Exercise Sheet
Topics in Mathematical Physics

Sheet Number 11

Due: Monday 26.01.26, 10 a.m., Letterbox 3.13, Ernst-Zemelo-Str. 1.
Please try handing in as pairs

Exercise 29: (4 Points)

Show that $\Phi(x) := w(x) - \frac{Z}{D(x)}$ is continuous on $\mathbb{R}^3$, harmonic in each cell Γ_j, but not harmonic on $\partial\Gamma_j$.

HINT: Recall the definitions:

- $D(x) = \min\{|x - R_i| : 1 \le i \le M\}$ where $R_1, \dots, R_M \in \mathbb{R}^3$ are the positions of the nuclei.
- $w(x) = Z \sum_{k=1}^{M} \frac{1}{|x-R_k|}$, where Z ist the charge.
- $\Gamma_j := \{x \in \mathbb{R}^3 : |x - R_j| < |x - R_i| \, \forall i \neq j\} \subset \mathbb{R}^3$.

Exercise 30: (8 Points)

Let

$$V(\underline{x}, \underline{R}) = \sum_{i<j} \frac{1}{|x_i - x_j|} - \sum_{i=1}^{N}\sum_{j=1}^{M} \frac{Z}{|x_i - R_j|} + \sum_{k<l}^{M} \frac{Z^2}{|R_k - R_l|},$$

where $\underline{x} = (x_1, \dots, x_N) \in \mathbb{R}^{3N}$ and $\underline{R} = (R_1, \dots, R_M) \in \mathbb{R}^{3M}$.

(i) Consider the measure μ_i on $\mathbb{R}^3$ with

$$d\mu_i(x) = \frac{1}{\pi D(x_i)} \delta(|x - x_i| - D(x_i)/2)$$

with $D(x_i) := \min\{|x - R_i| : 1 \le i \le M\}$ and show that μ_i is a probability measure.

(ii) Using Newton's Theorem, prove that

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

(iii) Using (i),(ii), $\mu := \sum_{i=1}^{N} \mu_i$ and $\int \frac{Z}{|y-R_j|} d\mu_i(y) = \frac{Z}{|x_i - R_j|}$, prove the following lower bound:

$$V(\underline{x}, \underline{R}) \ge D(\mu, \mu) - \sum_{i=1}^{N} D(\mu_i, \mu_i) - Z \sum_{j=1}^{N} \int \frac{1}{|x - R_j|} d\mu(x) + \sum_{l<k}^{M} \frac{Z^2}{|R_l - R_k|}.$$

(iv) Use that $D(\mu_i, \mu_i) = \frac{1}{D(x_i)}$ to show that

$$V(\underline{x}, \underline{R}) = D(\mu, \mu) - Z \sum_{j=1}^{N} \int \frac{1}{|x - R_j|} d\mu(x) + \sum_{k<l}^{M} \frac{Z^2}{|R_k - R_l|} - \sum_{i=1}^{N} \frac{1}{D(x_i)}.$$

(v) Apply the Electrostatic Inequality with

$$\phi(x) = Z \sum_{k=1}^{M} \frac{1}{|x - r_k|} - \frac{Z}{D(x)}$$

to prove the lower bound

$$V(\underline{x},\underline{R}) \geq -\sum_{i=1}^{N}\left[\int \frac{Z}{D(x)}d\mu_i(x) + \frac{1}{D(x_i)}\right] + \frac{Z^2}{8}\sum_{j=1}^{M}\frac{1}{D_j},$$

where $D_j := \min\{|R_i - R_j|,\, i \neq j\}$.

(vi) Using that for $x \in \mathrm{supp}(\mu_i)$ the inequality $D(x) \geq D(x_i)/2$ holds, prove the lower bound

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