Mathematisches Institut der LMU
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Functional Analysis II
Winter Semester 2017/18
2. 2. 2018

Excercise Sheet 14 for 9. 2. 2018

14.1. Prove the following inequality, which has been used in the proof of Lieb's theorem,

$$\mathrm{Re}\,\langle \varphi, |x|(-\Delta)\varphi\rangle \geq 0, \quad \forall \varphi \in C_c^\infty(\mathbb{R}^3).$$

Hint: You can use IMS formular (or integration by parts) and Hardy's inequality.

14.2. Let $Z, N > 0$, $K_{\mathrm{cl}} = \frac{3}{5}(6\pi^2)^{2/3}$. Consider the non-interacting Thomas-Fermi energy

$$E^{\mathrm{TF}}(N,Z) := \inf\left\{ K_{\mathrm{cl}} \int_{\mathbb{R}^3} \rho^{5/3}(x)\,\mathrm{d}x - Z\int_{\mathbb{R}^3} \frac{\rho(x)}{|x|}\,\mathrm{d}x : 0 \leq \rho \in L^1 \cap L^{5/3}, \int_{\mathbb{R}^3} \rho = N \right\}.$$

Given (you don't need to prove) that $E^{\mathrm{TF}}(N,Z)$ has a minimizer ρ_0 which is radially symmetric decreasing (i.e. $|x| \mapsto \rho_0(x)$ is decreasing). Show that ρ_0 satisfies the following Thomas-Fermi equation, for some constant $\mu > 0$,

$$\frac{5K_{\mathrm{cl}}}{3}\rho_0(x)^{2/3} = \left[\frac{Z}{|x|} - \mu\right]_+.$$

Deduce that

$$E^{\mathrm{TF}}(N,Z) = -\frac{3^{1/3}}{4}Z^2 N^{1/3}.$$

Note: This energy matches the leading order of the sum of hydgogen eigenvalues.

14.3. Let ρ^{TF} be the minimizer of the atomic Thomas-Fermi functional

$$\mathcal{E}^{\mathrm{TF}}(\rho) = K_{\mathrm{cl}} \int_{\mathbb{R}^3} \rho^{5/3}(x)\,\mathrm{d}x - Z\int_{\mathbb{R}^3} \frac{\rho(x)}{|x|}\,\mathrm{d}x + \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y$$

under the constraints $0 \leq \rho \in L^1 \cap L^{5/3}$ and $\int \rho = Z$. Consider the Thomas-Fermi potential $V(x) = Z|x|^{-1} - \rho^{\mathrm{TF}} * |x|^{-1}$. Prove that V satisfies the equation

$$\Delta V(x) = \frac{2}{3\pi} V(x)^{3/2}, \quad \forall x \neq 0,$$

and

$$-L_{\mathrm{cl}} \int_{\mathbb{R}^3} |V(x)|^{5/2}\,\mathrm{d}x = \mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) + \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho^{\mathrm{TF}}(x)\rho^{\mathrm{TF}}(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y.$$

Hint: You can use the Thomas-Fermi equation. Here $K_{\mathrm{cl}} = \frac{3}{5}(6\pi^2)^{2/3}$ and $L_{\mathrm{cl}} = (15\pi^2)^{-1}$.

14.4. Let Ψ_N be an anti-symmetric wave function in $L^2((\mathbb{R}^3)^N)$. Prove that for every open bounded set $\Omega \subset \mathbb{R}^3$

$$\left\langle \Psi_N, \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|}\Psi_N \right\rangle \geq \frac{1}{2\,\mathrm{diam}(\Omega)}(N_\Omega^2 - N_\Omega)$$

where N_Ω is the expectation of the number of particles in Ω, namely

$$N_\Omega = \left\langle \Psi_N, \sum_{i=1}^N 1_\Omega(x_i)\Psi_N \right\rangle = \int_\Omega \rho_{\Psi_N}(x)$$

with ρ_{Ψ_N} the one-body density of Ψ_N, and $\mathrm{diam}(\Omega)$ is the diameter of Ω.

This is the last homework. Congratulations for completing all 55 Problems!