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Mathematical Methods in Quantum Mechanics I

13th Exercise Sheet

Exercise 44:
Let A be a self-adjoint operator on $\mathcal{H}$. Then, $A = U^{-1}T_fU$ (see Theorem 9.1). We define $\phi(h) = U^{-1}T_{h(f)}U$, for any h bounded and Borel function. Prove that ϕ satisfies the properties of Theorem 9.2.

Exercise 45:
1) Let $f \in H^s(\mathbb{R}^d)$ where $s > \frac{d}{2}$. Using the inverse Fourier transform, Cauchy-Schwarz inequality and the Dominated convergence Theorem, show that f is a continuous and bounded function.

2) Consider $f \in H^2(\mathbb{R}^3)$ and assume that $g(x) = |x|f(x) \in H^1(\mathbb{R}^3)$. Using partial integration show

$$-Re\int_{\mathbb{R}^3} \bar{g}(x)\Delta\Big[g(x)\frac{1}{|x|}\Big]dx = \int_{\mathbb{R}^3}\frac{1}{|x|}|\nabla g(x)|^2dx - \frac{1}{2}\int_{\mathbb{R}^3}|g(x)|^2\Delta\frac{1}{|x|}dx.$$

Finally, using the above equality and the fact that $\Delta\frac{1}{|x|} = -C\delta$ in the sense of distributions prove that

$$Re\langle |x|f, -\Delta f\rangle \geq 0.$$

Exercise 46:
The purpose of this exercise is to present Lieb's estimate on maximum ionization. That is, to estimate the maximum number of electrons that a nucleus can bind. To this direction, consider the Hamiltonian

$$H_{N,Z} = \sum_{i=1}^{N}\Big(-\frac{1}{2}\Delta_i - \frac{Z}{|x_i|}\Big) + \sum_{1\leq i<j\leq N}\frac{1}{|x_i - x_j|}$$

and assume that

$$E(N,Z) := \inf_{\|\psi\|=1}\langle\psi, H_{N,Z}\psi\rangle$$

is an eigenvalue of $H_{N,Z}$ with corresponding normalized eigenfunction $\psi_{N,Z}$. If the binding condition $E(N,Z) < E(N-1,Z)$ holds, then

$$N < 2Z + 1.$$

The proof follows from the steps:

1. Start with the Schrödinger equation

$$(H_{N,Z} - E(N,Z))\psi_{N,Z} = 0,$$

   multiply by $|x_N|\psi_{N,Z}$ to arrive at

$$\langle |x_N|\psi_{N,Z}, (H_{N,Z} - E(N,Z))\psi_{N,Z}\rangle = 0$$

— **Turn the page!** —

and split the Hamiltonian into a system with $N-1$ electrons and contributions from the Nth electron:

$$H_{N,Z} = H_{N-1,Z} - \frac{1}{2}\Delta_N + \Big[- \frac{Z}{|x_N|} + \sum_{j=1}^{N-1} \frac{1}{|x_j - x_N|} \Big].$$

Hence, we obtain three terms that sum up to zero.

2. Use the fact that $H_{N,Z}$ does not act on the variable x_N and that $E(N-1,Z) \geq E(N,Z)$ to estimate the first term

$$\langle |x_N| \psi_{N,Z}, (H_{N-1,Z} - E(N,Z))\psi_{N,Z} \rangle$$

from below and obtain that it is non-negative.

3. For the second term

$$\frac{1}{2} \, \langle |x_N| \psi_{N,Z}, -\Delta_N \psi_{N,Z} \rangle$$

notice that $\psi_{N,Z}$ is an eigenfunction and use Exercise 45 to conclude that also this term is non-negative.

4. For the last term

$$\Big\langle \psi_{N,Z}, \Big[- Z + \sum_{j=1}^{N-1} \frac{|x_N|}{|x_j - x_N|} \Big] \psi_{N,Z} \Big\rangle$$

observe that assuming and using the symmetry of $|\psi_{N,Z}|^2$ (that is for all $\sigma \in S_N$, the symmetric group of N elements, $|\psi(x_1, \ldots, x_N)|^2 = |\psi(x_{\sigma(1)}, \ldots, x_{\sigma(N)})|^2$) we have an invariance under exchanging x_N with any other variable x_j, $j \neq i$, and thus, we may rewrite the last expression as

$$\Big\langle \psi_{N,Z}, \Big[- Z + \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq i} \frac{|x_i|}{|x_j - x_i|} \Big] \psi_{N,Z} \Big\rangle.$$

Conclude the argument by showing that the condition for this last term to be non-positive implies that

$$N < 2Z + 1.$$