Mathematisches Institut
LMU München
WS 2013-14

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# Mathematical Quantum Mechanics

## Homework Sheet 8

**Exercise 1:** Prove that every solution of the Thomas–Fermi equation which belongs to the domain of the Thomas–Fermi functional is actually a minimizer. Conclude that such solution is unique.

**Exercise 2 (12 points):** We prove the Teller's result that molecules do not bind in the Thomas–Fermi theory: The energy functional for $K$ atomic nuclei with positions $\mathbf{R} = (R_k \in \mathbb{R}^3)_{k=1}^K$ and charges $\mathbf{Z} = (Z_k \geqslant 0)_{k=1}^K$ is given by

$$\begin{aligned}\mathcal{E}_K(\rho; \mathbf{R}; \mathbf{Z}) = \frac{3}{5}\gamma \int \rho^{5/3}(x)\mathrm{d}x - \int \sum_{k=1}^K \frac{Z_k}{|x - R_k|}\rho(x)\mathrm{d}x \\ + \frac{1}{2}\iint \frac{\rho(x)\rho(y)}{|x-y|}\mathrm{d}x\mathrm{d}y + \sum_{k<l} \frac{Z_k Z_l}{|R_k - R_l|}.\end{aligned}$$

We denote the minimum of this functional by $E_K(\mathbf{R}; \mathbf{Z})$ and the corresponding minimizer by $\rho_K(x; \mathbf{R}; \mathbf{Z})$.

1. Prove that

$$\begin{aligned}\lim_{Z_K \to 0} E_K(R_1, \ldots, R_K; Z_1, \ldots, Z_K) \\ = E_{K-1}(R_1, \ldots, R_{K-1}; Z_1, \ldots, Z_{K-1}).\end{aligned}$$

2. Prove that

$$\frac{\partial E_K}{\partial Z_k}(\mathbf{R}; \mathbf{Z}) = \lim_{x \to R_k} \left( \phi_K(x; \mathbf{R}; \mathbf{Z}) - \frac{Z_k}{|x - R_k|} \right)$$

provided $Z_k > 0$. Here

$$\phi_K(x; \mathbf{R}; \mathbf{Z}) := \sum_{k=1}^K \frac{Z_k}{|x - R_k|} - \int \frac{\rho_K(y; \mathbf{R}; \mathbf{Z})}{|x - y|}\mathrm{d}y$$

is the Thomas–Fermi potential.

3. Prove that, for fixed $x$ and $\mathbf{R}$, $\phi_K(x; \mathbf{R}; \mathbf{Z})$ is a monotone increasing function of the entries of $\mathbf{Z}$.
*Hint:* Every superharmonic function in a domain $\Omega$ attains its minimum on the boundary $\partial\Omega$.

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4. Conclude that

$$E_{K+L}(R_1, \ldots, R_{K+L}; Z_1, \ldots, Z_{K+L}) \geqslant E_K(R_1, \ldots, R_K; Z_1, \ldots, Z_K) \\ + E_L(R_{K+1}, \ldots, R_{K+L}; Z_{K+1}, \ldots, Z_{K+L}).$$

Thus we cannot gain energy by bringing two sets of nuclei close together. This result shows that Thomas–Fermi theory is appropriate to describe matter (extensivity of the energy).

The solutions should be put to the box marked "Mathematical Quantum Mechanics" on the first floor **by 16:00 on Tuesday, Dezember 10**.

**Every solution must be an original work of its single author!**
**Violations of this rule will be penalized!**