Advanced Mathematical Quantum Mechanics

Mathematisches Institut der LMU – SS2009
Prof. Dr. L. Erdős, Dr. A. Michelangeli

Individual project no. 3: Instability of an atom with sufficiently many electrons

- ✓ Work out individually the details of the problem outlined in the scheme below.
- ✓ Results and techniques discussed in the class as well as in the tutorial sessions and in the weekly homeworks will be needed.
- ✓ Questions, info, further clarifications: Alessandro, usual times and places.
- ✓ Please return your completed project by July, Wednesday 22.

Consider the Hamiltonian of a three-dimensional atom with nucleus charge Z and with N electrons

$$H_{N,Z} \;=\; \sum_{j=1}^{N}\Big(-\Delta_{x_j}-\frac{Z}{|x_j|}\Big)+\sum_{1\leqslant j<k\leqslant N}\frac{1}{|x_j-x_k|}$$

where $x_1,\dots,x_N\in\mathbb{R}^3$, N,Z integers, $Z\geqslant 1$. By physical reasoning one would expect that the nucleus can bind only a limited number of electrons, because at some point the attraction of the nucleus should be dominated by the mutual repulsion of the electrons. The goal of this problem is to prove this expectation in the following form.

Theorem. *Consider $H_{N,Z}$ above as an operator on $\bigwedge^N L^2(\mathbb{R}^3)$. Let $E(N,Z):=\inf\sigma(H_{N,Z})$. For any positive integer Z there exists an integer $N_{\max}(Z)\leqslant 2Z$ such that*

$$E(N+1,Z) \;=\; E(N,Z) \qquad (\blacklozenge)$$

for every $N\geqslant N_{\max}(Z)$.

Remarks.

1. When $H_{N+1,Z}$ is defined as an operator on $\bigwedge^N L^2(\mathbb{R}^3)$, the following spectral property holds (assume it without proof):

$$\sigma_{\mathrm{ess}}(H_{N+1,Z}) \;=\; [E(N,Z),+\infty) \tag{1}$$

for any integers $Z\geqslant 1$ and $N\geqslant 0$. Then, in particular,

$$E(N+1,Z) \;\leqslant\; E(N,Z) \tag{2}$$

and $(\blacklozenge)$ translates indeed the instability of the atom.

2. Notice that the estimate $N_{\max}(Z) \leqslant 2Z$ given by the Theorem is still off by a factor of 2 with respect to the physically natural behaviour $N_{\max}(Z) \sim Z$. At least for large Z's this can be proved as well, but the proof requires a different strategy than the one suggested here below. Instead, the true ionisation conjecture is still a major open problem.

Hints.

- Show that remark 1 implies that if $E(N,Z) < E(N-1,Z)$ then $H_{N,Z}$ has an isolated eigenvalue at the bottom of its spectrum. Call Ψ the corresponding ground state. Use (without proof) that
  - $\rightarrow$ $\Psi(x_1,\dots,x_N)$ decays fast at infinity so that $x_j\Psi \in L^2(\mathbb{R}^{3N})$
  - $\rightarrow$ $\Psi(x_1,\dots,x_N)$ may be assumed to be real.
- Exploit the identity $0 = \big\langle\, |x_1|\Psi\,,\big(H_{N,Z} - E(N,Z)\big)\Psi\,\big\rangle$ by estimating conveniently the r.h.s. from below, i.e., expanding the r.h.s. in a number of terms and neglecting some of the positive ones. A convenient expansion is to write $H_{N,Z}$ in terms of $H_{N-1,Z}$ (the Hamiltonian of electrons $2,\dots,N$) and $H_{1,Z}$ (the Hamiltonian of electron 1).
- You will need to show that the term $\langle\,|x_1|\Psi\,,(-\Delta_{x_1})\Psi\rangle$ has a definite sign. To this aim, use the fact that Ψ is real-valued and prove and use the *operator identity*

$$\frac{1}{2}\Big(p^2|x| + |x|p^2\Big) \;=\; |x|\,p\,\frac{1}{|x|}\,p\,|x| \tag{3}$$

  ($p = -i\nabla_x$) on $H^2(\mathbb{R}^3) \cap \{\Phi \in L^2(\mathbb{R}^3) : x\Phi \in L^2(\mathbb{R}^3)\}$. For this project it is enough that you prove (3) at least on a formal level, i.e., manipulating the operators p, $|x|$, and $|x|^{-1}$ irrespectively of their domains in $L^2(\mathbb{R}^3)$.