Advanced Mathematical Physics, Assignment 1

Johannes Agerskov

Dated: May 19, 2020

1 Stability through Lieb-Oxford inequality

We are given the Lieb-Oxford inequality: For any bosonic or fermionic wave function $\psi \in L^2(\mathbb{R}^{3N})$ with $\|\psi\|_2 = 1$ we have

$$\sum_{1\leq i<j\leq N} \int_{\mathbb{R}^{3N}} \frac{|\psi(x_1,...,x_N)|^2}{|x_i - x_j|} \,\mathrm{d}x_1 ... \,\mathrm{d}x_N - D(\rho_\psi, \rho_\psi) \geq -C_{LO} \int_{\mathbb{R}^3} \rho_\psi(x)^{4/3} \,\mathrm{d}x, \tag{1.1}$$

with constant $0 \leq C_{LO} \leq 1.636$ independent of ψ and N. We now proceed to prove stability of the second kind through this inequality.

(a)

Let $\delta > 0$ then

$$\int_{\mathbb{R}^3} \rho_\psi(x)^{4/3} \,\mathrm{d}x \leq \frac{\delta}{2} \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \,\mathrm{d}x + \frac{N}{2\delta}. \tag{1.2}$$

Proof. Notice first first that $\rho_\psi(x)^{4/3} = \rho_\psi(x)^{5/6} \rho_\psi(x)^{1/2}$. Thus by Cauchy-Schwartz inequality, we have

$$\int_{\mathbb{R}^3} \rho_\psi(x)^{4/3} \,\mathrm{d}x \leq \left(\int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \,\mathrm{d}x \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^3} \rho_\psi(x) \,\mathrm{d}x \right)^{\frac{1}{2}} = \left(\int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \,\mathrm{d}x \right)^{\frac{1}{2}} \sqrt{N}, \tag{1.3}$$

where we used that $\int_{\mathbb{R}^3} \rho_\psi(x) \,\mathrm{d}x = N$. Now using that for $\delta > 0$ and $a, b \in \mathbb{R}$ is holds that $\frac{\delta}{2} a^2 + \frac{1}{2\delta} b^2 \geq ab$ (this is simply $(\sqrt{\delta} a - \frac{1}{\sqrt{\delta}} b)^2 \geq 0$) we find that

$$\int_{\mathbb{R}^3} \rho_\psi(x)^{4/3} \,\mathrm{d}x \leq \frac{\delta}{2} \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \,\mathrm{d}x + \frac{N}{2\delta} \tag{1.4}$$

$\square$

(b)

Let V_{C} be defined as in the lecture notes with fixed $R_1, ..., R_M \in \mathbb{R}^3$ and $Z_1 = ... = Z_N = Z$. We prove that if $\psi \in H^1(\mathbb{R}^{3N})$ is fermionic, then

$$\begin{aligned}\mathcal{E}(\psi) &= T_\psi + (V_{\mathrm{C}})_\psi \\ &\geq C_1 \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \,\mathrm{d}x + D(\rho_\psi, \rho_\psi) - \sum_{j=1}^M \int_{\mathbb{R}^3} \frac{Z\rho_\psi}{|x-R_j|} \,\mathrm{d}x + \sum_{1\leq j<k\leq M} \frac{Z^2}{|R_j - R_k|} - C_2 N,\end{aligned}$$

with some constants $C_1, C_2 > 0$ independent of ψ and N.

Proof. By definition we have

$$(V_{\mathrm{C}})_\psi = \int_{\mathbb{R}^{3N}} \sum_{1\leq i<j\leq N} \frac{|\psi(x_1,...,x_N)|^2}{|x_i - x_j|} - \sum_{i=1}^N \sum_{j=1}^M \frac{Z\,|\psi(x_1,...,x_N)|^2}{|x_i - R_j|} \,\mathrm{d}x_1 ... \,\mathrm{d}x_N + \sum_{1\leq j<k\leq M} \frac{Z^2}{|R_j - R_k|}. \tag{1.5}$$

Using that ψ is fermionic we find that

$$\int_{\mathbb{R}^{3N}} \sum_{i=1}^N \sum_{j=1}^M \frac{Z\,|\psi(x_1,...,x_N)|^2}{|x_i - R_j|} \,\mathrm{d}x_1 ... \,\mathrm{d}x_N = \sum_{j=1}^M \frac{1}{N} \sum_{i=1}^N \int_{\mathbb{R}^3} \frac{Z\rho_\psi(x_i)}{|x_i - R_j|} \,\mathrm{d}x_i = \sum_{j=1}^M \int_{\mathbb{R}^3} \frac{Z\rho_\psi(x)}{|x - R_j|} \,\mathrm{d}x. \tag{1.6}$$

Furthermore, using the Lieb-Oxford inequality we find that

$$(V_{\mathrm{C}})_\psi \geq -C_{LO} \int_{\mathbb{R}^3} \rho_\psi(x)^{4/3} \,\mathrm{d}x + D(\rho_\psi, \rho_\psi) - \sum_{j=1}^M \int_{\mathbb{R}^3} \frac{Z\rho_\psi(x)}{|x - R_j|} \,\mathrm{d}x + \sum_{1\leq j<k\leq M} \frac{Z^2}{|R_j - R_k|}. \tag{1.7}$$

Therefore, by (a) we have

$$(V_{\mathrm{C}})_\psi \geq -C_{LO} \left(\frac{\delta}{2} \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \,\mathrm{d}x + \frac{N}{2\delta} \right) \mathrm{d}x + D(\rho_\psi, \rho_\psi) - \sum_{j=1}^M \int_{\mathbb{R}^3} \frac{Z\rho_\psi(x)}{|x - R_j|} \,\mathrm{d}x + \sum_{1\leq j<k\leq M} \frac{Z^2}{|R_j - R_k|} \tag{1.8}$$

Now we use the fact that there exist a constant $C > 0$ such that $T_\psi \geq C \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \,\mathrm{d}x$. This can be seen by considering the Lieb-Thirring inequality with potential $V = -\alpha \rho_\psi^{2/3}$ with some $\alpha > 0$. Notice that then $V \in L^{5/2}(\mathbb{R}^3)$ by Sobolev's inequality and the fact that $\rho_\psi \in L^{3/2}(\mathbb{R}^3)$. Thus we may apply the Lieb-Thirring inequality

$$\sum_i |E_i| \leq L_{1,3} \int_{\mathbb{R}^3} V_-(x)^{5/2} \,\mathrm{d}x = \alpha^{5/2} L_{1,3} \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \,\mathrm{d}x. \tag{1.9}$$

Notice however, that from the very definition of the eigenvalues we have $T_\psi \geq -V_\psi + E_0$. Thus we may conclude that

$$T_\psi \geq \alpha \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \,\mathrm{d}x - \alpha^{5/2} L_{1,3} \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \,\mathrm{d}x. \tag{1.10}$$

Thereby we see that if we choose $\alpha < 1$ and $\alpha^{3/2} < L_{1,3}^{-1}$ we see that there exist some constant $C = \alpha(1 - \alpha^{3/2} L_{1,3}) > 0$ such that

$$T_\psi \geq C \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \, \mathrm{d}x. \tag{1.11}$$

Combining this with (1.8) we find that

$$\begin{aligned} \mathcal{E}(\psi) \geq \left(C - C_{LO}\frac{\delta}{2}\right) \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \, \mathrm{d}x + D(\rho_\psi, \rho_\psi) - \sum_{j=1}^{M} \int_{\mathbb{R}^3} \frac{Z\rho_\psi(x)}{|x - R_j|} \, \mathrm{d}x \\ + \sum_{1 \leq j < k \leq M} \frac{Z^2}{|R_j - R_k|} - C_{LO}\frac{N}{2\delta} \end{aligned}. \tag{1.12}$$

Now choosing $0 < \delta < \frac{2C}{C_{LO}}$, we find that $C_1 = \left(C - C_{LO}\frac{\delta}{2}\right) > 0$ and $C_2 = \frac{C_{LO}}{2\delta} > 0$ and

$$\mathcal{E}(\psi) \geq C_1 \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \, \mathrm{d}x + D(\rho_\psi, \rho_\psi) - \sum_{j=1}^{M} \int_{\mathbb{R}^3} \frac{Z\rho_\psi(x)}{|x - R_j|} \, \mathrm{d}x + \sum_{1 \leq j < k \leq M} \frac{Z^2}{|R_j - R_k|} - C_2 N. \tag{1.13}$$

as desired. $\square$

(c)

We now prove that for any $\psi \in H_1(\mathbb{R}^{3N})$ that is fermionic it hold for any $b > 0$ that

$$\mathcal{E}(\psi) \geq C_1 \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \, \mathrm{d}x - Z \int_{\mathbb{R}^3} \rho_\psi(x) \left(\frac{1}{\mathfrak{D}(x)} - b\right) \mathrm{d}x - ZbN - C_2 N. \tag{1.14}$$

with some constants $C_1, C_2 > 0$ independent of ψ and N.

Proof. First notice that by the basic electrostatic inequality with measure $\mu(\mathrm{d}x) = \rho_\psi(x)\, \mathrm{d}x$ (which indeed defines a measure since $\rho_\psi \in L^1(\mathbb{R}^3)$ and $\rho_\psi \geq 0$) and the result of (b) it follows that

$$\mathcal{E}(\psi) \geq C_1 \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \, \mathrm{d}x - Z \int_{\mathbb{R}^3} \rho_\psi(x) \frac{1}{\mathfrak{D}(x)} \, \mathrm{d}x - C_2 N. \tag{1.15}$$

Now using that $\int_{\mathbb{R}^3} \rho_\psi(x) \, \mathrm{d}x = N$ we see that

$$- Z \int_{\mathbb{R}^3} \rho_\psi(x) \frac{1}{\mathfrak{D}(x)} \, \mathrm{d}x = -Z \int_{\mathbb{R}^3} \rho_\psi(x) \left(\frac{1}{\mathfrak{D}(x)} - b\right) \mathrm{d}x - ZbN, \tag{1.16}$$

from which the claim follows:

$$\mathcal{E}(\psi) \geq C_1 \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} \, \mathrm{d}x - Z \int_{\mathbb{R}^3} \rho_\psi(x) \left(\frac{1}{\mathfrak{D}(x)} - b\right) \mathrm{d}x - ZbN - C_2 N. \tag{1.17}$$

$\square$

(d)

From calculus of variations it can be shown that the functional obtained in (c) is minimized by some ρ_ψ of the form

$$\rho_\psi(x) = d\left(\frac{1}{\mathfrak{D}(x)} - b\right)^{3/2} \chi_{\{\frac{1}{\mathfrak{D}(x)}-b\geq c\}}(x) \tag{1.18}$$

for some $d > 0$ and $c \geq 0$ independent of ψ and N. Thereby, we may conclude that $\mathcal{E}(\psi) \geq C(Z)(N+M)$. To see this notice that by inserting the minimizer on the left-hand side of (1.17) we obtain

$$\begin{aligned}\mathcal{E}(\psi) &\geq (C_1 d^{5/3} - Zd)\int_{\{\frac{1}{\mathfrak{D}(x)}-b\geq c\}} \left(\frac{1}{\mathfrak{D}(x)} - b\right)^{5/2} \mathrm{d}x - ZbN - C_2N \\ &\geq \min\left\{0, (C_1 d^{5/3} - Zd)\right\}\int_{\{\frac{1}{\mathfrak{D}(x)}\geq c+b\}} \left(\frac{1}{\mathfrak{D}(x)}\right)^{5/2} \mathrm{d}x - (Zb + C_2)N\end{aligned} \tag{1.19}$$

Now defining $\alpha := (c+b)^{-1}$ we have

$$\int_{\{\frac{1}{\mathfrak{D}(x)}\geq c+b\}} \left(\frac{1}{\mathfrak{D}(x)}\right)^{5/2} \mathrm{d}x \leq \sum_{j=1}^{M} \int_{\{|x-R_j|\leq\alpha\}} \left(\frac{1}{|x-R_j|}\right)^{5/2} \mathrm{d}x = 8\pi\sqrt{\alpha}M, \tag{1.20}$$

where we used that $\left(\frac{1}{\mathfrak{D}(x)}\right)^{5/2} \chi_{\{\frac{1}{\mathfrak{D}(x)}\geq\frac{1}{\alpha}\}} \leq \sum_{j=1}^M \left(\frac{1}{|x-R_j|}\right)^{5/2} \chi_{\{|x-R_j|\leq\alpha\}}$, which is obvious from the fact that, for any $x \in \mathbb{R}^3$ the left-hand side will equal at least one of the terms on the right-hand side, and since all on the terms on the right-hand side are non-negative the inequality follows. From this it follows that

$$\mathcal{E}(\psi) \geq -K_1(Z)M - K_2(Z)N \geq -C(Z)(N+M) \tag{1.21}$$

with $K_1(Z) = \max\left\{0, -(C_1 d^{5/3} - Zd)\right\} 8\pi\sqrt{\alpha}$, $K_2(Z) = (Zb + C_2)$, and $C(Z) = \max\{K_1(Z), K_2(Z)\}$. Many of these estimates were quite rough and can be optimized. For example one can optimize w.r.t b. Notice to find the exact d and c we would have to minimize w.r.t to d and c. Thus we find $d = \left(\frac{3Z}{5C_1}\right)^{3/2}$ and $c = 0$.

2 The volume occupied by matter

Let $\psi \in L^2(\mathbb{R}^{3N})$ ($\psi \in H^1(\mathbb{R}^{3N})$) be a fermionic wave function with $\|\psi\|_2 = 1$.

(a)

It holds that $\mathcal{E}(\psi) = T_\psi + (V_{\mathrm{C}})_\psi \geq -CN$ where $C > 0$ depends on Z and the ratio M/N. This is a direct consequence of the result from problem 1. Since we have $\mathcal{E}(\psi) \geq -C(Z)(M+N) = -C(Z)(M/N+1)N = -CN$ where $C = C(Z)(M/N+1)$.

(b)

Using a scaling argument, it is possible to conclude from (a) that

$$(1-\lambda)T_\psi + (V_\mathrm{C})_\psi \geq -\frac{CN}{1-\lambda}, \tag{2.1}$$

for any $0<\lambda<1$. From this it follows that

$$T_\psi \leq \frac{\mathcal{E}(\psi)+CN}{\lambda} + \frac{CN}{1-\lambda} \tag{2.2}$$

Proof. To see this, notice that from (2.1) we have

$$-\lambda T_\psi \geq -\frac{CN}{1-\lambda} - \mathcal{E}(\psi), \tag{2.3}$$

from which it follows that

$$T_\psi \leq \frac{CN}{\lambda(1-\lambda)} + \frac{\mathcal{E}(\psi)}{\lambda} = \frac{\mathcal{E}(\psi)+CN}{\lambda} + \frac{CN}{1-\lambda}, \tag{2.4}$$

where we in the last equality used the partial fraction decomposition $\frac{CN}{\lambda(1-\lambda)} = \frac{CN}{\lambda} + \frac{CN}{1-\lambda}$. □

From this we may conclude that

$$T_\psi \leq (\sqrt{\mathcal{E}(\psi)+CN} + \sqrt{CN})^2. \tag{2.5}$$

Proof. For $\mathcal{E}(\psi)=0$ it follows by choosing $\lambda = 1/2$ in (2.2). Now assume $\mathcal{E}(\psi)\neq 0$, we then optimize (2.2) w.r.t λ:

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{\mathcal{E}(\psi)+CN}{\lambda} + \frac{CN}{1-\lambda}\right) = -\frac{\mathcal{E}(\psi)+CN}{\lambda^2} + \frac{CN}{(1-\lambda)^2} = 0 \tag{2.6}$$

using that $0<\lambda<1$, this is equivalent

$$-(1-\lambda)^2(\mathcal{E}(\psi)+CN) - \lambda^2 CN = 0, \tag{2.7}$$

which has the solutions $\lambda_\pm = \frac{\mathcal{E}(\psi)+CN\pm\sqrt{\mathcal{E}(\psi)CN+C^2N^2}}{\mathcal{E}(\psi)}$, where we see that only the λ_- solution is consistent with $0<\lambda<1$ (it is consistent since $\mathcal{E}(\psi)\geq -CN$). Inserting this λ_- back into (2.2) we find that

$$T_\psi \leq (\sqrt{\mathcal{E}(\psi)+CN} + \sqrt{CN})^2, \tag{2.8}$$

as desired. □