Advanced Mathematical Physics, Assignment 2

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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[1] 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 $\rho_\psi \in L^1(\mathbb{R}^3)$[2]. 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

[1] This is Problem 23(c) in the exercises for stability of matter.

[2] $\|V\|_{5/2}^{5/2} = \alpha^{5/2} \int_{\mathbb{R}^3} \rho_\psi^{5/3}(x)\, \mathrm{d}x \leq \alpha^{5/2} \|\rho_\psi\|_3 \left(\int_{\mathbb{R}^3} \rho_\psi(x)\, \mathrm{d}x\right)^{2/3} < \infty$ where the last inequality follows from Sobolev's inequality with $\psi \in H_1(\mathbb{R}^3)$ and $\rho_\psi \in L^1(\mathbb{R}^3)$.

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 $\alpha > 0$ and $\alpha^{3/2} < L_{1,3}^{-1}$, 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 fermionic $\psi \in H_1(\mathbb{R}^{3N})$ 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 non-negative Borel 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:

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

□

(d)

Seeking to find the minimizer of the right hand side of (1.17), we notice that we restrict ρ_ψ to be non-negative, for it to be bounded from below. Thus we may rewrite the rhs. of (1.17) as

$$C_1 \int_{\mathbb{R}^3} \left(\sqrt{\rho_\psi(x)^2}\right)^{5/3} \mathrm{d}x - Z \int_{\mathbb{R}^3} \left(\sqrt{\rho_\psi(x)^2}\right) \left(\frac{1}{\mathfrak{D}(x)} - b\right) \mathrm{d}x - ZbN - C_2 N. \tag{1.18}$$

In this way we may allow ρ_ψ to take negative values which enables us to do the variation without restrictions. Thus we can write down the Euler-Lagrange equations (for $\rho_\psi(x) \neq 0$) in order to minimize (1.18). We find

$$\frac{5}{3} C_1 \rho_\psi(x) \left(\sqrt{\rho_\psi(x)^2}\right)^{-1/3} - Z\rho_\psi(x) \left(\sqrt{\rho_\psi(x)^2}\right)^{-1} \left(\frac{1}{\mathfrak{D}(x)} - b\right) = 0. \tag{1.19}$$

Notice that all terms are well behaved in the limits $\rho_\psi(x) \to 0_\pm$, however the second term does have a discontinuity in approaching zero so we assume $\rho_\psi(x) \neq 0$. We observe that for $\left(\frac{1}{\mathfrak{D}(x)} - b\right) > 0$ this equation have the solution

$$\rho_\psi(x) = \pm \left(\frac{3Z}{5C_1}\right)^{3/2} \left(\frac{1}{\mathfrak{D}(x)} - b\right)^{3/2}, \tag{1.20}$$

Since we are seeking solutions satisfying $\rho_\psi \geq 0$, we of course choose the positive solution. It is not hard to check that letting $\rho_\psi = 0$ on any subset of $\left\{\left(\frac{1}{\mathfrak{D}(x)} - b\right) > 0\right\}$ with positive measure, will increase the lower bound of the energy, thus this is indeed a minimizer.
For $\left(\frac{1}{\mathfrak{D}(x)} - b\right) \leq 0$ there is no solution, however by observing (1.18) directly we easily see that in this domain $\rho_\psi = 0$ is the minimizer. Combining these domains we find that the functional obtained in (c) is minimized by

$$\rho_\psi(x) = d\left(\frac{1}{\mathfrak{D}(x)} - b\right)^{3/2} \chi_{\{\frac{1}{\mathfrak{D}(x)} - b \geq 0\}}(x) \tag{1.21}$$

with $d = \left(\frac{3Z}{5C_1}\right)^{3/2}$ which is 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

$$\begin{aligned} \mathcal{E}(\psi) &\geq (C_1 d^{5/3} - Zd) \int_{\{\frac{1}{\mathfrak{D}(x)} - b \geq 0\}} \left(\frac{1}{\mathfrak{D}(x)} - b\right)^{5/2} \mathrm{d}x - ZbN - C_2 N \\ &\geq \min\left\{0, (C_1 d^{5/3} - Zd)\right\} \int_{\{\frac{1}{\mathfrak{D}(x)} \geq b\}} \left(\frac{1}{\mathfrak{D}(x)}\right)^{5/2} \mathrm{d}x - (Zb + C_2)N \end{aligned} \tag{1.22}$$

Now defining $\alpha := b^{-1}$ we have

$$\int_{\{\frac{1}{\mathfrak{D}(x)}\geq b\}}\left(\frac{1}{\mathfrak{D}(x)}\right)^{5/2}\mathrm{d}x \leq \sum_{j=1}^{M}\int_{\{|x-R_j|\leq\alpha\}}\left(\frac{1}{|x-R_j|}\right)^{5/2}\mathrm{d}x = 8\pi\sqrt{\alpha}M, \tag{1.23}$$

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 the terms on the right-hand side are non-negative the inequality follows. From this it follows that

$$\mathcal{E}(\psi) \geq -K_1(Z)M - K_2(Z)N \geq -C(Z)(N+M) \tag{1.24}$$

with $K_1(Z) = \max\left\{0, -(C_1 d^{5/3} - Zd)\right\}\frac{8\pi}{\sqrt{b}}$, $K_2(Z) = (Zb+C_2)$, and $C(Z) = \max\{K_1(Z), K_2(Z)\}$. Inserting the value of d in $K_1(Z)$ we find $K_1(Z) = \frac{6}{25}\sqrt{\frac{3}{5}}Z\left(\frac{Z}{C_1}\right)^{3/2}\frac{8\pi}{\sqrt{b}}$.[3].

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

$$\mathcal{E}(\psi) \geq -C(Z)(M+N) = -C(Z)(M/N+1)N = -CN, \tag{2.1}$$

where $C = C(Z)(M/N+1)$.

(b)

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

$$(1-\lambda)T_\psi + (V_{\mathrm{C}})_\psi \geq -\frac{CN}{1-\lambda}, \tag{2.2}$$

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

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

[3] Using the bound from the lecture notes on page 45 (mid)

$$\int_{\mathbb{R}^3}\left(b - \frac{1}{\mathfrak{D}(x)}\right)_-^{5/2}\mathrm{d}x \leq M\frac{5\pi^2}{4\sqrt{b}} \tag{1.25}$$

in the proof above one could have gotten the even tighter bound $K_1(Z) = \frac{6}{25}\sqrt{\frac{3}{5}}Z\left(\frac{Z}{C_1}\right)^{3/2}\frac{5\pi^2}{4\sqrt{b}}$.

Proof. To see this, notice that from (2.2) we have

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

from which it follows that

$$T_\psi \leq \frac{CN}{\lambda(1-\lambda)} + \frac{\mathcal{E}(\psi)}{\lambda} = \frac{\mathcal{E}(\psi)+CN}{\lambda} + \frac{CN}{1-\lambda}, \tag{2.5}$$

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

$$T_\psi \leq (\sqrt{\mathcal{E}(\psi)+CN} + \sqrt{CN})^2. \tag{2.6}$$

Proof. For $\mathcal{E}(\psi) = 0$ it follows by choosing $\lambda = 1/2$ in (2.3). Now assume $\mathcal{E}(\psi) \neq 0$, we then optimize (2.3) w.r.t λ:

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{\mathcal{E}(\psi)+CN}{\lambda} + \frac{CN}{1-\lambda}\right) = -\frac{\mathcal{E}(\psi)+CN}{\lambda^2} + \frac{CN}{(1-\lambda)^2} = 0. \tag{2.7}$$

Using that $0<\lambda<1$, this is equivalent to

$$-(1-\lambda)^2(\mathcal{E}(\psi)+CN) - \lambda^2 CN = 0, \tag{2.8}$$

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 $\mathcal{E}(\psi)\geq -CN$). We now insert this λ_- back into (2.3). First notice that by combining (2.3) and (2.7) we have

$$T_\psi/\lambda_- \leq \frac{\mathcal{E}(\psi)+CN}{\lambda_-^2} + \frac{CN}{(1-\lambda_-)\lambda_-} = \frac{CN}{(1-\lambda_-)^2} + \frac{CN}{(1-\lambda_-)\lambda_-} = \frac{CN}{(1-\lambda_-)^2\lambda_-}. \tag{2.9}$$

Thus, we find

$$\begin{aligned} T_\psi \leq \frac{CN}{(1-\lambda_-)^2} &= \frac{\mathcal{E}(\psi)^2 CN}{(-CN+\sqrt{\mathcal{E}(\psi)CN+C^2N^2})^2} = \frac{\mathcal{E}(\psi)^2}{(-\sqrt{CN}+\sqrt{\mathcal{E}(\psi)+CN})^2} \\ &= \frac{(\sqrt{\mathcal{E}(\psi)+CN}+\sqrt{CN})^2(\sqrt{\mathcal{E}(\psi)+CN}-\sqrt{CN})^2}{(-\sqrt{CN}+\sqrt{\mathcal{E}(\psi)+CN})^2} \\ &= (\sqrt{\mathcal{E}(\psi)+CN}+\sqrt{CN})^2, \end{aligned} \tag{2.10}$$

such that we have

$$T_\psi \leq (\sqrt{\mathcal{E}(\psi)+CN} + \sqrt{CN})^2, \tag{2.11}$$

as desired. □

(c)

It is known that for any $p > 0$ there exist a $C_p > 0$ independent of ρ_ψ such that

$$\left(\int_{\mathbb{R}^3} \rho_\psi(x)^{5/3}\,\mathrm{d}x\right)^{p/2} \int_{\mathbb{R}^3} |x|^p\,\rho_\psi(x)\,\mathrm{d}x \geq C_p \left(\int_{\mathbb{R}^3} \rho_\psi(x)\,\mathrm{d}x\right)^{1+\frac{5p}{6}}, \tag{2.12}$$

Thus from the previous sections it follows that

$$\left(\frac{1}{N}\int_{\mathbb{R}^3} \rho_\psi(x)\,|x|^p\,\mathrm{d}x\right)^{1/p} \geq C_p' \left(\sqrt{\mathcal{E}(\psi)/N + C} + \sqrt{C}\right)^{-1} N^{1/3}. \tag{2.13}$$

Proof. By the proof of problem 1.(b) we know that there exist C' independent of ρ_ψ such that

$$\int_{\mathbb{R}^3} \rho_\psi(x)^{5/3}\,\mathrm{d}x \leq C' T_\psi. \tag{2.14}$$

Combining this with problem 2.(b) we find that

$$\int_{\mathbb{R}^3} \rho_\psi(x)^{5/3}\,\mathrm{d}x \leq C'(\sqrt{\mathcal{E}(\psi) + CN} + \sqrt{CN})^2. \tag{2.15}$$

Now using that $\int_{\mathbb{R}^3} \rho_\psi(x)\,\mathrm{d}x = N$ we get from (2.12) the inequality

$$\left(\sqrt{C'}(\sqrt{\mathcal{E}(\psi) + CN} + \sqrt{CN})\right)^p \int_{\mathbb{R}^3} |x|^p\,\rho_\psi(x)\,\mathrm{d}x \geq C_p N^{1+5p/6}. \tag{2.16}$$

Using monotonicity of $x \mapsto x^{1/p}$ with $p > 0$, we find

$$\left(\sqrt{C'}(\sqrt{\mathcal{E}(\psi) + CN} + \sqrt{CN})\right)\left(\int_{\mathbb{R}^3} |x|^p\,\rho_\psi(x)\,\mathrm{d}x\right)^{1/p} \geq C_p N^{5/6} N^{1/p}, \tag{2.17}$$

which is equivalent to (since all quantities are positive)

$$\begin{aligned}\left(\frac{1}{N}\int_{\mathbb{R}^3} |x|^p\,\rho_\psi(x)\,\mathrm{d}x\right)^{1/p} &\geq \left(\sqrt{C'}(\sqrt{\mathcal{E}(\psi) + CN} + \sqrt{CN})\right)^{-1} C_p N^{5/6} \\ &= C_p' \left((\sqrt{\mathcal{E}(\psi)/N + C} + \sqrt{C})\right)^{-1} N^{1/3},\end{aligned} \tag{2.18}$$

where we defined $C_p' = C_p/\sqrt{C'}$ which is clearly independent of ρ_ψ. Setting $p = 1$ we find that the average distance from all the particles to the centre scales (at least) like $N^{1/3}$. $\square$

3 Local and locally bounded Hamiltonians are bounded

We are considering the Hilbert space $l^2(\mathbb{Z}^d;\mathbb{C}^N)$. We denote by $|y,\sigma_i\rangle$ the function $x\mapsto\delta_{x,y}|\sigma_i\rangle$ where $(|\sigma_i\rangle)_{i\in\{1,\dots,N\}}$ forms an orthonormal basis of $\mathbb{C}^N$. Thus, $(|x,\sigma_i\rangle)_{(x,i)\in\mathbb{Z}^d\times\{1,\dots,N\}}$ forms a basis of $l^2(\mathbb{Z}^d;\mathbb{C}^N)$. Letting P_x denote the orthogonal projection $P_x=\sum_{i=1}^N|x,\sigma_i\rangle\langle x,\sigma_i|$, we specify a Hamiltonian H, on $l^2(\mathbb{Z}^d;\mathbb{C}^N)$ by specifying its hopping matrices $H_{yx}=P_yHP_x$ and requiring:

- *R-locality*: $H_{yx}=0$ if $\|x-y\|_1\geq R$,
- *local boundedness*: There is a $c>0$ such that for all $x,y\in\mathbb{Z}^d$ we have $\|H_{yx}\|\leq c$.

A priori, it is not clear that specifying the hopping matrices defines the Hamiltonian uniquely. However, we show in this exercise that the hopping matrices, R-locality, and local boundedness indeed defines a unique Hamiltonian that, furthermore, is bounded.

Notice first that the set of all finite linear combination of $(|x,\sigma_i\rangle)_{(x,i)\in\mathbb{Z}^d\times\{1,\dots,N\}}$, denoted by $\langle|x,\sigma_i\rangle\rangle_{(x,i)\in\mathbb{Z}^d\times\{1,\dots,N\}}$, forms a dense subset of $l^2(\mathbb{Z}^d,C^N)$ (which is also why they form a basis). Furthermore, we note that the action of H on $\langle|x,\sigma_i\rangle\rangle_{(x,i)\in\mathbb{Z}^d\times\{1,\dots,N\}}$ is clearly defined by the hopping matrices since the hopping matrices defines the action on each basis vector

$$H|x,\sigma_i\rangle=\sum_{y\in\mathbb{Z}^d}H_{yx}|x,\sigma_i\rangle\,, \tag{3.1}$$

and this action can be linearly extended to all finite linear combinations of the basis vectors by

$$\begin{aligned}H\left(\sum_{(l,i)=(1,1)}^{(K,M)}c_{l,i}|x_l,i\rangle\right)=\sum_{(l,i)=(1,1)}^{(K,M)}c_{l,i}H|x_l,\sigma_i\rangle&=\sum_{(l,i)=(1,1)}^{(K,M)}\sum_{y\in\mathbb{Z}^d}c_{l,i}H_{yx_l}|x_l,\sigma_i\rangle\\&=\sum_{l=1}^{K}\sum_{y\in\mathbb{Z}^d}c_lH_{yx_l}|x_l,\sigma^l\rangle\,.\end{aligned} \tag{3.2}$$

where we introduced $|x_l,\sigma^l\rangle=\frac{1}{c_l}\sum_{i=1}^M c_{l,i}|x_l,\sigma_i\rangle$ and $c_l=(\sum_{i=1}^M|c_{l,i}|^2)^{1/2}$. Notice also that $M\leq N$. We clearly have that $(|x_l,\sigma^l\rangle)_{l\in\mathbb{Z}^d}$ are orthonormal vectors and $(c_l)_{l\in\mathbb{Z}^d}\in l^2(\mathbb{Z}^d)$. Here R-locality ensures that the sums in (3.1) and (3.2) are finite. Now notice that H is actually bounded on $\langle|x,\sigma_i\rangle\rangle_{(x,i)\in\mathbb{Z}^d\times\{1,\dots,N\}}$. This can be seen by the following estimate. Let $|v\rangle=\sum_{(l,i)=(1,1)}^{(K,M)}c_{l,i}|x_l,i\rangle$ be some finite linear combination of the basis vectors $|x,\sigma_i\rangle$. First for notational convenience we introduce the notation $|l\rangle=|x_l,\sigma^l\rangle$, with $|x_l,\sigma^l\rangle=\frac{1}{c_l}\sum_{i=1}^M c_{l,i}|x_l,\sigma_i\rangle$ and $c_l=(\sum_{i=1}^M|c_{l,i}|^2)^{1/2}$, such that $|v\rangle=\sum_{l=1}^K c_l|l\rangle$. Then we find

$$\left\|H\left(\sum_{l=1}^K c_l|l\rangle\right)\right\|_2^2=\sum_{l=1}^K\sum_{l'=1}^K\sum_{y\in Z^d}\sum_{y'\in Z^d}\langle l'|\,\overline{c_{l'}}(H_{y'x_{l'}})^*H_{yx_l}c_l|l\rangle\,. \tag{3.3}$$

Since $(H_{yx})^*$ is also R-local and locally bounded[4], and we have $(H_{yx})^* = (P_y H P_x)^* = (P_x H^* P_y) = H^*_{xy}$, we conclude that

$$\left\| H\left(\sum_{l=1}^{K} c_l \left|l\right\rangle\right)\right\|_2^2 = \sum_{l=1}^{K}\sum_{l'=1}^{K}\sum_{y\in Z^d} \left\langle l'\right| \overline{c_{l'}} H^*_{x_{l'}y} H_{yx_l} c_l \left|l\right\rangle . \tag{3.4}$$

Notice that $H^*_{x_{l'}y}H_{yx_l}$ is only non-zero if $\|x_l - x_{l'}\|_1 \leq \|x_l - y\|_1 + \|y - x_{l'}\|_1 \leq 2(R-1)$. Thereby we have

$$\begin{aligned}
\left\| H\left(\sum_{l=1}^{K} c_l \left|l\right\rangle\right)\right\|_2^2 &= \sum_{l=1}^{K}\sum_{l'=1}^{K}\sum_{y\in Z^d} \left\langle l'\right| \overline{c_{l'}} H^*_{x_{l'}y} H_{yx_l} c_l \left|l\right\rangle \\
&\leq \sum_{l=1}^{K} \sum_{\substack{l'=1\\ \|x_l - x_{l'}\|_1\leq 2(R-1)}}^{K} \sum_{y\in Z^d} \chi_{\{\|y-x_l\|_1<R\}}\chi_{\{\|y-x_{l'}\|_1<R\}} \left|c_l\right| \left|c_{l'}\right| c^2 \\
&\leq \mathrm{Num}(R)(2\mathrm{Num}(2R-1)-1)\sum_{l=1}^{K} \left|c_l\right|^2 c^2,
\end{aligned} \tag{3.5}$$

where $\mathrm{Num}(R)$ denotes the number of lattice points in

$$B_{\mathbb{Z}^d}(0,R)^{\|\cdot\|_1} = \{x\in\mathbb{Z}^d : \|x\|_1 < R\}, \tag{3.6}$$

i.e. the ball of radius R in the Manhattan metric. The first inequality of (3.5) is simply the triangle inequality of the sums followed by Cauchy-Schwartz and use of bounds $\|H_{yx}\| \leq c$ and $\left\|H^*_{x_{l'}y}\right\| \leq c$. To understand the second inequality notice that

$$\sum_{y\in\mathbb{Z}^d} \chi_{\{\|y-x_l\|_1<R\}}\chi_{\{\|y-x_{l'}\|_1<R\}} \leq \sum_{y\in\mathbb{Z}^d} \chi_{\{\|y-x_l\|_1<R\}} = \mathrm{Num}(R). \tag{3.7}$$

Furthermore, we used the following bound of the finite sum

$$\sum_{l=1}^{K} \sum_{\substack{l'=1\\ \|x_l - x_{l'}\|_1\leq 2(R-1)}}^{K} \left|c_l\right| \left|c_l'\right| \leq (2\mathrm{Num}(2R-1)-1)\sum_{l=1}^{K}\left|c_l\right|^2 . \tag{3.8}$$

This bound can be shown as follows, take the $\beta\in\{1,...,K\}$ such that $|c_\beta| \geq |c_l|$ for all $l\in\{1,...,K\}$. Then we observe

$$\sum_{l=1}^{K} \sum_{\substack{l'=1\\ \|x_l - x_{l'}\|_1\leq 2(R-1)}}^{K} \left|c_l\right| \left|c_l'\right| \leq (2\mathrm{Num}(2R-1)-1)\left|c_\beta\right|^2 + \sum_{\substack{l=1\\ l\neq\beta}}^{K} \sum_{\substack{l'=1\\ l'\neq\beta\\ \|x_l - x_{l'}\|_1\leq 2(R-1)}}^{K} \left|c_l\right| \left|c_l'\right|, \tag{3.9}$$

[4]This follows from the fact that $(H_{yx})^* = 0$ when $H_{yx} = 0$ and $\|(H_{yx})^*\| = \|(H_{yx})\| \leq c$.

where we have simply taken all terms in the sum of the form $|c_\beta||c_l|$ and replaced with the larger term $|c_\beta|^2$, and used that there is a maximal of $(2\mathrm{Num}(2R-1)-1)$ such terms. Here $2\mathrm{Num}(2R-1)-1$ comes from the bound on the distance between x_l and $x_{l'}$. By induction of (3.9) we find (3.8).
Notice now that $\sum_{l=1}^K |c_l|^2 = \left\|\sum_{l=1}^K c_l |l\rangle\right\|_2^2$. Thus, we have shown in (3.5) that

$$\left\|H\left(\sum_{l=1}^K c_l |l\rangle\right)\right\|_2^2 \leq \mathrm{Num}(R)(2\mathrm{Num}(2R-1)-1)c^2\left\|\sum_{l=1}^K c_l |l\rangle\right\|_2^2, \tag{3.10}$$

which implies $\|H\| \leq c\sqrt{\mathrm{Num}(R)(2\mathrm{Num}(2R-1)-1)}$. Therefore, we only need to bound $\mathrm{Num}(R)$. This can be done most easily by noticing that the ball $B_{\mathbb{Z}^d}(0,R)^{\|\cdot\|_1}$ can be embedded in $\mathbb{R}^d$. Now imagine forming unit d-dimensional cubes symmetrically around each lattice point in $B_{\mathbb{Z}^d}(0,R)^{\|\cdot\|_1}$, *i.e.* with the lattice point in the centre. Then the cubes overlap at most on a set of (Lebesgue) measure zero, and this collection of cubes is contained in a d-dimensional cube, $\mathcal{K}$, with diagonal $D = 2R$. Since D can be related to the side lengths, a, by $D = \sqrt{d}a$, we have $\mathrm{Vol}(\mathcal{K}) = (2R)^d d^{-d/2}$. Thus, as each lattice point corresponds to a cube of volume exactly 1, the number of of lattice point in $B_{\mathbb{Z}^d}(0,R)^{\|\cdot\|_1}$ can be bounded by

$$\mathrm{Num}(R) \leq (2R)^d d^{-d/2}. \tag{3.11}$$

Thereby, we arrive at the bound

$$\|H\| \leq c\sqrt{d^{-d/2}(2R)^d\left(2d^{-d/2}(2R-1)^d-1\right)} \leq c\sqrt{2}\left(\frac{2R}{\sqrt{d}}\right)^d, \tag{3.12}$$

where the second inequality presents a less tight bound, but more simple, expression. Now that it is known that H is bounded (and thus continuous) on the dense subspace $\langle |x,\sigma_i\rangle\rangle_{(x,i)\in\mathbb{Z}^d\times\{1,\ldots,N\}}$, it is clear that it extends to a bounded operator on all of $l^2(\mathbb{Z}^d;\mathbb{C}^N)$. We simply extend H to all limit-points of $\langle |x,\sigma_i\rangle\rangle_{(x,i)\in\mathbb{Z}^d\times\{1,\ldots,N\}}$ by continuity.

4 Wannier states

Cosider the Fermi projector of a one-dimensional transnationally invariant insulator with one occupied band. It is described by an analytic projection valued map $\mathbb{T}\to\mathrm{Proj}_1(\mathbb{C}^N) : k\mapsto\tilde{P}(k)$, where $\mathbb{T}$ is the one dimensional Brillouin zone (the circle). Suppose we have an analytic unit section $k\mapsto v(k)\in\mathbb{C}^N$ with $\|v(k)\| = 1$ and $\tilde{P}(k) = |v(k)\rangle\langle v(k)|$. We then define the Wannier states $w_x \in l^2(\mathbb{Z};\mathbb{C}^N)$ by

$$w_x(y) = \frac{1}{2\pi}\int_{\mathbb{T}} \mathrm{d}k\ \mathrm{e}^{-ik(x-y)}v(k), \quad \text{for any } x\in\mathbb{Z}. \tag{4.1}$$

(a)

We show first that the Wannier states $\{w_x : x \in \mathbb{Z}\}$ form an orthonormal basis of $\operatorname{Ran}(P)$ where $(P_{yx})_{j,i} = \langle y, \sigma_j | P | x, \sigma_i \rangle = \frac{1}{2\pi} \int_{\mathbb{T}} \mathrm{d}k \mathrm{e}^{ik(y-x)} \langle \sigma_j | \tilde{P}(k) | \sigma_i \rangle$. Let $|v\rangle \in \operatorname{Ran}(P)$ *i.e.* $|v\rangle = P|u\rangle$ for some $|u\rangle \in l^2(\mathbb{Z}; \mathbb{C}^N)$. We may calculate $|v\rangle$ by expanding

$$|u\rangle = \sum_{x\in\mathbb{Z}} \sum_{i=1}^{N} c_{x,i} |x, \sigma_i\rangle, \tag{4.2}$$

and using

$$\begin{aligned} \langle y, \sigma'_j | P |u\rangle &= \langle y, \sigma'_j | \sum_{x\in\mathbb{Z}} \sum_{i=1}^{N} c_{x,i} P |x, \sigma_i\rangle \\ &= \sum_{x\in\mathbb{Z}} \sum_{i=1}^{N} c_{x,i} \frac{1}{2\pi} \int_{\mathbb{T}} \mathrm{d}k \mathrm{e}^{ik(y-x)} \langle \sigma'_j | v(k)\rangle \langle v(k) | \sigma_i\rangle . \end{aligned} \tag{4.3}$$

Now notice that (Fourier inversion theorem)

$$v(k) = \sum_{x'\in\mathbb{Z}} w_{x'}(y') \mathrm{e}^{ik(x'-y')}. \tag{4.4}$$

where y' is arbitrary. Combining (4.3) and (4.4) we obtain

$$\begin{aligned} \langle y, \sigma'_j | P |u\rangle &= \sum_{x\in\mathbb{Z}} \sum_{x'\in\mathbb{Z}} \sum_{i=1}^{N} c_{x,i} \frac{1}{2\pi} \int_{\mathbb{T}} \mathrm{d}k \mathrm{e}^{ik(y-x)} \mathrm{e}^{ik(x'-y)} \langle \sigma'_j | w_{x'}(y)\rangle \langle v(k) | \sigma_i\rangle \\ &= \sum_{x\in\mathbb{Z}} \sum_{x'\in\mathbb{Z}} \sum_{i=1}^{N} c_{x,i} \frac{1}{2\pi} \int_{\mathbb{T}} \mathrm{d}k \mathrm{e}^{ik(x'-x)} \langle \sigma'_j | w_{x'}(y)\rangle \langle v(k) | \sigma_i\rangle \\ &= \langle y, \sigma'_j | \sum_{x'\in\mathbb{Z}} \tilde{c}_{x'} w_{x'} . \end{aligned} \tag{4.5}$$

where $\tilde{c}_{x'} = \sum_{x\in\mathbb{Z}} \sum_{i=1}^{N} c_{x,i} \frac{1}{2\pi} \int_{\mathbb{T}} \mathrm{d}k \mathrm{e}^{ik(x'-x)} \langle v(k) | \sigma_i\rangle = \sum_{x\in\mathbb{Z}} \sum_{i=1}^{N} c_{x,i} \langle w_{x'}(x) | \sigma_i\rangle = \langle w_{x'} | u\rangle$. Since $|y, \sigma'_j\rangle$ was arbitrary we conclude that $P|u\rangle = \sum_{x'\in\mathbb{Z}} \langle w_{x'} | u\rangle w_{x'}$. We note that the x' sum in the above calculation is absolutely convergent as a consequence of Parseval's identity with the fact that $v(k)$ is analytic. This shows that the Wannier states span $\operatorname{Ran}(P)$. It Remains to show that they are orthonormal and thus form an orthonormal basis.

To see this consider the inner product

$$\langle w'_x, w_x\rangle = \sum_{y\in\mathbb{Z}} \langle w_{x'}(y) | w_x(y)\rangle . \tag{4.6}$$

To calculate this we notice that $(w_x(y))_{y\in\mathbb{Z}^d}$ are the Fourier coefficients of $\mathrm{e}^{-ikx} v(k)$, and $(w'_x(y))_{y\in\mathbb{Z}^d}$ are similarly the Fourier coefficients of $\mathrm{e}^{-ikx'} v(k)$. Thus by analyticity of $v(k)$

and Parselval's identity we immediately conclude

$$\langle w_x', w_x \rangle = \sum_{y\in\mathbb{Z}} \langle w_{x'}(y)|w_x(y)\rangle = \frac{1}{2\pi}\int_{\mathbb{T}} \mathrm{d}k\mathrm{e}^{ik(x'-x)} \langle v(k)|v(k)\rangle = \frac{1}{2\pi}\int_{\mathbb{T}} \mathrm{d}k\mathrm{e}^{ik(x'-x)} = \delta_{x,x'}. \tag{4.7}$$

This concludes that the Wannier states are orthonormal.

(b)

Now as we have already seen the Wannier states are the Fourier coefficients of $v(k)$ as seen in (4.4). Thus, by analyticity of $k \mapsto v(k)$ it is a well-known fact that the Fourier coefficients and thus $w_x(y)$ must have exponential decay, *i.e.* there exist $C > 0$ and $\mu > 0$ such that

$$|w_x(y)| \leq C\mathrm{e}^{-\mu|x-y|} \tag{4.8}$$

(c)

We now show that the Wannier functions translates to each other *i.e.*

$$w_x(y) = w_{x+r}(y+r), \qquad \text{for all } x, y, z \in \mathbb{Z}. \tag{4.9}$$

This may be seen directly from the definition

$$w_x(y) = \frac{1}{2\pi}\int_{\mathbb{T}} \mathrm{d}k\ \mathrm{e}^{-ik(x-y)}v(k) = \frac{1}{2\pi}\int_{\mathbb{T}} \mathrm{d}k\ \mathrm{e}^{-ik((x+r)-(y+r))}v(k) = w_{x+r}(y+r) \tag{4.10}$$

(d)

We now show the converse, namely that if $\mathrm{Ran}\,(P)$ is spanned by an orthonormal family of Wannier states, w_x that are exponentially localized and are translated to each other, then P admits an analytic unit section. To do this notice that $\sum_{x\in\mathbb{Z}} w_x(y)\mathrm{e}^{ik(x-y)}$ is a finite sum due to the exponential localization. Furthermore, it is independent of y since

$$\sum_{x\in\mathbb{Z}} w_x(y)\mathrm{e}^{ik(x-y)} = \sum_{x\in\mathbb{Z}} w_{x-y}(0)\mathrm{e}^{ik(x-y)} = \sum_{z\in\mathbb{Z}} w_z(0)\mathrm{e}^{ikz}. \tag{4.11}$$

Thus we define $v(k) := \sum_{x\in\mathbb{Z}} w_x(y)\mathrm{e}^{ik(x-y)}$, then clearly $w_x(y) = \frac{1}{2\pi}\int_{\mathbb{T}} \mathrm{d}k\mathrm{e}^{-ik(x-y)}v(k)$. Furthermore, $v(k)$ defines a section of $\tilde{P}(k)$ since w_x spans $\mathrm{Ran}\,(P)$. Notice namely that

$$P = \sum_{x\in\mathbb{Z}} |w_x\rangle\langle w_x|, \tag{4.12}$$

since $(w_x)_{x\in\mathbb{Z}}$ is an orthonormal set spanning $\mathrm{Ran}\,(P)$. Thus we have

$$(P_{yx})_{j,i} = \sum_{x'\in\mathbb{Z}} \langle \sigma_j|w_{x'}(y)\rangle\langle w_{x'}(x)|\sigma_i\rangle = \frac{1}{2\pi}\int_{\mathbb{T}} \mathrm{d}k\mathrm{e}^{ik(y-x)} \langle\sigma_j|v(k)\rangle\langle v(k)|\sigma_i\rangle \tag{4.13}$$

where we used Parseval's identity in the second equality with the facts that $(\langle\sigma_j|w_{x'}(y)\rangle)_{x'\in\mathbb{Z}}$ are the Fourier coefficients of $\mathrm{e}^{iky}\langle\sigma_j|v(k)\rangle$ and that $(\langle w_{x'}(x)|\sigma_i\rangle)_{x'\in\mathbb{Z}}$ are the Fourier coefficients of $\mathrm{e}^{-ikx}\langle v(k),\sigma_i\rangle$. However, knowing that

$$(P_{yx})_{j,i} = \frac{1}{2\pi}\int_{\mathbb{T}} \mathrm{d}k \mathrm{e}^{ik(y-x)}\langle\sigma_j|\tilde{P}(k)|\sigma_i\rangle\,, \tag{4.14}$$

we conclude[5] that $\tilde{P}(k) = |v(k)\rangle\langle v(k)|$. Therefore, $\tilde{P}(k)v(k) = v(k)$ and $k\mapsto v(k)$ forms a section of $k\mapsto\tilde{P}(k)$. That $\langle v(k), v(k)\rangle = 1$ follows from Parseval's identity and the normalization of w_x again. Finally we notice that $k\mapsto v(k)$ is analytic as its Fourier coefficients are exponentially localized (thus the Cauchy-Riemann conditions can be verified in a neighbourhood of the real line by allowing k to take values in $\mathbb{C}$ and differentiating under the sum). This proves that $k\mapsto\tilde{P}(k)$ admits an analytic unit section.

[5]This is Fourier's inversion theorem applied to each matrix element (i,j).