Mathematisches Institut
LMU München
WS 2013-14

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Mathematical Quantum Mechanics

Homework Sheet 9

Exercise 1: Let ξ be the Slater determinant of N orthonormal orbitals $\xi_1, \dots, \xi_N \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^q$. Compute its one–particle reduced density $\rho_\xi^{(1)}$ and density matrix $\gamma_\xi^{(1)}$. Express the two–particle reduced density and density matrix of ξ through $\rho_\xi^{(1)}$ and $\gamma_\xi^{(1)}$.

Exercise 2: Consider the atomic Hartree–Fock functional on

$$D := \Big\{ \gamma \in \mathfrak{S}^1\big(L^2(\mathbb{R}^3) \otimes \mathbb{C}^4\big) : 0 \leqslant \gamma \leqslant 1, \quad T_\gamma < \infty \Big\}.$$

1. Prove that if γ is a minimizer of $\mathcal{E}_{HF}$ over $D_N := \{\gamma \in D : \operatorname{tr} \gamma = N\}$ with $N \in \mathbb{R}_+$ then $\gamma = P + |\xi\rangle\langle\xi|$, where P is an orthogonal projector with $\operatorname{tr} P = [N]$, and $\xi \in \mathfrak{H}$ satisfies $P\xi = 0$ and $\|\xi\|^2 = N - [N]$. Here $[N] := \max\{M \in \mathbb{N}_0 : M \leqslant N\}$ is the integer part of N.

2. Prove that the charge is quantized in the Hartree–Fock theory: If there exists a minimizer of $\mathcal{E}_{HF}$ in D then there exists a minimizer with an integer trace.

Exercise 3:

1. For $\gamma \in D$ let the Hartree–Fock two–particle density be

   $$\rho_{HF}^{(2)}(\mathfrak{x}, \mathfrak{y}) := \frac{1}{2} \sum_{\sigma,\tau=1}^{q} \big(\gamma(x,x)\gamma(y,y) - \gamma(x,y)\gamma(y,x)\big).$$

   Prove that

   $$\iint_{\mathbb{R}^6} \rho_{\gamma,HF}^{(2)}(\mathfrak{x}, \mathfrak{y}) \mathrm{d}\mathfrak{x} \mathrm{d}\mathfrak{y} \geqslant \binom{N}{2}$$

   with the strict inequality unless γ is a projector.

2. For $\gamma \in D$ let the Müller two–particle density be

   $$\rho_{M}^{(2)}(\mathfrak{x}, \mathfrak{y}) := \frac{1}{2} \sum_{\sigma,\tau=1}^{q} \big(\gamma(x,x)\gamma(y,y) - \gamma^{1/2}(x,y)\gamma^{1/2}(y,x)\big).$$

   Prove that

   $$\iint_{\mathbb{R}^6} \rho_{\gamma,M}^{(2)}(\mathfrak{x}, \mathfrak{y}) \mathrm{d}\mathfrak{x} \mathrm{d}\mathfrak{y} = \binom{N}{2}.$$

The solutions should be put to the box marked “Mathematical Quantum Mechanics” on the first floor **by 12:00 on Thursday, Dezember 19**.

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