Advanced Mathematical Quantum Mechanics – Homework 5

Mathematisches Institut der LMU – SS2009
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Exercise 5.1. (*Instability of matter for Bosons*). Consider the standard three-dimensional many-body non-relativistic spinless molecular Hamiltonian H with M nuclei and N electrons. Assume for simplicity that each nucleus has the same positive charge Z. The goal of this exercise is to prove that there exists a (normalised) many-body wave function Ψ_N of N boson coordinates and there exists a choice of positions $(R_1, \dots, R_M)$ of the nuclei such that

$$\langle \Psi_N, H\Psi_N \rangle \leqslant -C\alpha^2 Z^{4/3} \min\{N, ZM\}^{5/3} \tag{1}$$

for some constant $C > 0$. This shows that non-relativistic matter made out of bosons is unstable of the second kind.

(*a*) Introduce the bosonic trial function $\Psi_N(x_1, \dots, x_N) := \prod_{i=1}^N \phi_\lambda(x_i)$ with some one-body wave function $\phi_\lambda(x) := \lambda^{3/2}\phi(\lambda x)$ and some scaling parameter $\lambda > 0$ to be optimised later. Assume that the unscaled ϕ is a normalised ($\|\phi\|_2 = 1$) smooth and compactly supported function. Prove by direct computation that

$$\begin{aligned}\langle \Psi_N, H\Psi_N \rangle \;=\; N\lambda^2 \int_{\mathbb{R}^3} |\nabla\phi(x)|^2 \mathrm{d}x \;+\; \lambda\alpha \Bigg\{ \frac{N(N-1)}{2} \iint_{\mathbb{R}^2\times\mathbb{R}^3} \frac{|\phi(x)|^2|\phi(y)|^2}{|x-y|} \mathrm{d}x\,\mathrm{d}y \\ -\; ZN \sum_{k=1}^M \int_{\mathbb{R}^3} \frac{|\phi(x)|^2}{|x-R_k|} \mathrm{d}x + U(\underline{R}) \Bigg\} .\end{aligned} \tag{2}$$

(*b*) Let $W_{N,\underline{R}} := \{\cdots\}$ the potential term in (2). Show that if there exists an $\underline{R}$ such that

$$W_{N,\underline{R}} \leqslant -CZ^{2/3}N^{4/3} \tag{3}$$

for some constant $C > 0$ then by optimising on λ in (2) one gets the desired bound (1).

(*c*) In order to obtain (3), divide the support of ϕ in M cells $\Gamma_1, \dots, \Gamma_M \subset \mathbb{R}^3$ in such a way that $\int_{\Gamma_k} |\phi(x)|^2 \mathrm{d}x = \frac{1}{M}$. Place one nucleus in each cell Γ_k, and in the expression (2) for $W_{N,\underline{R}}$ average each nuclear coordinate R_k with respect to the weight $M|\phi(x)|^2$, restricted to Γ_k. The quantity you get this way is certainly above $W_{N,\underline{R}}$ for some choice of $\underline{R}$ because an average is never less than the minimum. Under the assumption $N = ZM$, show that you can drop a number of negative terms in the estimate of $W_{N,\underline{R}}$ from above so to obtain

$$W_{N,\underline{R}} \leqslant -\frac{1}{2}Z^2M^2 \sum_{k=1}^M \iint_{\Gamma_k\times\Gamma_k} \frac{|\phi(x)|^2|\phi(y)|^2}{|x-y|} \mathrm{d}x\,\mathrm{d}y\,. \tag{4}$$

(*d*) In order to estimate $\frac{1}{2}\iint_{\Gamma_k\times\Gamma_k}\frac{|\phi(x)|^2|\phi(y)|^2}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y$ from below, observe that this quantity is certainly larger than the smallest possible self-energy of a charge distribution of total charge $1/M$ confined to the smallest ball containing Γ_k (denote by r_k its radius). Thus, prove that

$$\frac{1}{2}Z^2M^2\sum_{k=1}^{M}\iint_{\Gamma_k\times\Gamma_k}\frac{|\phi(x)|^2|\phi(y)|^2}{|x-y|}\mathrm{d}x\,\mathrm{d}y \;\geqslant\; \frac{1}{2}Z^2\sum_{k=1}^{M}\frac{1}{r_k}\,. \tag{5}$$

(*e*) Use Jensen's inequality in the r.h.s. of (5) and show that (3) reads

$$W_{N,\underline{R}} \;\leqslant\; -\frac{1}{2}Z^2M\frac{1}{\frac{1}{M}\sum_{k=1}^{M}r_k}\,. \tag{6}$$

(*f*) You are then left with estimating $\frac{1}{M}\sum_{k=1}^{M}r_k$, the mean value of the radius of the smallest ball containing Γ_k. Show that the freedom that you still have in choosing the decomposition of the support of ϕ into the Γ_k's with the constraint $\int_{\Gamma_k}|\phi(x)|^2\mathrm{d}x=\frac{1}{M}$ allows you to organise the cells so that

$$\frac{1}{M}\sum_{k=1}^{M}r_k \;\leqslant\; C\frac{1}{M^{1/3}}\,. \tag{7}$$

Conclude the proof, showing that (6) and (7) yield the desired bound (3).

Exercise 5.2. (*Instability of relativistic matter for large α*) Consider the standard three-dimensional many-body pseudo-relativistic spinless molecular Hamiltonian H with M nuclei and N electrons. Assume for simplicity that each nucleus has the same positive charge Z. The goal of this exercise is to prove that there exists a constant $D<128/(15\pi)$ such that if $\alpha>D$ then the system is unstable of the first kind for N and M large enough.

(*a*) Show by a scaling argument that to prove instability it suffices merely to show that the energy can be made negative.

(*b*) To this aim, pick $\phi\in H^{1/2}(\mathbb{R}^3)$ with $\|\phi\|_2=1$. Let $N=1$ and compute the expectation value $\langle\phi,H\phi\rangle$ in terms of $\alpha,Z,\underline{R}$.

(*c*) For an upper bound on $\langle\phi,H\phi\rangle$, average it over the nuclear positions, with weight given by $\prod_{k=1}^{M}|\phi(R_k)|^2$ and show that

$$\langle\phi,H\phi\rangle \;\leqslant\; \langle\phi,|p|\phi\rangle \;-\; \Big(Z\alpha M-\frac{1}{2}Z^2\alpha M(M-1)\Big)\underbrace{\iint_{\mathbb{R}^2\times\mathbb{R}^3}\frac{|\phi(x)|^2|\phi(y)|^2}{|x-y|}\mathrm{d}x\,\mathrm{d}y}_{=:\mathcal{I}}\,. \tag{8}$$

(*d*) Show that for a given value of Z you can choose M so that the above bound reads

$$\langle\phi,H\phi\rangle \;\leqslant\; \langle\phi,|p|\phi\rangle \;-\frac{1}{2}\,\alpha\,\mathcal{I} \tag{9}$$

(*e*) Complete the proof of the main statement by plugging the trial function $\phi(x)=\frac{1}{\sqrt{\pi}}e^{-|x|}$ in.