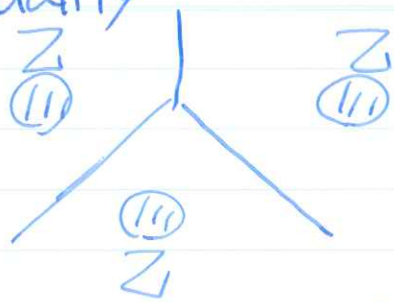
§5.2 Basic Electrostatic Inequality

Voronoi cell



$R_1, \dots, R_M \in \mathbb{R}^3$

$\Gamma_j = \{ x \in \mathbb{R}^3 : |x - R_j| < |x - R_i| \ \forall i \neq j \}$

○ Γ_j open

$\because)$ $\forall x \in \Gamma_j$ $\quad d = \mathrm{dist}(x, \partial\Gamma_j)$

$$B(x, \tfrac{d}{2}) = \{ y \in \mathbb{R}^3 : |y - x| < \tfrac{d}{2} \}$$
$$\subset \Gamma_j \ //$$

○ Γ_j convex

$\stackrel{\text{def}}{\iff})$ $x, y \in \Gamma_j \implies \lambda x + (1-\lambda) y \in \Gamma_j$
$\quad 0 < {}^\forall \lambda < 1$

$\because)$ $x \in \Gamma_j \iff |x - R_j| < |x - R_i| \quad \forall i \neq j$

$$\iff (x - R_j)\cdot(R_i - R_j) < \frac{1}{2} |R_i - R_j|^2$$

$$\left(\lambda x + (1-\lambda) y - R_j\right)\cdot(R_i - R_j)$$

$$= \Big(\lambda (x - R_j) + (1-\lambda)(y - R_j)\Big)\cdot(R_i - R_j)$$

$$= \lambda \underline{(x - R_j)\cdot(R_i - R_j)} + (1-\lambda)\underline{(y - R_j)\cdot(R_i - R_j)}$$

$$< \frac{\lambda + (1-\lambda)}{2} |R_i - R_j|^2$$

$$\therefore \lambda x + (1-\lambda) y \in \Gamma_j \ //$$

$$D_j := \frac{1}{2} \min_{i \neq j} |R_i - R_j| = \mathrm{dist}(R_j, \partial \Gamma_j)$$

equal

$$W(x) = Z \sum_k \frac{1}{|x - R_k|}$$

W : harmonic

$\Longleftrightarrow \Delta W = 0$ in $\mathbb{R}^3 \setminus \{R_1, \dots, R_M\}$

$$D(x) = \min_{i=1,\dots,M} |x - R_i|$$

$$\Phi(x) = W(x) - \frac{Z}{D(x)}$$

$\Rightarrow$ Φ : continuous on $\mathbb{R}^3$

$\because$) $x \in \partial \Gamma_j \cap \partial \Gamma_k$

$D(x) = |x - R_j| = |x - R_k|$ //

Φ : harmonic in Γ_j (not in $\mathbb{R}^3$)

$-\Delta \Phi = 0$ in Γ_j

$\Phi \notin C^1(\mathbb{R}^3)$

$$Z^2 \sum_{k<l} \frac{1}{|R_k - R_l|} = \frac{1}{2} Z \sum_j \Phi(R_j)$$

Theorem 5.3
(Basic Electrostatic Inequality)

$$\mu = \mu_+ - \mu_-$$

$$D(\mu_+, \mu_+),\ D(\mu_-, \mu_-) < \infty$$

$$R_1, \dots, R_M \in \mathbb{R}^3$$

$$\Longrightarrow D(\mu, \mu) - \int \Phi(x)\, \mu(dx) + \sum_{k<l} \frac{Z^2}{|R_k - R_l|} \geq \frac{1}{8} \sum_j \frac{Z^2}{D_j}$$

Step 1.

Find ν

s.t. $\Phi(x) = \int_{\mathbb{R}^3} \frac{\nu(dy)}{|x-y|}$

or $-\Delta \Phi = 4\pi \nu$

$f \in C_c^\infty(\mathbb{R}^3)$

$$\int_{\mathbb{R}^3} \Phi(x) \Delta f(x)\, dx$$

$$= \sum_j \int_{\Gamma_j} \Phi(x) \Delta f(x)\, dx$$

$\#$ $\nabla \cdot (\Phi \nabla f) = (\nabla \Phi)\cdot(\nabla f) + \Phi \Delta f$

$$= \underbrace{\sum_j \int_{\Gamma_j} \nabla \cdot (\Phi \nabla f)(x)\, dx} - \sum_j \int_{\Gamma_j} \nabla \Phi(x) \cdot \nabla f(x)\, dx$$

$$= \int_{\partial \Gamma_j} \underbrace{\Phi(x)} \hat{n}_j \cdot \underbrace{\nabla f(x)}\, dS \quad (\because \text{Gauß})$$

$\Phi,\ \nabla f \in C$

$$\sum_j \int_{\partial \Gamma_j} \Phi(x) \hat{n}_j \cdot \nabla f(x)\, dS = 0.$$

$$-\sum_j \int_{\Gamma_j} \nabla f(x) \cdot \nabla \Phi(x)\, dx$$

$$= -\sum_j \int_{\Gamma_j} \nabla \cdot (f \nabla \Phi)(x)\, dx + \sum_j \int_{\Gamma_j} f(x) \underbrace{\Delta \Phi(x)}_{\shortparallel}\, dx$$

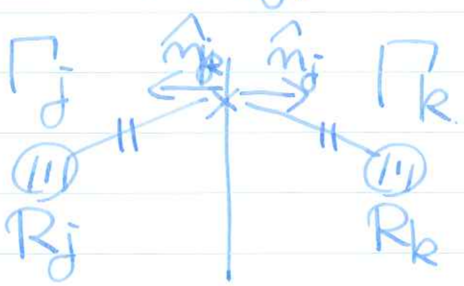
$$\therefore \int_{\mathbb{R}^3} \Phi(x)\,\Delta f(x)\,dx = -\sum_j \int_{\partial\Gamma_j} f(x)\,\hat{n}_j\cdot\nabla \underbrace{\Phi(x)}_{W(x)-\frac{Z}{D(x)}}\,dS$$

$$W \in C^\infty(\mathbb{R}^3\setminus\{R_1,\dots,R_m\})$$

$$= \sum_j \int_{\partial\Gamma_j} f(x)\,\hat{n}_j\cdot\nabla \frac{Z}{D(x)}\,dS$$

$$\hat{n}_j\cdot\nabla\frac{1}{|x-R_j|} = \hat{n}_k\cdot\nabla\frac{1}{|x-R_k|}$$

$$\forall x\in\partial\Gamma_j\cap\partial\Gamma_k$$



$$= 2Z\int_{\bigcup_j\partial\Gamma_j} f(x)\,\hat{n}_j\cdot\nabla\frac{1}{|x-R_j|}\,dS$$

$$-\Delta\Phi = 4\pi\nu$$

$$-\frac{Z}{2\pi}\underbrace{\hat{n}_j\cdot\nabla\frac{1}{|x-R_j|}}_{-\hat{n}_j\cdot\frac{x-R_j}{|x-R_j|^2}} = -\frac{Z}{2\pi}\hat{n}_k\cdot\nabla\frac{1}{|x-R_k|}$$

$\therefore \nu \ge 0$ $\qquad \hat{n}_j\cdot(x-R_j)\ge 0\ \forall x\in\partial\Gamma_j$

(Γ_j convex !)

Step 2.

$$\underbrace{D(\mu,\mu) - \int \Phi(x)\,\mu(dx)} + \sum_{k<l} \frac{Z^2}{|R_k - R_l|}$$

$$= D(\mu,\mu) - 2D(\mu,\nu) + D(\nu,\nu) - D(\nu,\nu)$$

$$= D(\mu-\nu,\mu-\nu) - D(\nu,\nu)$$

$$\geq -D(\nu,\nu) \quad (\because \text{Th } 5.1)$$

$$\geq -D(\nu,\nu) + \sum_{k<l} \frac{Z^2}{|R_k - R_l|}$$

$$W(x) = Z \sum_j \frac{1}{|x - R_j|} = Z \sum_j \int_{\mathbb{R}^3} \frac{1}{|y-x|}\,\delta(y - R_j)\,dy$$

$$\Rightarrow \int_{\mathbb{R}^3} W(x)\,\nu(dx) = Z \sum_j \int \underbrace{\left(\int_{\mathbb{R}^3} \frac{\nu(dx)}{|x-y|} \right)}_{\Phi(y)} \delta(y - R_j)\,dy$$

$$= Z \sum_j \Phi(R_j)$$

$$D(\nu,\nu) = \frac{1}{2} \int_{\mathbb{R}^3} \Phi(x)\,\nu(dx)$$

$$= \underbrace{\frac{1}{2} \int_{\mathbb{R}^3} W(x)\,\nu(dx)}_{\# \frac{Z}{2} \sum_j \Phi(R_j)} - \frac{1}{2} \int_{\mathbb{R}^3} \frac{Z}{D(x)}\,\mu(dx)$$

$$= \sum_{k<l} \frac{Z^2}{|R_k - R_l|}$$

Step 3

$$\frac{1}{2}\int_{\mathbb{R}^3} \frac{Z}{D(x)} \, \nu(dx)$$

$$= -\frac{Z^2}{8\pi} \sum_j \int_{\partial\Gamma_j} \frac{1}{|x-R_j|} \hat{n}_j \cdot \nabla \frac{1}{|x-R_j|} \, dS$$

$\because)$ $\nu = -\frac{1}{4\pi} \Delta \Phi$

$$\int_{\mathbb{R}^3} f(x) \, \nu(dx)$$

$$= -\frac{1}{4\pi} \int_{\mathbb{R}^3} \Phi(x) \Delta f(x) \, dx$$

$$= -\frac{Z}{4\pi} \sum_j \int_{\partial\Gamma_j} \cancel{f}(x) \, \hat{n}_j \cdot \nabla \frac{1}{|x-R_j|} \, dS$$

where $\cancel{f}(x)_j = \cancel{\frac{1}{|x-R_j|}} \frac{1}{D(x)}$

$$\nabla \frac{1}{|x-R_j|^2} = \nabla \left(\frac{1}{|x-R_j|} \cdot \frac{1}{|x-R_j|} \right) = 2 \frac{1}{|x-R_j|} \nabla \frac{1}{|x-R_j|}$$

$$= -\frac{Z^2}{16\pi} \sum_j \int_{\partial\Gamma_j} \hat{n}_j \cdot \nabla \frac{1}{|x-R_j|^2} \, dS$$

$$= \cancel{\pm} \frac{Z^2}{16\pi} \sum_j \int_{\Gamma_j^c} \underbrace{\Delta \frac{1}{|x-R_j|^2}} \, dx \quad (\because \text{Gauß})$$

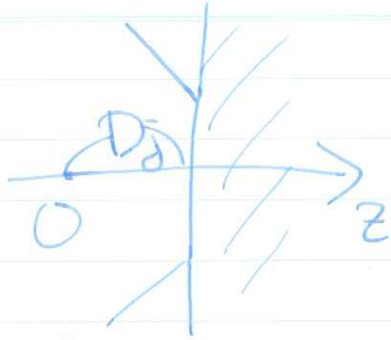
$$\Delta \frac{1}{|x-R_j|^2} = \frac{2}{|x-R_j|^4}$$

$$\nabla \frac{1}{|x-R_j|^2} = -2 \frac{x-R_j}{|x-R_j|^{\cancel{3}\,4}}$$

∇ $-2 \, \frac{1 \cdot |\;\;|^4 - (x-R_j) \cdot 2|x-R_j|^2 \cdot 2(x-R_j)}{|\;\;|^8}$

$\sum$ $-2 \left(\frac{3}{|\;\;|^4} - \frac{4}{|\;\;|^4} \right)$

$$\frac{Z_i}{2}\int_{\mathbb{R}^3}\frac{\nu(dx)}{D(x)} = \frac{Z_i^2}{8\pi}\sum_j\int_{\Gamma_j^c}\frac{dx}{|x-R_j|^4}$$



$\forall\ T, R$

$$\int_{\Gamma_j^c}\frac{dx}{|x-R_j|^4} \geq \int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{D_j}^{\infty}\frac{dz}{(x^2+y^2+z^2)^2}$$

$$\begin{pmatrix}x\\y\end{pmatrix} = r\omega,\quad \omega\in S^1$$

$$dx\,dy\,dz = r\,dr\,d\omega$$

$$\int_{D_j}^{\infty}\int_0^{\infty}\frac{r\,dr}{(r^2+z^2)^2}\underbrace{\int_{S^1}d\omega}_{\substack{\shortparallel\\2\pi}}$$

$$-\frac{1}{2}\left[\frac{1}{r^2+z^2}\right]_0^{\infty} = \frac{1}{2z^2}$$

$$= \pi\int_{D_j}^{\infty}\frac{dz}{z^2} = \pi\left[-\frac{1}{z}\right]_{D_j}^{\infty} = \frac{\pi}{D_j}$$

$$\therefore \frac{Z_i}{2}\int_{\mathbb{R}^3}\frac{\nu(dx)}{D(x)} \geq \frac{Z_i^2}{8\pi}\sum_j\frac{\pi}{D_j} = \frac{Z_i^2}{8}\sum_j\frac{1}{D_j}\quad //$$