Mathematical Quantum Mechanics, 2014/15 Homework Problems, LMU

Issued: December 2, 2014; deadline for handing in the solutions: December 9, 2014, 4 pm

24. Determine the form of the Hartree-Fock energy for a two-electron system with

$$H = \sum_{i=1}^{2} (-\Delta_i - \frac{Z}{|x_i|}) + \frac{1}{|x_1 - x_2|} \tag{24}$$

on $\Lambda_{i=1,2} H^2(\mathbb{R}^3)$ and γ_ψ, γ_χ associated with the Slaterdeterminants $\psi(x_1, x_2) = (1/\sqrt{2})|\phi(x_1)\alpha\,\phi(x_2)\beta|$ and $\chi(x_1, x_2) = (1/\sqrt{2})|\phi_1(x_1)\alpha\,\phi_2(x_2)\alpha|$, where α and β stand for up and down spin, respectively,

$$\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{25}$$

and $\phi, \phi_1, \phi_2 \in H^2(\mathbb{R}^3)$ with ϕ_1, ϕ_2 being orthonormal.

25. Prove that the Gaussian coherent states

$$\psi_{p,q}(x) = c e^{\mathrm{i}\hbar^{-1} p x} e^{-a(x-q)^2} \tag{26}$$

with $q, p \in \mathbb{R}$, $c \in \mathbb{C}$, $a > 0$, yield an equality in the uncertainty relation

$$\Delta_\psi p_{\mathrm{op}}\, \Delta_\psi x_{\mathrm{op}} \geq \hbar/2 \tag{27}$$

for the momentum operator $p_{\mathrm{op}} = -i\hbar\, d/dx$ and position operator x_{op} in $L^2(\mathbb{R})$, and where the variance $\Delta_\psi A$ of an operator A is given by $\Delta_\psi A = \sqrt{\langle \psi, A^2\psi \rangle - \langle \psi, A\psi \rangle^2}$.

26. Consider the functional $\mathcal{E}(\psi) = -(1/8\pi)\int |\nabla\psi(x)|^2 d^3x - (2/5)\int [V(x) - \psi(x)]_+^{5/2} d^3x$, where $V(x) = -Z/|x|$, $Z > 0$, and $[g(x)]_+$ denotes the nonnegative part of a function, i.e., $[g(x)]_+ = g(x)$ if $g(x) > 0$, and $[g(x)]_+ = 0$ otherwise, and where $\mathcal{E}$ is defined on $\mathcal{D}_{\mathcal{E}} = \{\psi \in \mathcal{S}'(\mathbb{R}^3) \cap L^1_{\text{loc}}(\mathbb{R}^3),\ \nabla\psi \in L^2(\mathbb{R}^3), \exists c_0, R_0 > 0$ such that $|\psi(x)| \leq c_0|x|^{-1}$ a.e. for $|x| > R_0\}$

(i) Show that $\mathcal{E}$ is strictly concave and therefore there is at most one maximizer.

(ii) Demonstrate that each maximizer of $\mathcal{E}$ has to obey the distributional equation $-\Delta\psi = 4\pi[V(x) - \psi(x)]_+^{3/2}$. Compare this equation with the Thomas-Fermi equation.