac{1}{2}\sum_{i,j} q_i q_j = -\frac{1}{2}\sum_i q_i^2 \qquad = \frac{1}{2}\left[|\tilde{\rho}(\mathbf{k})|^2 - \sum_i q_i^2\right]$$

$$- \frac{8\pi}{\Omega}\sum_{\mathbf{k}}{}' \frac{k_a k_b}{k^4}(1+\gamma^2k^2)\, e^{-\gamma^2k^2} \underbrace{\sum_{i<j} q_i q_j\, e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}}_{\frac{1}{2}\left[\sum_{i,j} q_i q_j e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} - \sum_i q_i^2\right]}$$

$$= \frac{1}{2}\left[|\tilde{\rho}(\mathbf{k})|^2 - \sum_i q_i^2\right]$$

$$+ \sum_{i<j} q_i q_j \sum_{\nu} (\mathbf{r}_{ij}-\nu)_a(\mathbf{r}_{ij}-\nu)_b \left(-\frac{1}{r}\frac{du}{dr}\right)_{|\mathbf{r}_{ij}-\nu|}$$

$$\therefore\ \Omega\Pi = \delta_{ab}\left[\frac{\overset{2}{\cancel{4}}\pi\gamma^2}{\Omega}\left(\sum_i q_i^2\right) + \frac{1}{2\Omega}\sum_{\mathbf{k}}{}' \frac{4\pi}{k^2}e^{-\gamma^2k^2}\left(|\tilde{\rho}(\mathbf{k})|^2 - \sum_i q_i^2\right)\right]$$

$$- \frac{4\pi}{\Omega}\sum_{\mathbf{k}}{}' \frac{k_a k_b}{k^4}(1+\gamma^2k^2)e^{-\gamma^2k^2}\left(|\tilde{\rho}(\mathbf{k})|^2 - \sum_i q_i^2\right)$$

$$+ \sum_{i<j} q_i q_j \sum_{\boldsymbol{\nu}} (\mathbf{r}_{ij}-\boldsymbol{\nu})_a(\mathbf{r}_{ij}-\boldsymbol{\nu})_b\left(-\frac{1}{r}\frac{du}{dr}\right)_{|\mathbf{r}_{ij}-\boldsymbol{\nu}|} \qquad (56)$$

where

$$\tilde{\rho}(\mathbf{k}) = \sum_{i=1}^{N} q_i\, e^{-i\mathbf{k}\cdot\mathbf{r}_i} \qquad (57)$$

$$-\frac{1}{r}\frac{du}{dr} = \frac{1}{r^3}\operatorname{erfc}\left(\frac{r}{2\gamma}\right) + \frac{1}{\sqrt{\pi}\,\gamma r^2}e^{-(r/2\gamma)^2} \qquad (58)$$