Advanced Mathematical Physics, Assignment 1

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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

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

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

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

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

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

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

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

$\square$

(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

$$\mathcal{E}(\psi) = T_\psi + (V_C)_\psi$$

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

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

Proof. By definition we have

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

Using that ψ is fermionic we find that

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

Furthermore, using the Lieb-Oxford inequality we find that

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

Therefore, by (a) we have

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

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

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

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

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

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

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

Combining this with (1.8) we find that

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

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

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

as desired. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad\square$

(c)

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

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

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

Proof. First notice that by the basic electrostatic inequality with measure $\mu(dx) = \rho_\psi(x) \, dx$ (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

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

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

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

from which the claim follows:

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

$$\square$$

(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 $d, c > 0$ 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

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

Now choose $b > \frac{2}{d}$ where $d = \min\left\{|R_i - R_j| : 1 \leq i < j \leq M\right\}$, then

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

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 $K_1(Z) = \min\left\{0, (C_1 d^{5/3} - Zd)\right\}8\pi\sqrt{d/2}$, $K_2(Z) = (Zb + C_2)$, and $C(Z) = \max\{K_1(Z), K_2(Z)\}$.