HOMEWORK ASSIGNMENT 07–08
Hand-in deadline: Tuesday 18 December 2012 (**TWO WEEKS**) 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 25. Consider the Hamiltonian $H = -\Delta - V$ in three dimensions, where V does not vanish almost everywhere, $V \in L^1_{\mathrm{loc}}(\mathbb{R}^3)$ and $V \geqslant 0$. Assume that some $f \in C^2(\mathbb{R}^3)$, $f \geqslant 0$, satisfies $-\Delta f(\mathbf{x}) - Vf(\mathbf{x}) = 0$ $\forall \mathbf{x} \in \mathbb{R}^3$. Show that either $f(\mathbf{x}) > 0$ $\forall \mathbf{x} \in \mathbb{R}^3$ or $f(\mathbf{x}) = 0$ $\forall \mathbf{x} \in \mathbb{R}^3$.

(*Hint:* prove that $f(\mathbf{x}) \geqslant \frac{1}{4\pi r^2}\int_{|\mathbf{x}-\mathbf{y}|=r} f(\mathbf{y})\mathrm{d}\mathbf{y}$ $\forall \mathbf{x} \in \mathbb{R}^3$.)

Exercise 26. The purpose of this problem is to show that the ground state of a single-well potential has only a single peak.

Consider the Hamiltonian $H = -\dfrac{\mathrm{d}^2}{\mathrm{d}x^2} - V(x)$ on $L^2(\mathbb{R})$, where $V \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R}) \cap C^1(\mathbb{R})$, $V \geqslant 0$, $V'(x) > 0$ $\forall x \in (-\infty, 0)$, $V'(x) < 0$ $\forall x \in (0, +\infty)$.

(i) Prove that H admits a ground state ψ_0 with ground state energy $E_0 < 0$. (Recall that in this case ψ_0 can be assumed to be strictly positive.)

(ii) Prove that ψ_0 has only one local maximum (which then, of course, is global). I.e., show that ψ_0 cannot have a shape of, e.g., two peaks as in Fig (a), the correct behaviour is shown in Fig (b).

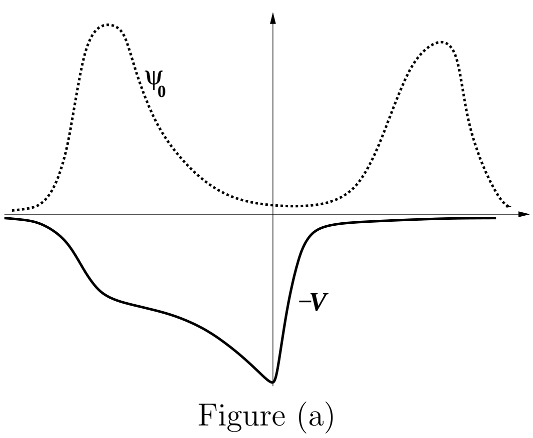

Figure (a)

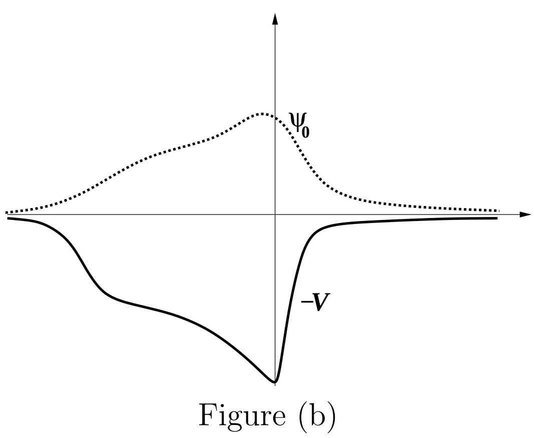

Figure (b)

Exercise 27. Consider the following Hamiltonian for the Helium atom in normalised units:

$$H^{\mathrm{He}} \;=\; -\Delta_{\mathbf{x}_1} - \Delta_{\mathbf{x}_2} - \frac{2}{|\mathbf{x}_1|} - \frac{2}{|\mathbf{x}_2|} + \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} \qquad \text{on } L^2(\mathbb{R}^3 \times \mathbb{R}^3, \mathrm{d}\mathbf{x}_1 \mathrm{d}\mathbf{x}_2)\,.$$

Note that H^{He} describes two *spinless* electrons moving around a nucleus with charge $Z = 2$. Further simplification: we shall *not* restrict H^{He} to fermionic wave-functions only.

(i) Assume first that the electron-electron interaction is absent, that is, consider $H_0^{\mathrm{He}} := H^{\mathrm{He}} - \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|}$. 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 28. Consider two families $\{\phi_j\}_{j=1}^N$ and $\{\psi_\ell\}_{\ell=1}^N$ of functions in $L^2(\mathbb{R}^d)$ $(d, N \in \mathbb{N})$.

(i) Prove that $\langle \phi_1 \wedge \cdots \wedge \phi_N, \psi_1 \wedge \cdots \wedge \psi_N \rangle_{L^2(\mathbb{R}^{Nd})} \;=\; \det \begin{pmatrix} \langle \phi_1, \psi_1 \rangle & \cdots & \langle \phi_1, \psi_N \rangle \\ \vdots & \ddots & \vdots \\ \langle \phi_N, \psi_1 \rangle & \cdots & \langle \phi_N, \psi_N \rangle \end{pmatrix}.$

(ii) Let A be a $N \times N$ matrix with complex entries. Define the functions

$$\xi_i \;:=\; \sum_{j=1}^{N} A_{ij} \psi_j\,, \qquad i = 1, 2, \ldots, N\,.$$

Prove that

$$\xi_1 \wedge \cdots \wedge \xi_N \;=\; (\det A)\, \psi_1 \wedge \cdots \wedge \psi_N\,.$$