Exercise Sheet 12

Exercise 35. Ground state in quantum mechanics. The spatial density distribution of the electron in a hydrogen atom is given in terms of the density $\rho : \Omega \to [0, \infty[$, where for simplicity we let $\Omega = B_R(0) \subset \mathbb{R}^3$. The wave function $\psi : \Omega \to \mathbb{C} \simeq \mathbb{R}^2$ defines the density ρ via $\rho(x) = |\psi(x)|^2$. The ground state is the minimizer of the total energy $I(\psi) = I_{\text{kin}}(\psi) + I_{\text{Coul}}(\psi)$ under the constraint $\int_\Omega |\psi(x)|^2 \,\mathrm{d}x = \int_\Omega \rho(x) \,\mathrm{d}x = 1$.

The kinetic energy $I_{\text{kin}}(\psi) = \int_\Omega \mu |\nabla\psi(x)|^2 \,\mathrm{d}x$ and the Coulomb-interaction energy $I_{\text{Coul}}(\psi) = \int_\Omega -\frac{\gamma}{|x|} |\psi(x)|^2 \,\mathrm{d}x$ are given via positive physical constants μ and γ.

(a) Show that a ground state exists for all $R \in \,]0, \infty[$.

Hint: Show and use $(x \mapsto 1/|x|) \in \mathrm{L}^2(\Omega)$ and $\|u\|_{\mathrm{L}^4} \leq C \|u\|_{\mathrm{L}^2}^{1/4} \|u\|_{\mathrm{H}^1}^{3/4}$.

(b) Show that there is a real and nonnegative ground state, i.e. $\psi(x) = \operatorname{Re}\psi(x) \geq 0$ a.e.

(c) For the physical case $R = \infty$ show that a solution of the form $\psi(x) = \alpha \mathrm{e}^{-\beta|x|}$ satisfies the Euler–Lagrange equations.

Exercise 36. Variational inequality. We consider a string which is fixed rigidly on the left end and which is elastically supported on the right end under the constraint that the support is in a given interval.

Characterize the minimizer of $I(u) = \int_0^1 \left\{\frac{1}{2} u'(x)^2 - h(x)u\right\} \mathrm{d}x + \frac{k}{2}(u(1) - u_0)^2$ under the constraint $u(1) \in [-1, 2]$, where $h \in \mathrm{L}^2(0, 1)$, $k > 0$ and $u_0 \in \mathbb{R}$ and are given.

(a) Give a functions space and a constraint set, such that always a minimizer exists. Is it unique?

(b) Solve the constraint minimization problem for the case $h = 0$ explicitly, and characterize the set of (k, u_0) for which one of the two constraints is active.