Mathematisches Institut
LMU München
WS 2016-17

Prof. H. Siedentop
Dr. R. Helling
Dr. J.-C. Cuenin

Mathematical Quantum Mechanics

Problem Sheet 9

Hand-in deadline: 12/23/2016 before noon in the designated MQM box (1st floor, next to the library).

Ex. 1: Let $d = 3$. Prove that for all $\psi \in \mathcal{D}(-\Delta) \cap \mathcal{D}(|x|)$, the following inequality holds,

$$\operatorname{Re} \langle \psi, |x|(-\Delta)\psi \rangle \geq 0.$$

Proceed as follows:

(a) For $x \in \mathbb{R}^3$ and $\varepsilon > 0$ set $\rho_\varepsilon(x) := (|x|^2) + \epsilon^2)^{1/2}$. Prove that for $\psi \in \mathcal{D}(-\Delta) \cap \mathcal{D}(|x|)$, the following identity holds,

$$\operatorname{Re} \langle \psi, \rho_\varepsilon(-\Delta)\psi \rangle = \int_{\mathbb{R}^3} \frac{|\nabla(\rho_\varepsilon \psi)(x)|^2}{\rho_\varepsilon(x)} \mathrm{d}x + \frac{3}{2}\varepsilon^2 \int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{\rho_\varepsilon(x)^3} \mathrm{d}x.$$

(b) By taking the limit $\varepsilon \to 0$, prove that

$$\operatorname{Re} \langle \psi, \rho_\varepsilon(-\Delta)\psi \rangle = \int_{\mathbb{R}^3} \frac{|\nabla(|x|\psi(x)|^2}{|x|} \mathrm{d}x.$$

Ex. 2: (a) Show that the number of electrons that can be bound to a nucleus of charge Z in Thomas-Fermi theory satisfies $N < 2Z$, using the following argument: Multiply the Thomas-Fermi equation by $\rho(x)|x|$ and integrate.

(b) Using the same argument as above, show that the number of electrons that can be bound to a nucleus of charge Z in Hartree-Fock theory satisfies $N < 2Z + 1$.

Ex. 3: Prove that the Hartree-Fock functional $\mathcal{E}_{\mathrm{HF}} : F \to \mathbb{C}$ is continuous. Here,

$$F = \{\gamma \in \mathfrak{S}_1(\mathfrak{h}) : (1-\Delta)^{1/2}\gamma(1-\Delta)^{1/2} \in \mathfrak{S}_1(\mathfrak{h})\},$$

endowed with the norm

$$\|\gamma\|_F := \operatorname{tr} |(1-\Delta)^{1/2}\gamma(1-\Delta)^{1/2}|, \quad \gamma \in F.$$