§7.2 An Alternative Proof of Stability

(Thm. 5.4)

$$V_c(\underline{X},\underline{R}) \geq -(2Z+1)\sum_{i=1}^{N}\frac{1}{D(x_i)} + \cancel{\frac{Z^2}{8}\sum_{j=1}^{M}\frac{1}{D_j}}$$

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

$$D(x)^{-1} = \left(D(x)^{-1} - b\right) + b \qquad (b>0)$$

$(\psi, H\psi)$

$$H = \frac{1}{2}\sum_{j=1}^{N}(-\Delta_j) + \alpha V_c(\underline{X},\underline{R})$$

$$\geq \frac{1}{2}\sum_{j}(-\Delta_j) - \alpha(2Z+1)\sum_{i=1}^{N}\frac{1}{D(x_i)}$$

$$= \frac{1}{2}\sum_{i=1}^{N}\Big[\underbrace{-\Delta_i - 2(2Z+1)\alpha\Big\{\Big(\frac{1}{D(x_i)} - b\Big)}_{H_i} + b\Big\}\Big]$$

$$h = -\Delta \underbrace{- 2(2Z+1)\alpha\left(\frac{1}{D(x)} - b\right)}_{= V(x)}$$

$$\sum_{i=1}^{N} H_i = \operatorname{Tr} h\,\gamma_\psi^{(1)}$$

$$\geq \|\gamma_\psi^{(1)}\|_\infty \sum_{j=1}^{N} E_j$$

$$\geq -q L_{1,3}\int_{\mathbb{R}^3} V_-(x)^{1+\frac{3}{2}}\,dx$$

$$\geq -q L_{1,3}\, 2^{\frac{5}{2}}(2Z+1)^{\frac{5}{2}}\alpha^{\frac{5}{2}}\underbrace{\int_{\mathbb{R}^3}\left[\frac{1}{D(x)} - b\right]_+^{\frac{5}{2}} dx}_{\leq \frac{5\pi^2}{4} M b^{-\frac{1}{2}}}$$

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

$$Z - \underbrace{q L_{1,3}\, 2^{\frac{3}{2}} (2Z+1)^{\frac{5}{2}} \alpha^{\frac{5}{2}} \cdot \frac{5\pi^2}{4} M}_{A}\, b^{-\frac{1}{2}} - \underbrace{(2Z+1)\alpha N}_{B}\, b$$

$$- A b^{-\frac{1}{2}} - B b$$

$$\frac{1}{2} A b^{-\frac{3}{2}} - B = 0 \qquad b^* = \left(\frac{A}{2B}\right)^{\frac{2}{3}}$$

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

$(\psi, H\psi)$

$$Z - \frac{3}{2} (q L_{1,3})^{\frac{2}{3}}\, \cancel{2}\, (2Z+1)^{\frac{5}{3}} \alpha^{\frac{5}{3}} \left(\frac{5\pi^2}{\cancel{4}}\right)^{\frac{2}{3}} M^{\frac{2}{3}}$$

$$\times\ \cancel{2^{\frac{1}{3}}} (2Z+1)^{\frac{1}{3}} \alpha^{\frac{1}{3}} N^{\frac{1}{3}}$$

$$= \underbrace{-\frac{3}{2} (5\pi^2)^{\frac{2}{3}} L_{1,3}^{\frac{2}{3}}}_{1.073}\ q^{\frac{2}{3}} \left[(2Z+1)\alpha\right]^2 M^{\frac{2}{3}} N^{\frac{1}{3}}$$

$$L_{1,3} \le \frac{\pi}{\sqrt{3}} L_{1,3}^{cl} \quad \frac{1}{15\pi^2}$$

$$= \frac{1}{15\sqrt{3}\pi} \approx 0.0123$$

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

$30.64\ M$ Ry.

§7.3 Stability of Matter via Thomas-Fermi Theory

$$\mathcal{E}^{TF}(\rho) = \frac{3}{10}\gamma q^{-\frac{2}{3}}\int_{\mathbb{R}^3}\rho(x)^{\frac{5}{3}}dx - \sum_{j=1}^{M} Z_j \alpha \int_{\mathbb{R}^3}\frac{\rho(x)}{|x-R_j|}dx$$

$$+\frac{\alpha}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho(x)\rho(y)}{|x-y|}dxdy + \sum_{i<j}\frac{Z_i Z_j \alpha}{|R_i - R_j|}$$

$$\gamma = (6\pi^2)^{\frac{2}{3}}$$

$$E^{TF}(N, \underline{Z}, \underline{R}, \gamma)$$

$$= \inf\left\{\mathcal{E}^{TF}(\rho) : \rho \in L^{\frac{5}{3}}(\mathbb{R}^3),\ \rho(x) \geq 0,\ \int_{\mathbb{R}^3}\rho(x)dx = N\right\}$$

Rem.

$$E^{TF}(N, \underline{Z}, \underline{R}, \gamma) = E^{TF}\left(\sum_i Z_i, \underline{Z}, \underline{R}, \gamma\right)$$

$$\forall N \geq \sum_i Z_i$$

$$N \leq \sum_i Z_i \Longrightarrow \exists \rho \text{ s.t. } \mathcal{E}^{TF}(\rho) = E^{TF}(N, \underline{Z}, \underline{R}, \gamma).$$

Rem. (no-binding theorem)

$$E^{TF}(N, \underline{Z}, \underline{R}, \gamma)$$

$$\geq \min\left\{\sum_{i=1}^{M} E^{TF}(N_i, Z_i, R_i, \gamma) : N_i \geq 0, \sum_{i=1}^{M} N_i = N\right\}$$

Rem. (scaling)

$$E^{TF}(N, Z, 0, \gamma) = Z^{\frac{7}{3}} \gamma^{-1} E^{TF}\left(\frac{N}{Z}, 1, 0, 1\right)$$

$$(\text{LHS}) = \inf\left\{ \mathcal{E}^{TF}(\rho) : \int \rho(x)\,dx = N \right\}$$

$$\mathcal{E}^{TF}(\rho)$$

$$= \frac{3}{10}\gamma q^{-\frac{2}{3}} \int \rho(x)^{\frac{5}{3}} dx - Z\alpha \int \frac{\rho(x)}{|x|} dx + \frac{\alpha}{2} \iint \frac{\rho(x)\rho(y)}{|x-y|} dx dy$$

$$E^{TF}\left(\frac{N}{Z}, 1, 0, 1\right) = \inf\left\{ \mathcal{E}^{TF}(\rho') : \int \rho'(x)\,dx = \frac{N}{Z} \right\}$$

$$\mathcal{E}^{TF}(\rho')$$

$$= \frac{3}{10}(1) q^{-\frac{2}{3}} \int \rho'(x)^{\frac{5}{3}} dx - (1)\alpha \int \frac{\rho'(x)}{|x|} dx + \frac{\alpha}{2} \iint \frac{\rho'(x)\rho'(y)}{|x-y|} dx dy$$

$$\rho'(x) = C \rho(\lambda x)$$

$$\underbrace{\int \rho'(x)\,dx}_{\frac{N}{Z}} = C\lambda^{-3} \int \rho(\lambda x) \lambda^3 dx = C\lambda^{-3} \underbrace{\int \rho(x')\,dx'}_{N}$$

$$\therefore \quad C\lambda^{-3} = Z^{-1}.$$

(1^{st} term)

$$\int \rho'(x)^{\frac{5}{3}} dx = C^{\frac{5}{3}} \lambda^{-3} \int \rho(\lambda x)^{\frac{5}{3}} \lambda^3 dx$$

$$\int \rho(x')^{\frac{5}{3}} dx'$$

$$\therefore C^{\frac{5}{3}} \lambda^{-3} = (Z^{\frac{7}{3}} \gamma^{-1})^{-1} \gamma = Z^{-\frac{7}{3}} \gamma^2$$

(2^{nd} term)

$$\int \frac{\rho'(x)}{|x|} dx = C \lambda^{-2} \int \frac{\rho(\lambda x)}{|\lambda x|} \lambda^3 dx = C \lambda^{-2} \int \frac{\rho(x')}{|x'|} dx'$$

$$\therefore C \lambda^{-2} = (Z^{\frac{7}{3}} \gamma^{-1})^{-1} Z = Z^{-\frac{4}{3}} \gamma$$

(3^{rd} term)

$$\iint \frac{\rho'(x) \rho'(y)}{|x-y|} dx dy = C^2 \lambda^{-5} \iint \frac{\rho(\lambda x) \rho(\lambda y)}{|\lambda x - \lambda y|} \lambda^3 dx \cdot d^3 \lambda y$$

$$\therefore C^2 \lambda^{-5} = (Z^{\frac{7}{3}} \gamma^{-1})^{-1} = Z^{-\frac{7}{3}} \gamma$$

$$\Longrightarrow \begin{cases} C = Z^{-2} \gamma^3 \\ \lambda = Z^{-\frac{1}{3}} \gamma \end{cases}$$

$$\therefore \rho'(x) = Z^{-2} \gamma^3 \rho(Z^{-\frac{1}{3}} \gamma x).$$

$$
\begin{aligned}
\therefore\ & E^{TF}(N, \underline{Z}, \underline{R}, \gamma) \\
& \geq \sum_{i=1}^{M} E^{TF}(N_i, Z_i, R_i, \gamma) \\
& = \gamma^{-1} \underbrace{E^{TF}(1,1,0,1)}_{\approx\, -7.356\,\alpha^2} \underbrace{\sum_i Z_i^{\frac{7}{3}}}_{\leq\, Z^{\frac{7}{3}} M}
\end{aligned}
$$

$$K \geq \left(\frac{3}{\pi^2}\right)^{\frac{1}{3}} K^{cl} = \left(\frac{3}{\pi^2}\right)^{\frac{1}{3}} \cdot \frac{3}{5}(6\pi^2)^{\frac{2}{3}} = \frac{9}{5}(2\pi)^{\frac{2}{3}}$$

$$\gamma = 6\left(\frac{\pi^2}{2}\right)^{\frac{1}{3}}$$

$$\Longrightarrow \frac{1}{2}\frac{3}{5}\cdot 6\left(\frac{\pi^2}{2}\right)^{\frac{1}{3}} = \frac{1}{2}\cdot\frac{9}{5}(2\pi)^{\frac{2}{3}}$$

(Lieb-Oxford)

$$\int \rho(x)^{\frac{4}{3}}dx \leq \left(\cancel{a}\int \rho(x)^{\frac{5}{3}}dx\right)^{\frac{1}{2}}\left(\cancel{\tfrac{1}{a}}\int \rho(x)\,dx\right)^{\frac{1}{2}}$$

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

$$-1.68\,\cancel{\alpha}\int \rho(x)^{\frac{4}{3}}dx$$

$$\geq -1.68\,\cancel{\alpha}\,\frac{a}{2}\int \rho(x)^{\frac{5}{3}}dx - 1.68\,\frac{N\cancel{\alpha}}{2a}$$

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

$$\geq E^{TF}\left(N, Z, R, 6\left(\frac{\pi^2}{2}\right)^{\frac{1}{3}} - \frac{5}{3}q^{\frac{2}{3}}\,1.68\,\cancel{\alpha}\,a\right) - 1.68\frac{N\cancel{\alpha}}{2a}$$

$$\geq \left\{6\left(\frac{\pi^2}{2}\right)^{\frac{1}{3}} - \frac{5}{3}q^{\frac{2}{3}}\,1.68\,\cancel{\alpha}\,a\right\}^{-1} E^{TF}(1,1,0,1)\sum_j Z_j^{\frac{7}{3}}$$

$$-1.68\frac{N\cancel{\alpha}}{2a}$$

$$\begin{cases} a = \dfrac{6\left(\frac{\pi^2}{2}\right)^{\frac{1}{3}}}{\frac{5}{3} q^{\frac{2}{3}}\, 1.68\,\alpha}\, \varepsilon \qquad (0 < \forall \varepsilon < 1) \end{cases}$$

$$= -\left\{\left(-E^{TF}(1,1,0,1) \sum_j Z_j^{\frac{7}{3}}\right)\left\{6\left(\frac{\pi^2}{2}\right)^{\frac{1}{3}}(1-\varepsilon)\right\}^{-1} - \frac{1.68\, N\alpha}{2} \cdot \frac{\frac{5}{3} q^{\frac{2}{3}}\, 1.68\,\alpha}{6\left(\frac{\pi^2}{2}\right)^{\frac{1}{3}}} \frac{1}{\varepsilon}\right\}$$

$$\frac{A}{1-\varepsilon} + \frac{B}{\varepsilon} \geq \left(\sqrt{A} + \sqrt{B}\right)^2$$

$(\psi, H\psi)$

$$\geq -\left\{\left[\frac{-E^{TF}(1,1,0,1) \sum_j Z_j^{\frac{7}{3}}}{6\left(\frac{\pi^2}{2}\right)^{\frac{1}{3}}}\right]^{\frac{1}{2}} + \left[\frac{1.68^2\, N\alpha^2\, \frac{5}{3} q^{\frac{2}{3}}}{2 \cdot 6\left(\frac{\pi^2}{2}\right)^{\frac{1}{3}}}\right]^{\frac{1}{2}}\right\}^2$$

$$= -\underbrace{\frac{\frac{5}{3}\, 1.68^2\, q^{\frac{2}{3}}\, \alpha^2 N}{2 \cdot 6\left(\frac{\pi^2}{2}\right)^{\frac{1}{3}}}}_{0.2302\ldots\, q^{\frac{2}{3}} \alpha^2 N} \Bigg(1 + \underbrace{\sqrt{D \sum_{j=1}^{M} Z_j^{\frac{7}{3}}}}_{1.97\sqrt{\frac{1}{N}\sum_j Z_j^{\frac{7}{3}}}\ (\text{for } q=2)}\Bigg)^2$$

$$D = \frac{-2E^{TF}(1,1,0,1)}{\frac{5}{3}\, 1.68^2\, q^{\frac{2}{3}} \alpha^2 N}$$

$\longrightarrow$ 6.45 Ry/M ?

§7.4 Other Routes to a Proof of Stability

(III) Dyson-Lenard 1967

10^{14} Ry.

(III) Federbush 1975

(III) Lieb-Thirring

(III) Fefferman 1983

(III) Graf 1997