MATHEMATISCHES INSTITUT
LMU MÜNCHEN
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Mathematical Quantum Mechanics

Problem Sheet 6

Hand-in deadline: 12/01/2016 before noon in the designated MQM box (1st floor, next to the library).

Exercise 1: Find a potential of the form $c|x|^{-a}$, $x \neq 0$, $c \neq 0$, $a > 0$, that obeys the neutral atomic Thomas-Fermi equation

$$-\Delta\varphi_{\mathrm{TF}} = -4\pi(\varphi_{\mathrm{TF}}/\gamma)^{3/2}. \tag{1}$$

Exercise 2: Consider the unique minimizer ρ_{TF} of the atomic Thomas-Fermi functional. It satisfies the Thomas-Fermi equation

$$\gamma\rho_{\mathrm{TF}}(x)^{2/3} = \varphi_{\mathrm{TF}}(x) := \frac{1}{|x|} - \left(\rho_{\mathrm{TF}} * \frac{1}{|\cdot|}\right)(x). \tag{2}$$

(a) Define $\rho_{\mathrm{TF},Z} := Z^2\rho_{\mathrm{TF}}(Z^{1/3}\cdot)$ and $\varphi_{\mathrm{TF},Z} = Z^{4/3}\varphi_{\mathrm{TF}}(Z^{1/3}\cdot)$. Show that

$$\gamma\rho_{\mathrm{TF},Z}(x)^{2/3} = \varphi_{\mathrm{TF},Z}(x).$$

Moreover, let

$$\mathcal{E}_{\mathrm{TF}}(\rho; Z) := \int_{\mathbb{R}^3}\left(\frac{3\gamma}{5}\rho(x)^{5/3} - \frac{Z}{|x|}\rho(x)\right)dx + \frac{1}{2}\iint \frac{\rho(x)\rho(y)}{|x-y|}\mathrm{d}x\mathrm{d}y$$

and let $E_{\mathrm{TF}}(Z)$ be the minimum of the functional. Show that $E_{\mathrm{TF}}(Z) = Z^{7/3}E_{\mathrm{TF}}(1)$.

(b) Since φ_{TF} is radially symmetric, we can write φ_{TF} in (2) as $\varphi_{\mathrm{TF}}(x) = \phi(|x|)$. Show that $\eta(r) := r\phi(r)$, $r > 0$, solves the following ODE (also called Thomas-Fermi equation),

$$y'' = \zeta\frac{y^{3/2}}{r^{1/2}},$$

where $\zeta := 4\pi/\gamma^{3/2}$.

(c) Infer from (b) that $\varphi_{\mathrm{TF},Z}(x) \leq \min\{Z|x|^{-1}, 144/(\zeta^2|x|^4)\}$ by comparing η with the *Sommerfeld solution* $\xi(r) := 144/(\zeta^2 r^3)$.

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Exercise 3: 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 $\rho_K(x; \mathbf{R}; \mathbf{Z})$.

(a) Prove that

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

(b) 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.