Theorem 5.4 (Baxter's Inequality)

$$V_c(\underline{X},\underline{R}) = \sum_{i<j} \frac{1}{|x_i - x_j|} - \sum_i \sum_j \frac{Z}{|x_i - R_j|} + \sum_{k<l} \frac{Z^2}{|R_k - R_l|}$$

$$\Longrightarrow V_c(\underline{X},\underline{R}) \geq -(2Z+1)\sum_{i=1}^{N} \frac{1}{D(x_i)} + \frac{Z^2}{8}\sum_{j=1}^{M} \frac{1}{D_j}$$

$$D(x) := \min_j |x - R_j|$$

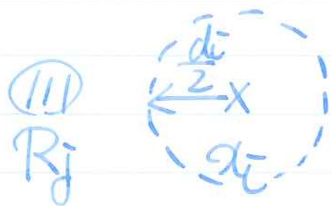
$$x \in \Gamma_j \Longrightarrow D(x) = |x - R_j|$$

$$D_j := \frac{1}{2} \min_{i \neq j} |R_i - R_j|$$

pf. $d_i = D(x_i)$

$$\mu_i(dx) = \frac{1}{d_i^2 \pi} \delta\left(|x - x_i| - \frac{d_i}{2}\right) dx$$

$$\mu = \sum_i \mu_i$$



$\left(\frac{d_i}{2} < d_i\right)$

$$\frac{Z}{|x_i - R_j|} = \int_{\mathbb{R}^3} \frac{Z}{|x - R_j|} \mu_i(dx) \quad (\forall_i j = 1, \dots, N)$$

$$\therefore \sum_i \frac{Z}{|x_i - R_j|} = \int_{\mathbb{R}^3} \frac{Z}{|x - R_j|} \mu(dx)$$

Calculation of $\Phi_j(x) = \int_{\mathbb{R}^3} \frac{\mu_j(dy)}{|x-y|}$

$\forall R > \frac{d_j}{2} \quad \mu_j\left(\{y \in \mathbb{R}^3 : |y - x_j| > R\}\right) = 0$

$$\underset{\text{Newton}}{\Longrightarrow} \quad \Phi_j(x) = \frac{1}{|x-x_j|} \underbrace{\mu_j(\mathbb{R}^3)}_{\shortparallel \atop 1} \qquad |\forall x - x_j| > R$$

$\forall R < \frac{d_j}{2} \quad \mu_j\left(\{y \in \mathbb{R}^3 : |y - x_j| < R\}\right) = 0$

$$\underset{\text{Newton}}{\Longrightarrow} \quad \Phi_j(x) = \int_{|y-x_j|>R} \frac{\mu_j(dy)}{|y-x_j|} \qquad |\forall x - x_j| < R$$

$$= \frac{1}{d_j^2 \pi} \int \frac{1}{|y-x_j|} \delta\left(|y-x_j| - \frac{d_j}{2}\right) dy$$

$$= \frac{1}{d_j^2 \pi} \int_{|y-x_j| = \frac{d_j}{2}} \frac{dy}{|y-x_j|}$$

$$y = x_j + \frac{d_j}{2}\omega$$

$$= \frac{1}{d_j^2 \pi} \left(\frac{d_j}{2}\right)^2 \int_{S^2} \frac{d\omega}{\left|\frac{d_j}{2}\omega\right|}$$

$$= \frac{1}{4\pi} \cdot \frac{2}{d_j} \underbrace{\int_{S^2} d\omega}_{\shortparallel \atop 4\pi} = \frac{2}{d_j}$$

$$\therefore \Phi_j(x) = \begin{cases} \dfrac{1}{|x-x_j|} & |x-x_j| > \dfrac{d_j}{2} \\[2ex] \dfrac{2}{d_j} & |x-x_j| < \dfrac{d_j}{2} \end{cases}$$

$$\boxed{2D(\mu_i, \mu_j) \le \frac{1}{|x_i - x_j|}}$$

Case I. $|x_i - x_j| > \frac{d_i + d_j}{2}$

Newton $\Longrightarrow$ $2D(\mu_i, \mu_j) = \frac{1}{|x_i - x_j|}$

Case II. $|x_i - x_j| \le \frac{d_i + d_j}{2}$

$$2D(\mu_i, \mu_j) = \int_{\mathbb{R}^3} \Phi_j(x)\, \mu_i(dx)$$

$$= \frac{1}{d_i^2 \pi} \int_{|x - x_i| = \frac{d_i}{2}} \Phi_j(x)\, dx$$

$$= \frac{1}{d_i^2 \pi} \left(\frac{d_i}{2}\right)^2 \int_{S^2} \Phi_j\!\left(x_i + \frac{d_i}{2}\omega\right) d\omega$$

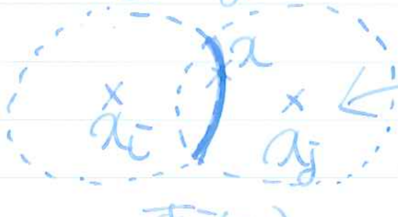
$$= \frac{1}{4\pi} \int_{S^2 \cap \Omega_j^c} \frac{d\omega}{|x_i + \frac{d_i}{2}\omega - x_j|} + \frac{1}{4\pi} \int_{S^2 \cap \Omega_j} \frac{2}{d_j}\, d\omega$$

$$= \frac{1}{4\pi} \int_{S^2} \frac{d\omega}{|x_i + \frac{d_i}{2}\omega - x_j|} - \frac{1}{4\pi} \int_{S^2 \cap \Omega_j} \left(\frac{1}{|\underbrace{x_i + \frac{d_i}{2}\omega}_{x} - x_j|} - \frac{2}{d_j} \right) d\omega$$

$$x = x_i + \frac{d_i}{2}\omega \in S^2 \cap \Omega_j \subset \Omega_j$$

$$\Longrightarrow |x - x_j| \le \frac{d_j}{2} \qquad \therefore\ -2^{\text{nd}} \text{ term} \le 0$$

$$\le \frac{1}{4\pi} \int_{S^2} \frac{d\omega}{|x_i + \frac{d_i}{2}\omega - x_j|} = \frac{1}{|x_i - x_j|} \quad //$$



$\Omega_j = B(x_j, \frac{d_j}{2})$

$\Phi_j(x)$

$$\boxed{D(\mu_i, \mu_i) = \frac{1}{d_i}}$$

$$
\begin{aligned}
D(\mu_i, \mu_i) &= \frac{1}{2}\int_{\mathbb{R}^3} \Phi_i(x)\, \mu_i(dx) \\
&= \frac{1}{\cancel{2}} \frac{1}{d_i^2 \pi} \int_{|x-x_i| = \frac{d_i}{2}} \frac{\cancel{2}}{d_i}\, dx \\
&= \frac{1}{d_i^2 \pi} \left(\frac{d_i}{2}\right)^2 \frac{1}{d_i} \underbrace{\int_{S^2} d\omega}_{= 4\pi} = \frac{1}{d_i} \quad //
\end{aligned}
$$

Rem. $D(\mu_i, \mu_i) = \frac{1}{2}\left(\frac{2}{d_i}\right)$

cont.

$V_c(\underline{x}, \underline{R})$

$$\geq \underbrace{\sum_{i<j} 2D(\mu_i, \mu_j)} - \sum_j \int_{\mathbb{R}^3} \frac{Z}{|x-R_j|}\mu(dx) + \underline{\sum_{k<l} \frac{Z^2}{|R_k-R_l|}}$$

$$= \sum_i \sum_j D(\mu_i, \mu_j) - \sum_i (\mu_i, \mu_i)$$

$$= \underline{D(\mu, \mu)} - \sum_i \frac{1}{d_i}$$

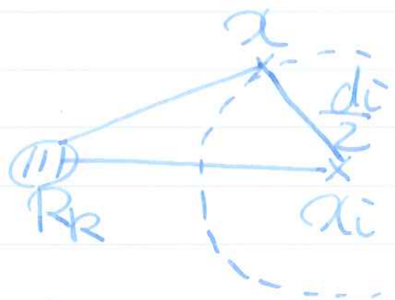
Th5.3

$$\geq \int_{\mathbb{R}^3} \Phi(x)\mu(dx) - \sum_j \int_{\mathbb{R}^3} \frac{Z}{|x-R_j|}\mu(dx) - \sum_i \frac{1}{d_i} + \frac{Z^2}{8}\sum_j \frac{1}{D_j}$$

$$\Phi(x) = \sum_j \frac{Z}{|x-R_j|} - \frac{Z}{\mathcal{D}(x)}$$

$$= -\sum_i \left(\int_{\mathbb{R}^3} \frac{Z}{\mathcal{D}(x)} \mu_i(dx) + \frac{1}{d_i} \right) + \frac{Z^2}{8} \sum_j \frac{1}{D_j}$$

$x \in \operatorname{supp} \mu_i$



$$\Rightarrow \mathcal{D}(x) = |x - R_k|$$

$$\geq \underbrace{|x_i - R_k|}_{\geq d_i} - \underbrace{|x - x_i|}_{= \frac{d_i}{2}}$$

$$\geq d_i - \frac{d_i}{2} = \frac{d_i}{2}$$

$$\therefore (\cdots) \geq (2Z+1) \cdot \frac{1}{d_i}$$

Q.E.D.