Exam "Modèles non-linéaires en mécanique quantique".

March 23, 2022 *D. Gontier, david.gontier@ens.fr*

Exercice 1. Hartree term in one-dimension.
For $f \in C_0^\infty(\mathbb{R})$, we set

$$V_f(x) := \int_{\mathbb{R}} f(x-y)G(y)\mathrm{d}y, \quad \textit{with} \quad G(y) := -\frac{1}{2}|y|.$$

1/ Let $R > 0$ be big enough so that $f(x) = 0$ for $|x| > R$. Prove that

$$\forall x > R, \quad V_f(x) = -\frac{x}{2}\int_{\mathbb{R}} f(y)\mathrm{d}y + \frac{1}{2}\int_{\mathbb{R}} f(y)y\mathrm{d}y$$
$$\forall x < -R, \quad V_f(x) = \frac{x}{2}\int_{\mathbb{R}} f(y)\mathrm{d}y - \frac{1}{2}\int_{\mathbb{R}} f(y)y\mathrm{d}y.$$

2/ Compute V_f'.
3/ Prove that $-V_f'' = f$ for all $x \in \mathbb{R}$.

We now set, for $f \in C_0^\infty(\mathbb{R})$,

$$\mathcal{D}(f) := -\frac{1}{2}\iint_{\mathbb{R}\times\mathbb{R}} \overline{f}(x)f(y)|x-y|\mathrm{d}x\mathrm{d}y,$$

4/ Let $f_1, f_2 \in C_0^\infty(\mathbb{R})$ and $t \in \mathbb{R}$. Prove that

$$\mathcal{D}(tf_1 + (1-t)f_2) - t\mathcal{D}(f_1) - (1-t)\mathcal{D}(f_2) = -t(1-t)\mathcal{D}(f_1 - f_2).$$

What happens if $f_1 - f_2 > 0$? Is the map $f \mapsto \mathcal{D}(f)$ convex on C_0^∞ ?
5/ Prove that, if $\int_{\mathbb{R}} f = 0$, then $V_f' \in C_0^\infty$, and

$$\mathcal{D}(f) = \int_{\mathbb{R}} |V_f'|^2.$$

Deduce that $f \mapsto \mathcal{D}(f)$ is strictly convex on $C_{00}^\infty := \left\{f \in C_0^\infty, \ \int_{\mathbb{R}} f = 0\right\}$.

Since $f \mapsto \mathcal{D}(f)$ is a positive definite quadratic form on C_{00}^∞, it defines a norm. One can close C_{00}^∞ for this norm to obtain a Banach space $\mathcal{C}$, called the (one-dimensional) Coulomb space. Elements in C_{00}^∞ have null integral. We admit that for $f \in \mathcal{C}$, we have

$$\lim_{x\to\infty} V_f(x) = \frac{1}{2}\int_{\mathbb{R}} f(y)y\mathrm{d}y, \quad \textit{and} \quad \lim_{x\to-\infty} V_f(x) = -\frac{1}{2}\int_{\mathbb{R}} f(y)y\mathrm{d}y.$$

Exercice 2. One dimensional Thomas–Fermi.
Let $p \geq 1$ and let $m \in C_0^\infty(\mathbb{R})$ be a positive charge distribution (fixed once for all). We introduce

$$\mathcal{R} := \left\{\rho \in L^p(\mathbb{R}) \cap L^1(\mathbb{R}), \quad \rho \geq 0, \quad \rho - m \in \mathcal{C}\right\},$$

(in particular, $\int \rho - m = 0$), and, for $\rho \in \mathcal{R}$, we define

$$\mathcal{E}^{\mathrm{TF}}(\rho) := \frac{1}{p}\int_{\mathbb{R}} \rho^p + \frac{1}{2}\mathcal{D}(\rho - m).$$

We admit that $\mathcal{E}^{\mathrm{TF}}(\rho)$ has a minimizer ρ_{TF} in $\mathcal{R}$, and we set $\Phi_{\mathrm{TF}} := V_{\rho_{\mathrm{TF}}-m}$, defined previously. We also admit that Φ_{TF} is continuous, and that Φ_{TF}' goes to 0 at infinity.

1/ For which power p do we have the «kinetic» scaling

$$\int_{\mathbb{R}} \rho_\lambda^p = \lambda^2 \int_{\mathbb{R}} \rho^p, \quad \text{where} \quad \rho_\lambda := \lambda\rho(\lambda x) \qquad ?$$

2/ Prove that $\mathcal{R}$ is a convex set. Deduce that ρ_{TF} is the unique minimizer of $\mathcal{E}^{\mathrm{TF}}$ on $\mathcal{R}$.
3/ Prove that if m is even $m(-x) = m(x)$, then so is ρ_{TF}.
4*/ Prove that there is $\mu \in \mathbb{R}$ so that

$$\forall x \in \mathbb{R}, \quad \rho_{\mathrm{TF}}^{p-1}(x) = (\mu - \Phi_{\mathrm{TF}}(x))_+ .$$

5/ Define $\Omega := \{x \in \mathbb{R},\ \mu - \Phi_{\mathrm{TF}} < 0\}$. Prove that for all $x \in \Omega$, we have $(\mu - \Phi_{\mathrm{TF}})''(x) \leq 0$.
6/ Deduce that $\Phi_{\mathrm{TF}} \leq \mu$ point-wise [1].
7/ Prove that

$$\lim_{x \to +\infty} \Phi_{\mathrm{TF}}(x) = \lim_{x \to -\infty} \Phi_{\mathrm{TF}}(x) = \mu.$$

8/ Deduce that

$$\int_{\mathbb{R}} (\rho_{\mathrm{TF}} - m)(x) \cdot x \mathrm{d}x = 0. \qquad \textit{(we say that the dipolar moment of } m \textit{ is perfectly screened in TF).}$$

Exercice 3. Sommerfeld estimates
We now focus on the Thomas-Fermi equation

$$\rho^{p-1}(x) = (\mu - \Phi(x)), \qquad \Phi''(x) = m(x) - \rho(x).$$

Recall that m is compactly supported, and set $R > 0$ big enough so that $m(x) = 0$ for $|x| > R$.
We admit that $\rho(x_0) > 0$ for some $x_0 > R$, and that $\Phi' \to 0$ at ∞.

1/ Prove that the function $f := (\mu - \Phi)$ satisfies

$$\forall x > R, \quad f''(x) = f^{\frac{1}{(p-1)}}(x).$$

2/ Deduce that

$$\forall x > R, \quad \frac{1}{2}|f'(x)|^2 = \frac{p-1}{p} f^{\frac{p}{p-1}}.$$

3/ Prove that $f'(x) \leq 0$ for $x > R$, and deduce that

$$\forall x > R, \quad f'(x) = -\left(\frac{2(p-1)}{p}\right)^{1/2} f^{\frac{p}{2(p-1)}}(x).$$

4/ Assume $1 < p < 2$. Prove that Cauchy-Lipschitz theorem applies. Deduce that there are constants $c_1 > 0$ and $c_2 > 0$, independent of m, and a constant $x_0 \in \mathbb{R}$ so that

$$\forall x > R, \quad f(x) = \frac{c_1}{(x - x_0)^{\frac{2(p-1)}{2-p}}}, \quad \text{and} \quad \rho(x) = \frac{c_2}{(x - x_0)^{\frac{2}{p-2}}}.$$

5**/ Assume $p > 2$. Prove that f and ρ are compactly supported.

---

1. In the one-dimensional case, μ can be different from 0