Mathematical Quantum Mechanics

TMP Programme, Munich – Winter Term 2010/2011

EXERCISE SHEET 5, issued on Tuesday 23 November 2010
Due: Tuesday 30 November 2010 by 8,15 a.m. in the designated "MQM" box on the 1st floor
Info: `www.math.lmu.de/~michel/WS10_MQM.html`

Each exercise is worth a full mark as specified below. Correct answers without proofs are not accepted. Each step should be justified. You can hand in the solutions either in German or in English. The exercise marked with ★ is for extra credit.

Exercise 17 [10 points]. Let d be a positive integer, let $\alpha > 0$, and define

$$H^\alpha(\mathbb{R}^d) \;:=\; \Big\{ f \in L^2(\mathbb{R}^d) \mid \|f\|^2_{H^\alpha} := \int_{\mathbb{R}^d} \big(1 + (2\pi|k|)^{2\alpha}\big)|\widehat{f}(k)|^2 \,\mathrm{d}k \;<\; \infty \Big\}.$$

By analogy with the proof of the Sobolev inequality for the space $H^1(\mathbb{R}^2)$ (Theorem 12.3 of the handout "*Crash course in Analysis*"), prove that if $d > 2\alpha$ and $p \in [2, \frac{2d}{d-2\alpha})$ then

$$\|f\|_p \;\leqslant\; C\,\|f\|_{H^\alpha} \qquad \forall f \in H^\alpha(\mathbb{R}^d)$$

for some constant C depending on d, p, and α, but independent of f.

Exercise 18 [15 points]. Recall the notation

$$|\alpha| := \alpha_1 + \cdots + \alpha_d\,, \qquad D^\alpha \;:=\; \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1}\cdots \partial x_d^{\alpha_d}}\,, \qquad x^\alpha \;:=\; x_1^{\alpha_1}\cdots x_d^{\alpha_d}$$

for any d-dimensional multi-index $\alpha = (\alpha_1, \dots, \alpha_d)$ ($x = (x_1, \dots, x_d) \in \mathbb{R}^d$). Recall also that for any positive integer k

$$D^k \;:=\; \sum_{\substack{\text{multi-indices } \alpha \\ \text{with } |\alpha| = k}} D^\alpha$$

(In particular, there are $\frac{d(d+1)}{2}$ terms in $D^2 = \sum_{i \leqslant j} \frac{\partial^2}{\partial x_i \partial x_j}$ and only d terms in $\Delta = \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2}$.)

(i) Prove that $\|\nabla f\|_2^2 \leqslant \|\Delta f\|_2 \|f\|_2$ $\forall f \in \mathcal{S}(\mathbb{R}^d)$.

(ii) Prove that $\|D^2 f\|_2 \leqslant \sqrt{\frac{d(d+1)}{2}}\;\|\Delta f\|_2$ $\forall f \in \mathcal{S}(\mathbb{R}^d)$.

(iii) Prove that for any multi-index α there exists a constant $C_{d,|\alpha|}$ such that

$$\|D^{|\alpha|} f\|_2^2 \;\leqslant\; C_{d,|\alpha|}\,\|\Delta^{|\alpha|} f\|_2\,\|f\|_2 \qquad \forall f \in \mathcal{S}(\mathbb{R}^d)\,.$$

(iv) Let $d > 2$, $p \in [2, \frac{2d}{d-2}]$, $a := d(\frac{1}{2} - \frac{1}{p})$. Prove that there exists a constant $C_{d,p}$ such that

$$\|f\|_p \;\leqslant\; C_{d,p}\,\|\nabla f\|_2^a\,\|f\|_2^{1-a} \qquad \forall f \in \mathcal{S}(\mathbb{R}^d)\,.$$

(v) Let $d > 2$, $p \in [2, \frac{2d}{d-2}]$, $b := \frac{d}{2}(\frac{1}{2} - \frac{1}{p})$. Deduce from (i) and (iv) that there exists a constant $C_{d,p}$ such that

$$\|f\|_p \leqslant C_{d,p} \, \|\Delta f\|_2^b \, \|f\|_2^{1-b} \qquad \forall f \in \mathcal{S}(\mathbb{R}^d)\,.$$

Exercise 19 [15 points]. Consider the Hamiltonian of the Helium atom in normalised units, i.e.,

$$H^{\mathrm{He}} \;=\; -\Delta_{x_1} - \Delta_{x_2} - \frac{2}{|x_1|} - \frac{2}{|x_2|} + \frac{1}{|x_1 - x_2|}\,.$$

Note that there are two electrons moving around a nucleus with charge $Z = 2$; H^{He} acts therefore on wave functions $\psi(x_1, x_2)$ with $x_j \in \mathbb{R}^3$, $j = 1, 2$. (Neglect the fact that electrons are fermions: in this case this is justified since we also neglected spins.)

(i) Assume first that the electron-electron interaction is absent, that is, consider $H_0^{\mathrm{He}} := H^{\mathrm{He}} - \frac{1}{|x_1 - x_2|}$. Compute the ground state energy E_0 of H_0^{He}.

(ii) Compute an upper bound E_+ of the ground state energy of H^{He} by means of the trial function that has the same form of the ground state wave function of H_0^{He} but with a generic charge Z to be optimised. (The optimal value $Z = Z_{\mathrm{eff}}$ turns out to be smaller than 2, which accounts for the physical intuition that each electron is effectively subject to a nuclear charge $Z_{\mathrm{eff}} < 2$ due to the "screening effect" of the other.)

(iii) Compute the relative (i.e., percentage) error of the approximate results E_0 and E_+ above with respect to the experimental value for the Helium ground state energy, that in *normalised units* amounts to $E_{\mathrm{exp}} = -1.45$ ($E_{\mathrm{exp}} = -78.8$ eV in *physical units*).

★ **Exercise 20 [15 points].** Consider the three-dimensional system made of two nuclei, both of charge Z, one placed at the origin and one placed at some point at distance R very far away from the origin, and 2 electrons subject to their mutual repulsion and to the attraction of the nuclei. The nuclei are fixed, the repulsion among them is neglected in this problem. Let $\mathcal{E}_{\mathrm{GS}}(R)$ be the ground state energy of such a system. Prove that

$$\lim_{R \to \infty} \mathcal{E}_{\mathrm{GS}}(R) \;=\; -\frac{Z^2}{2}\,.$$

(*Hint:* a good trial function for the upper bound, an IMS-type localisation in both variables for the lower bound, i.e., write $1 = \chi_0^2(x_j) + \chi_R^2(x_j) + \overline{\chi}^2(x_j)$, $j = 1, 2$, for suitable χ_0, χ_R, $\overline{\chi}$.)