Mathematisches Institut
LMU München
WS 2013-14

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Mathematical Quantum Mechanics

Homework Sheet 10

Exercise 1: Let $\rho_0 \geqslant 0$ be a radially symmetric function from $L^1(\mathbb{R}^3)$ with $\int_{\mathbb{R}^3} \rho_0(x)\mathrm{d}x = 1$. For $y \in \mathbb{R}^3$ let $\rho_y(x) := \rho_0(x-y)$. Prove that $2D(\rho_y, \rho_{y'}) \leqslant |y-y'|^{-1}$.

Exercise 2: Let the Hartree–Fock two–particle density $\rho^{(2)}_{HF}$ and the Müller two–particle density $\rho^{(2)}_{M}$ be as defined in Exrecise 3 of Homework Sheet 9.

1. Determine, whether $\rho^{(2)}_{HF}$ is non–negative.
2. Determine, whether $\rho^{(2)}_{M}$ is non–negative.
3. Show that on D_N (see Exercise 2.1 of Homework Sheet 9) the minimal energy of the atomic Hartree–Fock functional is greater then the one of the Müller functional.

Exercise 3:

1. For $\varphi \in L^{5/2}(\mathbb{R}^3)$ with $\varphi \geqslant 0$ compute
$$\left(\iint \big(p^2 - \varphi(q)\big)_- \mathrm{d}p\,\mathrm{d}q\right)\Big/ \int \varphi^{5/2}(x)\mathrm{d}x.$$
2. In $L^2(\mathbb{R}^3)$ consider the operator $H = -\hbar^2\Delta - \varphi(x)$ with $\varphi \in L^{5/2}(\mathbb{R}^3)$, $\varphi \geqslant 0$. Prove that the trace of the negative part of H satisfies
$$\operatorname{tr} H_- = h^{-3} \iint \big(p^2 - \varphi(q)\big)_- \mathrm{d}p\,\mathrm{d}q + o(h^{-3}).$$
3. Prove the equivalence of the two statements:
   (a) There exists $C > 0$ such that for every $N \in \mathbb{N}$ and every $\psi \in \wedge^N C_0^\infty(\mathbb{R}^3)$ the inequality $T_\psi \geqslant C \int \rho_\psi^{5/3}$ holds.
   (b) There exists $c > 0$ such that for every $\varphi \in C_0^\infty(\mathbb{R}^3)$ with $\varphi \geqslant 0$ the inequality $-\operatorname{tr}(-\Delta - \varphi)_- \leqslant c \int \varphi^{5/2}$ holds.

The solutions should be put to the box marked "Mathematical Quantum Mechanics" on the first floor **by 16:00 on Tuesday, January 7**.

Merry Christmas and Happy New Year!