Stability for relativistic systems; putting everything together

In this section we prove the our final result about relativistic stability. Recall that our functional is of the form

$$\mathcal{E}(\rho) = \beta(\sqrt{\rho}, \sqrt{-\Delta}\sqrt{\rho}) + \frac{3}{4}\gamma \int \rho^{4/3}(x)dx$$

$$+\alpha \left[-Z \sum_k \int \frac{\rho(x)}{|x-R_k|}dx + D(\rho,\rho) + Z^2 \sum_{k<l} \frac{1}{|R_k - R_l|} \right] .$$

We prove

Theorem 1 *The functional $\mathcal{E}$ is stable if $\beta \geq \pi Z\alpha/2$ and $\gamma \geq 4.8158 Z^{2/3}\alpha$.*

PROOF: Set $\beta = \pi Z\alpha/2$ and'pull the Coulomb tooth' (see section 15) to find that

$$\mathcal{E}(\rho) \geq \frac{3}{4}\gamma \int \rho^{4/3}(x)dx +$$

$$\alpha \left[- \int \rho(x)U(x)dx + D(\rho,\rho) + Z^2 \sum_{k<l} \frac{1}{|R_k - R_l|} \right] . \tag{1}$$

where

$$U(x) = Z \sum_k \frac{1}{|x-R_k|}(1-\chi_{B_k}) + \frac{\pi}{2}\chi_{B_k}\frac{1}{D_k}Y(\frac{|x-R_k|}{D_k}) .$$

Recall that

$$\Phi(x) = Z \sum_k \frac{1}{|x-R_k|} - \frac{Z}{\delta(x)}$$

which takes the value

$$Z \sum_{k \neq j} \frac{1}{|x-R_k|}$$

in the Voronoi cell Γ_j. Now we split $U(x)$ as

$$U(x) = [U(x) - \Phi(x)] + \Phi(x)$$

and the lower bound (1) takes the form

$$\mathcal{E}_1(\rho) + \alpha\mathcal{E}_2(\rho)$$

where

$$\mathcal{E}_1(\rho) = \frac{3}{4}\gamma \int \rho^{4/3}(x)dx - Z\alpha \int \rho(x)[U(x) - \Phi(x)]dx$$

and

$$\mathcal{E}_2(\rho) = D(\rho,\rho) - \int \Phi(x)\rho(x)dx + Z^2 \sum_{k<l} \frac{1}{|R_k - R_l|} .$$

The second functional is bounded below by

$$\frac{Z^2}{8}\sum_k \frac{1}{D_k}$$

by the electrostatic inequality in section 16. The first term we bound using Hölder's inequality by

$$\frac{3}{4}\gamma\|\rho\|_{4/3}^{4/3} - Z\alpha\|\rho\|_{4/3}\|U-\Phi\|_4$$

and optimizing over $X = \|\rho\|_{4/3}$ yields

$$-\frac{(Z\alpha)^4}{4\gamma^3}\int [U(x)-\Phi(x)]^4 dx$$

$$= -\frac{(Z\alpha)^4}{4\gamma^3}\sum_k (\frac{\pi}{2})^4 \int_{B_k} D_k^{-4} Y(\frac{|x-R_k|}{D_k})^4 dx + \int_{\Gamma_k - B_k} \frac{1}{|x-R_k|^4} dx \ .$$

Since the Voronoi cell Γ_k lies on one side of the mid plane defined by the nearest neighbor nucleus we get an upper bound on the last term by integrating over the outside of the ball B_k and then subtract the integral of the half space whose z-coordinate is greater or equals D_k. Thus

$$\int_{\Gamma_k - B_k} \frac{1}{|x-R_k|^4} dx \le \frac{4\pi}{D_k} - -\frac{1}{D_k}\int_1^\infty dz \int_0^\infty \frac{2\pi r}{(r^2+z^2)^2} dr = \frac{3\pi}{D_k} \ .$$

Hence we get that

$$\mathcal{E}_1(\rho) \ge -\frac{(Z\alpha)^4}{4\gamma^3}\left[(\frac{\pi}{2})^4 4\pi \int_0^1 Y(r)^4 r^2 dr + 3\pi\right]\sum_k \frac{1}{D_k}$$

$$= -\frac{(Z\alpha)^4}{4\gamma^3}\left[7.6245(\frac{\pi}{2})^4 + 3\pi\right]\sum_k \frac{1}{D_k}$$

Adding the bounds yields in total

$$\mathcal{E}(\rho) \ge \left[-\frac{(Z\alpha)^4}{4\gamma^3}\left[7.6245(\frac{\pi}{2})^4 + 3\pi\right] + \alpha\frac{Z^2}{8}\right]\sum_k \frac{1}{D_k}$$

and the condition on γ stated in the theorem yields the result. Next we apply this theorem to the full problem. We recall that

$$\beta = \frac{\pi}{2} Z\alpha$$

and

$$\gamma = \frac{4}{3}\left[1.63 q^{-1/3}(1-\frac{\pi}{2}Z\alpha) - 1.68\alpha\right]$$

which yields stability provided that

$$\frac{\pi}{2}Z + 2.2159q^{1/3}Z^{2/3} + 1.0307q^{1/3} \leq \frac{1}{\alpha} \ .$$

To summarize, we have proved the following theorem.

Theorem 2: *For all antisymmetric, normalized wave functions* Ψ *associated with particles having* q *spin states*

$$\sum_{j=1}^{N}(\Psi, \sqrt{-\Delta}\Psi) + \alpha(\Psi, V_c\Psi) \geq 0$$

provided that

$$\frac{\pi}{2}Z + 2.2159q^{1/3}Z^{2/3} + 1.0307q^{1/3} \leq \frac{1}{\alpha} \ .$$

This is one of the main theorems in this whole field of research. As an elementary application we use this theorem to prove stability of matter for non-relativistic systems.

PROOF: Note that by Schwarz's inequality

$$(\Psi, \sqrt{-\Delta}\Psi) \leq \|\Psi\|(\Psi, -\Delta\Psi)^{1/2} \ .$$

Hence, since Ψ is normalized

$$N^{1/2}\left[\sum_{j=1}^{N}(\Psi, -\Delta\Psi)\right]^{1/2} \geq \sum_{j=1}^{N}(\Psi, -\Delta\Psi)^{1/2} \geq \sum_{j=1}^{N}(\Psi, \sqrt{-\Delta}\Psi)$$

From this we get that for any $a > 0$

$$\sum_{j=1}^{N}(\Psi, -\Delta\Psi) \geq \frac{2}{a}\sum_{j=1}^{N}(\Psi, \sqrt{-\Delta}\Psi) - N\frac{1}{a^2} \ .$$

Thus,

$$\sum_{j=1}^{N}(\Psi, -\Delta\Psi) + (\Psi, V_c\Psi) \geq \frac{2}{a}\sum_{j=1}^{N}(\Psi, \sqrt{-\Delta}\Psi) + (\Psi, V_c\Psi) - N\frac{1}{a^2}$$

$$\geq -\frac{N}{a^2}$$

provided that a is chosen such that

$$\frac{\pi}{2}Z + 2.2159q^{1/3}Z^{2/3} + 1.0307q^{1/3} \leq \frac{2}{a} \ .$$

For $Z = 1$ and $q = 2$ we choose

$$\frac{2}{a} = 5.6611$$

and the lower bound

$$-8.012N \ .$$

Note that the bound depends only on N and not on K. Further, if we go back to the Lieb-Thirring result and take neutral hydrogen, i.e., $Z = 1$ and $N = K$ even the constants are comparable.