Advanced Mathematical Quantum Mechanics – Homework 4

Mathematatisches Institut der LMU – SS2009
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Exercise 4.1. (*Asymptotics of Thomas-Fermi density in the neutral case*). Consider the Thomas-Fermi equation $\gamma\rho^{2/3}(x) = [\phi_\rho(x) - \mu]_+$, $\phi_\rho(x) = -V(x) - (\frac{1}{|x|} * \rho)(x)$, with all the usual notation. Consider the *neutral case* $\mu = 0$: let ρ be a solution and ϕ be the corresponding ϕ_ρ.

(a) Take the distributional Laplacian in the TF equation and write the TF "*differential* equation" thus obtained. Note that the latter involves ϕ only. Check that the function $\psi(x) := \gamma^3(\frac{3}{\pi})^2|x|^{-4}$ solves the TF differential equation for $|x| > 0$ and away from the R_j's. Check also that it is the only power-law function that does so. (This was first noted by Sommerfeld, who thus argued heuristically that $\psi(x)$ gives the asymptotics of $\phi(x)$, and consequently the asymptotics $|x|^{-6}$ of $\rho(x)$.)

Here the goal is to prove rigorously that $\phi(x) \approx \psi(x)$ as $|x| \to \infty$. So let $R > 0$ be larger than the distance of any nucleus from the origin and consider $|x| \geqslant R$. To conveniently estimate the ratio ϕ/ψ from above and below and prove that *this ratio converges to 1*, define $\phi_\pm(r)$ to be the max (the min) of $\phi(x)$ on $|x| = r$ and $C_\pm(r) := \phi_\pm(r)/\psi(r)$.

(b) By comparing the functions $\gamma^{-3}\phi(x)$, $\gamma^{-3}\psi(x)$, and $\gamma^{-3}C_\pm(R)\psi(x)$ and by means of the "maximum principle argument" proved in Exercise 2.2, prove that (for all $|x| \geqslant R$)

- $C_+(R) \geqslant 1 \;\Rightarrow\; C_+(r) \leqslant C_+(R)\,, \qquad C_+(R) \leqslant 1 \;\Rightarrow\; C_+(r) \leqslant 1$
- $C_-(R) \leqslant 1 \;\Rightarrow\; C_-(r) \geqslant C_-(R)\,, \qquad C_-(R) \geqslant 1 \;\Rightarrow\; C_-(r) \geqslant 1.$

(c) Prove that $C_\pm(r)$ is continuous. Check that proving $\limsup C_+(r) \leqslant 1$ and $\liminf C_-(r) \geqslant 1$ leads to $C_\pm(r) \to 1$ as $r = |x| \to \infty$. Show in detail that $\limsup C_+(r) \leqslant 1$ follows trivially unless when $C_+(R) > 1$ and $C_+(r) > 1$ $\forall r \geqslant R$. If this is the case, prove that $C_+(r)$ is non increasing and the limit $C_+(\infty) := \lim_{r\to\infty} C_+(r)$ exists and $C_+(\infty) \geqslant 1$.

(d) It remains to investigate the case $C_+(R) > 1$, $C_+(r) > 1$ $\forall r \geqslant R$, $C_+(\infty) > 1$. To this aim, consider the sphere $|x| = R_1 > R$ for some arbitrarily large R_1. On this sphere compare the function ϕ with some $\widetilde{\psi}$ which is slightly larger than ψ on $|x| = R_1$, e.g., $\widetilde{\psi}(x) := \gamma^3(\frac{3}{\pi})^2(|x| - bR_1)^{-4}$ for some $0 < b < 1$ to be fixed conveniently. Show that it is possible to choose b so that $\phi(x) \leqslant \widetilde{\psi}(x)$ on $|x| = R_1$. Then show that one can apply the same "maximum principle argument" as in (b) to deduce that $\phi(x) \leqslant \widetilde{\psi}(x)$ on $|x| \geqslant R_1$ and, consequently, that $C_+(\infty) \leqslant 1$. Hence necessarily $C_+(\infty) = 1$. This, together with the other possible cases, yields the conclusion $\limsup C_+(r) \leqslant 1$.

(e) Revert inequalities and signs in the argument in (c) and (d) so to have $\liminf C_-(r) \geqslant 1$.

Exercise 4.2. Consider the Thomas-Fermi density ρ in the "*atomic case*". Prove that ρ is a *symmetric and decreasing* function. (*Hint:* one possible way is to evaluate the TF energy functional in the density ρ^* given by the symmetric decreasing rearrangement of ρ and to check term by term that $\mathcal{E}^{\mathrm{TF}}(\rho^*) \leqslant \mathcal{E}^{\mathrm{TF}}(\rho)$, thereby proving the statement.) Which of the two desired properties of ρ can be derived from the uniqueness of ρ? And which of the two properties can be derived from the Newton's theorem?