7. Stability of Non-Relativistic Matter

$$H = \frac{1}{2}\sum_{j=1}^{N}\left(-i\nabla_j + \sqrt{\alpha}A(x_j)\right)^2 + \alpha V_c(X,R)$$

$$V_c(X,R) = \sum_{1\le i<j\le N}\frac{1}{|x_i-x_j|} - \sum_{i=1}^{N}\sum_{j=1}^{M}\frac{Z_j}{|x_i-R_j|} + \sum_{1\le k<l\le M}\frac{Z_k Z_l}{|R_k-R_l|}$$

Th. 7.1

$$Z = \max_j\{Z_j\}$$

$$\psi \in \Lambda^N L^2(\mathbb{R}^3;\mathbb{C}^q)$$

$$(\psi,\psi) = 1$$

$$\Longrightarrow (\psi, H\psi) \ge -0.231\,\alpha^2 q^{\frac{2}{3}} N\left(1+2.16Z\left(\frac{M}{N}\right)^{\frac{1}{3}}\right)^2$$

Rem. $N\left(1+cZ\left(\frac{M}{N}\right)^{\frac{1}{3}}\right)^2$

$$= N + 2cZN^{\frac{2}{3}}M^{\frac{1}{3}} + c^2Z^2N^{\frac{1}{3}}M^{\frac{2}{3}}$$

$$N^{\frac{2}{3}}M^{\frac{1}{3}} \le N+M \quad (*)$$

$$\le (1+cZ)^2(N+M)$$

(*) $n^3+m^3-n^2m$

$= (n+m)^3 - 3nm(n+m) - n^2m$

$\ge \quad -4nm(n+m)$

$= (n+m)\{\underbrace{(n+m)^2-4nm}_{(n-m)^2}\} \ge 0$ //

Rem. "not optimal"

depends only on M for $M \ll N$

N $\quad N \ll M$

$\nwarrow$ rel. effect in Ch. 8

$$N \le \sum_{j=1}^{M} (2Z_j+1)q \le (2Z+1)M$$

cf. $N \geq (2Z+1)M$

Rem. neutral hydrogen ($Z=1$, $M=N$, $q=2$)

7.29 Ry./nucleus

$\because)$ $-0.231\,\alpha^2\, 2^{\frac{2}{3}} M (1+2.16)^2$

$= -7.29 \cancel{M} \frac{\alpha^2}{2}$

$K = K^{cl} = \frac{3}{5}(6\pi^2)^{\frac{2}{3}}$

$\Longrightarrow$ 4.90 Ry./M

pf.

$$Z_j = Z \quad (j = 1, \dots, M)$$

$$\rho_\psi(x) = \sum_{i=1}^{N} \rho_\psi^{i}(x)$$

$$\rho_\psi^{i}(x) = \int_{\mathbb{R}^{3(N-1)}} |\psi(x_1, \dots, x_{i-1}, \overset{i}{x}, x_{i+1}, \dots, x_N)|^2 \, dx_1 \cdots \widehat{dx_i} \cdots dx_N$$

Cor. 4.1 with $\|\gamma_\psi^{(1)}\|_\infty = q$

$$\gamma_\psi^{(1)}(x, x') = \sum_{\sigma=1}^{q} \gamma^1(x\sigma; x'\sigma)$$

(p.71)

$$\Longrightarrow \frac{1}{2}\Big(\psi, \sum_j (-i\nabla_j + \sqrt{\alpha} A(x_j))^2 \psi\Big)$$

$$\geq \frac{K}{2} q^{-\frac{2}{3}} \int_{\mathbb{R}^3} \rho_\psi(x)^{\frac{5}{3}} \, dx$$

$$K \geq \left(\frac{3}{\pi^2}\right)^{\frac{1}{3}} K^{cl} = \frac{9}{5}(4\pi^2)^{\frac{1}{3}}$$

$$\approx 6.129$$

Th. 6.1 with $\sum_{i=1}^{N} \underbrace{e_i}_{1} Q_i(x) = Q(x)$

$$\Longrightarrow \Big(\psi, \sum_{i<j} \frac{1}{|x_i - x_j|} \psi\Big)$$

$$\geq D(\rho_\psi, \rho_\psi) - 1.68 \int_{\mathbb{R}^3} \rho_\psi(x)^{\frac{4}{3}} \, dx$$

$$\left(\psi, \sum_i \sum_k \frac{Z}{|x_i - R_k|} \psi\right) = \sum_k \int_{\mathbb{R}^3} \frac{Z}{|x - R_k|} \rho_\psi(x)\, dx$$

$$\because) \quad \sum_i \left(\psi, \frac{Z}{|x_i - R_k|} \psi\right)$$

$$= \sum_i \int_{\mathbb{R}^{3N}} \overline{\psi(\underline{X})} \cdot \frac{Z}{|x_i - R_k|} \psi(\underline{X})\, d\underline{X} \quad \rho_\psi^i = \int \overline{\psi}\psi$$

$$= \sum_i \int_{\mathbb{R}^3} \frac{Z}{|\cancel{x_i}_{x} - R_k|} \rho_\psi^{\cancel{i}}(\cancel{x_i}_{x})\, d\cancel{x_i}_{x}$$

$$= \int_{\mathbb{R}^3} \frac{Z}{|x - R_k|} \rho_\psi(x)\, dx \;//$$

$$(\psi, V_c \psi) \geq D(\rho_\psi, \rho_\psi) - \sum_k \int_{\mathbb{R}^3} \frac{Z}{|x - R_k|} \rho_\psi(x)\, dx$$

$$+ U(R) - 1.68 \int_{\mathbb{R}^3} \rho_\psi(x)^{\frac{4}{3}}\, dx$$

$$\therefore \quad (\psi, H\psi)$$

$$= \frac{K}{2} q^{-\frac{2}{3}} \int_{\mathbb{R}^3} \rho(x)^{\frac{5}{3}}\, dx + \alpha D(\rho, \rho) + \alpha U(R)$$

$$- \sum_k \int_{\mathbb{R}^3} \frac{Z\alpha}{|x - R_k|} \rho(x)\, dx \underbrace{- 1.68\alpha \int_{\mathbb{R}^3} \rho(x)^{\frac{4}{3}}\, dx}_{\text{Dirac}}$$

$$=: \mathcal{E}^{\mathrm{TFD}}(\rho)$$

under $\int \rho(x)\, dx = N.$

Th. 5.3

$$D(\rho_\psi, \rho_\psi) - \int \Phi(x) \rho_\psi(x)\, dx + U(\underline{R}) \geq \frac{1}{8} \sum_j \frac{Z^2}{D_j}$$

$$\int \Phi(x)\rho_\psi(x)\,dx = \sum_k \int \frac{Z}{|x-R_k|}\rho_\psi(x)\,dx - \int \frac{Z}{D(x)}\rho_\psi(x)\,dx$$

$$D(x) := \min_k |x - R_k|$$

$$\Longrightarrow D(\rho_\psi, \rho_\psi) - \sum_k \int \frac{Z}{|x-R_k|}\rho_\psi(x)\,dx + U(\underline{R})$$

$$\geq 0 - \int \frac{Z}{D(x)}\rho_\psi(x)\,dx$$

$$\therefore (\psi, V_c\psi) \geq -1.68 \underbrace{\int \rho_\psi(x)^{\frac{4}{3}}\,dx} - \int \frac{Z}{D(x)}\rho_\psi(x)\,dx$$

$$\int \rho_\psi(x)^{\frac{4}{3}}\,dx = \int \rho_\psi(x)^{\frac{5}{6}}\rho_\psi(x)\,dx$$

$\frac{4}{3} = \frac{5}{6}+1$

$$\leq \left(a\int \rho_\psi(x)^{\frac{5}{3}}\,dx\right)^{\frac{1}{2}} \left(\frac{1}{a}\underbrace{\int \rho_\psi(x)\,dx}_{N}\right)^{\frac{1}{2}}$$

$$\leq \frac{a}{2}\int \rho_\psi(x)^{\frac{5}{3}}\,dx + \frac{N}{2a}$$

$(\forall a > 0)$

$(\psi, H\psi)$

$$\geq \frac{K}{2} q^{-\frac{2}{3}} \int \rho_\psi(x)^{\frac{5}{3}} dx$$

$$- 1.68\alpha \left(\frac{a}{2} \int \rho_\psi(x)^{\frac{5}{3}} dx + \frac{N}{2a} \right)$$

$$- \int \frac{Z\alpha}{D(x)} \rho_\psi(x) dx$$

$$= \left(\frac{K}{2} q^{-\frac{2}{3}} - \frac{1.68\alpha}{2} a \right) \int \rho_\psi(x)^{\frac{5}{3}} dx$$

$$- \frac{1.68\alpha N}{2a} - \int \frac{Z\alpha}{D(x)} \rho_\psi(x) dx$$

$$a := \frac{K q^{-\frac{2}{3}}}{1.68\alpha} \varepsilon \qquad (0 < \varepsilon < 1)$$

$$(\quad \cdots \quad) = \frac{K}{2} q^{-\frac{2}{3}} (1 - \varepsilon)$$

$$\frac{1.68\alpha N}{2} \frac{q^{\frac{2}{3}}}{K\varepsilon} 1.68\alpha = 1.68^2 \frac{\alpha^2 q^{\frac{2}{3}} N}{2K\varepsilon}$$

$\therefore (\psi, H\psi)$

$$\geq -0.84^2 \frac{2\alpha^2 q^{\frac{2}{3}} N}{K\varepsilon} + \frac{K}{2} q^{-\frac{2}{3}} (1 - \varepsilon) \int \rho_\psi(x)^{\frac{5}{3}} dx$$

$$- Z\alpha \int \underbrace{\frac{1}{D(x)}}_{(D(x)^{-1} - b) + b} \rho_\psi(x) dx$$

$$\int \left(\frac{1}{D(x)} - b \right) \rho_\psi(x) dx + bN.$$

$$\frac{K}{2}q^{-\frac{2}{3}}(1-\varepsilon)\int \rho_\psi(x)^{\frac{5}{3}}\,dx - Z\alpha\int\left(\frac{1}{D(x)}-b\right)\rho_\psi(x)\,dx$$

$$\geq -\frac{2q}{5}\left(\frac{6}{5K(1-\varepsilon)}\right)^{\frac{3}{2}}(Z\alpha)^{\frac{5}{2}}\int\left[\frac{1}{D(x)}-b\right]_+^{\frac{5}{2}}dx$$

$\because$ $$\int\left\{\underbrace{\frac{K}{2}q^{-\frac{2}{3}}(1-\varepsilon)}_{A}\,\rho_\psi(x)^{\frac{5}{3}} - \underbrace{Z\alpha\left[\frac{1}{D(x)}-b\right]_+}_{B}\,\rho_\psi(x)\right\}dx$$

$$f(\rho) = A\rho^{\frac{5}{3}} - B\rho$$

$$f'(\rho) = \frac{5}{3}A\rho^{\frac{2}{3}} - B = 0$$

$$\rho^* = \left(\frac{3B}{5A}\right)^{\frac{3}{2}}$$

$$f(\rho^*) = A\left(\frac{3B}{5A}\right)^{\frac{5}{2}} - B\left(\frac{3B}{5A}\right)^{\frac{3}{2}} = -\frac{2B}{5}\left(\frac{3B}{5A}\right)^{\frac{3}{2}}$$

$$\geq -\frac{2}{5}\left(\frac{3}{5}\right)^{\frac{3}{2}}A^{-\frac{3}{2}}B^{\frac{5}{2}}$$

$$= -\frac{2}{5}\left(\frac{3}{5}\right)^{\frac{3}{2}}\left(\frac{2q^{\frac{2}{3}}}{K(1-\varepsilon)}\right)^{\frac{3}{2}}\left(Z\alpha\left[\frac{1}{D(x)}-b\right]_+\right)^{\frac{5}{2}}$$

$$= -\frac{2q}{5}\left(\frac{6}{5K(1-\varepsilon)}\right)^{\frac{3}{2}}(Z\alpha)^{\frac{5}{2}}\left[\frac{1}{D(x)}-b\right]_+^{\frac{5}{2}} \quad //$$

Rem. $\rho_\psi : \mathbb{R}^3 \longrightarrow [0,\infty)$

$$\left[\frac{1}{\Phi(x)}-b\right]_+^{\frac{5}{2}} = \max_{1\le k\le M}\left[\frac{1}{|x-R_k|}-b\right]_+^{\frac{5}{2}}$$

$$\le \sum_{k=1}^{M}\left[\frac{1}{|x-R_k|}-b\right]_+^{\frac{5}{2}}$$

$$\therefore \int\left[\frac{1}{\Phi(x)}-b\right]_+^{\frac{5}{2}}dx \le M\underbrace{\int_{|x|\le\frac{1}{b}}\left(\frac{1}{|x|}-b\right)^{\frac{5}{2}}dx}_{(☆)} = \frac{5\pi^2}{4}M\,b^{-\frac{1}{2}}$$

$$\because)\ (☆) = 4\pi\underbrace{\int_0^{\frac{1}{b}}\left(\frac{1}{r}-b\right)^{\frac{5}{2}}r^2\,dr}_{\int_0^{\frac{1}{b}}(1-br)^{\frac{5}{2}}(br)^{-\frac{1}{2}}b^{\frac{1}{2}}\,dr}$$

$$br = \tilde{r}$$

$$= \int_0^1 (1-\tilde{r})^{\frac{5}{2}}\,\tilde{r}^{-\frac{1}{2}}\,dr\cdot\ b^{-\frac{1}{2}}$$

$$= \underbrace{B\left(\frac{1}{2},\frac{7}{2}\right)}_{\frac{\Gamma(\frac{1}{2})\Gamma(\frac{7}{2})}{\Gamma(\frac{1}{2}+\frac{7}{2})} = \frac{\sqrt{\pi}\cdot\frac{5}{2}\cdot\frac{3}{2}\cdot\frac{1}{2}\sqrt{\pi}}{3\cdot 2}} b^{-\frac{1}{2}}$$

$$\therefore (☆) = \cancel{4}\pi\cdot\frac{5\cdot\cancel{3}\ \pi}{\cancel{3}\cdot 2\cdot 2\cdot\cancel{2}\cdot\cancel{2}}\,b^{-\frac{1}{2}} = \frac{5\pi^2}{4}b^{-\frac{1}{2}} \quad //$$

$$-\underbrace{(Z\alpha)N}_{A}b-\underbrace{\frac{\cancel{2}q}{\cancel{5}}\left(\frac{6}{5K(1-\varepsilon)}\right)^{\frac{3}{2}}(Z\alpha)^{\frac{5}{2}}\cdot\frac{\cancel{5}\pi^2}{\cancel{4}_{2}}M}_{B}\,b^{-\frac{1}{2}}$$

$$g(b):=-Ab-Bb^{-\frac{1}{2}}$$

$$g'(b)=-A+\frac{1}{2}Bb^{-\frac{3}{2}}=0$$

$$b^*=\left(\frac{B}{2A}\right)^{\frac{2}{3}}$$

$$g(b^*)=-A\left(\frac{B}{2A}\right)^{\frac{2}{3}}-B\left(\frac{B}{2A}\right)^{-\frac{1}{3}}=2^{-\frac{2}{3}}\cdot 3A^{\frac{1}{3}}B^{\frac{2}{3}}$$

$$=-2^{-\frac{2}{3}}\cdot 3(Z\alpha)^{\frac{1}{3}}N^{\frac{1}{3}}\cdot q^{\frac{2}{3}}\frac{6}{5K(1-\varepsilon)}(Z\alpha)^{\frac{5}{3}}\left(\frac{\pi^2}{2}\right)^{\frac{2}{3}}M^{\frac{2}{3}}$$

$$=-N^{\frac{1}{3}}M^{\frac{2}{3}}(Z\alpha)^2\frac{18}{5K(1-\varepsilon)}\left(\frac{\pi^2 q}{4}\right)^{\frac{2}{3}}$$

$(\psi, H\psi)$

$$\geq -0.84^2 \frac{2\alpha^2 q^{\frac{2}{3}} N}{K} \frac{1}{\varepsilon} - N^{\frac{1}{3}} M^{\frac{2}{3}} (Z\alpha)^2 \frac{18}{5K(1-\varepsilon)} \left(\frac{\pi^2 q}{4}\right)^{\frac{2}{3}}$$

$$= -\frac{2 q^{\frac{2}{3}} \alpha^2}{K} N \left\{ \underbrace{0.84^2}_{A} \left(\frac{1}{\varepsilon}\right) + \underbrace{\left(\frac{M}{N}\right)^{\frac{2}{3}} Z^2 \, \frac{9}{5} \left(\frac{\pi^2}{4}\right)^{\frac{2}{3}}}_{B} \left(\frac{1}{1-\varepsilon}\right) \right\}$$

$$h(\varepsilon) = \frac{A}{\varepsilon} + \frac{B}{1-\varepsilon}$$

$$h'(\varepsilon) = -\frac{A}{\varepsilon^2} + \frac{B}{(1-\varepsilon)^2} = 0$$

$$\varepsilon^* = \frac{-A + \sqrt{AB}}{B-A}$$

$$h(\varepsilon^*) = (\sqrt{A} + \sqrt{B})^2$$

$$\geq -\frac{2 q^{\frac{2}{3}} \alpha^2}{K} N \left(0.84 + \left(\frac{M}{N}\right)^{\frac{1}{3}} Z \sqrt{\frac{9}{5}\left(\frac{\pi^2}{4}\right)^{\frac{2}{3}}} \right)^2$$

$$D = \frac{9}{5}\left(\frac{\pi^2}{4}\right)^{\frac{2}{3}} \approx 3.287$$

$$K \geq \frac{9}{5}(4\pi^2)^{\frac{1}{3}} \approx \underline{6.129}$$

$\Longrightarrow (\psi, H\psi)$

$$\geq -0.23\underline{0}\, \alpha^2 q^{\frac{2}{3}} N \left(1 + 2.16 Z \left(\frac{M}{N}\right)^{\frac{1}{3}}\right)^2$$

Q.E.D.