## Mathematical Quantum Mechanics

TMP Programme Munich - winter term 2012/2013

## HOMEWORK ASSIGNMENT 06

Hand-in deadline: Tuesday 4 December 2012 by 6 p.m. in the "MQM" drop box.
Rules: Each exercise is worth 10 points. Correct answers without proofs are not accepted. Each step should be justified. You can hand in your solutions in German or in English.
Info: www.math.lmu.de/~michel/WS12_MQM.html

Exercise 21. Let $d \in \mathbb{N}$.
(i) Construct two functions $\chi_{1}, \chi_{2} \in C^{\infty}\left(\mathbb{R}^{d}\right)$ with the following properties $\forall x \in \mathbb{R}^{d}$ : $0 \leqslant \chi_{j}(x) \leqslant 1, j=1,2, \chi_{1}(x)=1$ if $|x| \leqslant 1, \chi_{1}(x)=0$ if $|x| \geqslant 2$, and $\chi_{1}^{2}(x)+\chi_{2}^{2}(x)=1$.
(ii) Let $\left\{\chi_{j}\right\}_{j=1}^{M}(M \in \mathbb{N})$ be a family of bounded functions in $C^{\infty}\left(\mathbb{R}^{d}\right)$ such that $\sum_{j=1}^{M} \chi_{j}^{2}(x)=1$ $\forall x \in \mathbb{R}^{d}$. Prove the following identity of operators on $\mathcal{S}\left(\mathbb{R}^{d}\right)$ :

$$
-\Delta=\sum_{j=1}^{M}\left(\chi_{j}(-\Delta) \chi_{j}-\left|\nabla \chi_{j}\right|^{2}\right)
$$

Exercise 22. Consider the Hamiltonian $H=-\Delta+V$ in $d$ dimensions and its ground state energy

$$
E_{0}=\inf _{\substack{\|\psi\|_{2}=1 \\ \psi \in \mathcal{M}}}\left[\int_{\mathbb{R}^{d}}|\nabla \psi(x)|^{2} \mathrm{~d} x+\int_{\mathbb{R}^{d}} V(x)|\psi(x)|^{2} \mathrm{~d} x\right]
$$

with $\mathcal{M}:=H^{1}\left(\mathbb{R}^{d}\right) \cap\left\{\left.\psi\left|\int V_{-}\right| \psi\right|^{2} \mathrm{~d} x<\infty\right\}$. The potential $V$ is assumed not to vanish almost everywhere.
(i) Let $d \geqslant 3$. Assume that $V \in L^{d / 2}\left(\mathbb{R}^{d}\right)+L^{\infty}\left(\mathbb{R}^{d}\right)$ and $\mid\left\{x \in \mathbb{R}^{d}\right.$ s.t. $\left.|V(x)| \geqslant \varepsilon\right\} \mid<\infty$ $\forall \varepsilon>0$ (no assumption on the sign of $V$ ). $|\Omega|$ denotes the Lebesgue measure of the set $\Omega$. Prove that $E_{0} \leqslant 0$.
(ii) Assume that $V \in L^{1+\varepsilon}\left(\mathbb{R}^{2}\right)+L^{\infty}\left(\mathbb{R}^{2}\right)$ for some $\varepsilon>0$ and that $V(x) \leqslant 0$. Prove that $E_{0}<0$. (Hint: a convenient trial function that involves logarithm.)

Exercise 23. Consider the following two Hamiltonians in three dimensions and the corresponding ground state energies ( $\mathbf{R}$ is a fixed parameter in $\mathbb{R}^{3}$ ):

$$
\left\{\begin{array}{l}
H=-\Delta-\frac{1}{|\mathbf{x}|} \\
E_{\mathrm{GS}}=\inf _{\substack{\psi \in H^{1}\left(\mathbb{R}^{3}\right) \\
\|\psi\|_{2}=1}}\langle\psi, H \psi\rangle
\end{array}, \quad\left\{\begin{array}{l}
H^{(\mathbf{R})}=-\Delta-\frac{1}{|\mathbf{x}|}-\frac{1}{|\mathbf{x}-\mathbf{R}|} \\
E_{\mathrm{GS}}^{(\mathbf{R})}=\inf _{\substack{\psi \in H^{1}\left(\mathbb{R}^{3}\right) \\
\|\psi\|_{2}=1}}\left\langle\psi, H^{(\mathbf{R})} \psi\right\rangle
\end{array} .\right.\right.
$$

(i) Prove that

$$
E_{\mathrm{GS}}^{(\mathbf{R})} \leqslant E_{\mathrm{GS}}-\frac{1}{2} e^{-|\mathbf{R}|} \quad \forall \mathbf{R} \in \mathbb{R}^{3}
$$

(Hint: ground state wave-function of the Hydrogen atom as a trial function.)
(ii) Prove that there exists constants $c, r>0$ such that

$$
E_{\mathrm{GS}}^{(\mathbf{R})} \geqslant E_{\mathrm{GS}}-\frac{c}{|\mathbf{R}|}, \quad|\mathbf{R}| \geqslant r .
$$

(Hint: Exercise 21(ii).)

Exercise 24. Consider the Schrödinger Hamiltonian $H=-\Delta+V$ in $d$ dimensions. Assume that $V(\lambda x)=\frac{1}{\lambda} V(x) \forall \lambda>0$ and $\forall x \in \mathbb{R}^{d}$ (this is the case, for instance, for $\left.V(x)=\frac{c}{|x|}\right)$. Let $\psi \in L^{2}\left(\mathbb{R}^{d}\right),\|\psi\|_{2}=1$, such that $\Delta \psi \in L^{2}\left(\mathbb{R}^{d}\right), V \psi \in L^{2}\left(\mathbb{R}^{d}\right)$, and $H \psi=E \psi$ for some $E \in \mathbb{R}$, the equality being in the sense of $L^{2}$ functions. Prove that

$$
E=-\langle\psi,(-\Delta) \psi\rangle=\frac{1}{2}\langle\psi, V \psi\rangle
$$

and that therefore $E \leqslant 0$.
(Hint: introduce $U_{\lambda}: L^{2}\left(\mathbb{R}^{d}\right) \rightarrow L^{2}\left(\mathbb{R}^{d}\right),\left(U_{\lambda} \phi\right)(\cdot):=\lambda^{-d / 2} \phi(\cdot / \lambda)$ and check that both $U_{\lambda} H \psi$ and $H U_{\lambda} \psi$ belong to $L^{2}\left(\mathbb{R}^{d}\right)$. Use this to compute the expectation of $\left(U_{\lambda} H-H U_{\lambda}\right)$ in the state $\psi$ when $\lambda \rightarrow 1$.)

