

# Advanced Mathematical Physics, Assignment 1

Johannes Agerskov

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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

$$\sum_{1 \leq i < j \leq N} \int_{\mathbb{R}^{3N}} \frac{|\psi(x_1, \dots, x_N)|^2}{|x_i - x_j|} dx_1 \dots dx_N - D(\rho_\psi, \rho_\psi) \geq -C_{LO} \int_{\mathbb{R}^3} \rho_\psi(x)^{4/3} dx, \quad (1.1)$$

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

(a)

Let  $\delta > 0$  then

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

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

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

where we used that  $\int_{\mathbb{R}^3} \rho_\psi(x) dx = N$ . Now using that for  $\delta > 0$  and  $a, b \in \mathbb{R}$  it 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

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

□

(b)

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

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

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

*Proof.* By definition we have

$$(V_C)_\psi = \int_{\mathbb{R}^{3N}} \sum_{1 \leq i < j \leq N} \frac{|\psi(x_1, \dots, x_N)|^2}{|x_i - x_j|} - \sum_{i=1}^N \sum_{j=1}^M \frac{Z |\psi(x_1, \dots, x_N)|^2}{|x_i - R_j|} dx_1 \dots dx_N + \sum_{1 \leq j < k \leq M} \frac{Z^2}{|R_j - R_k|}. \quad (1.5)$$

Using that  $\psi$  is fermionic we find that

$$\int_{\mathbb{R}^{3N}} \sum_{i=1}^N \sum_{j=1}^M \frac{Z |\psi(x_1, \dots, x_N)|^2}{|x_i - R_j|} dx_1 \dots dx_N = \sum_{j=1}^M \frac{1}{N} \sum_{i=1}^N \int_{\mathbb{R}^3} \frac{Z \rho_\psi(x_i)}{|x_i - R_j|} dx_i = \sum_{j=1}^M \int_{\mathbb{R}^3} \frac{Z \rho_\psi(x)}{|x - R_j|} dx. \quad (1.6)$$

Furthermore, using the Lieb-Oxford inequality we find that

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

Therefore, by (a) we have

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

Now we use the fact that there exist a constant  $C > 0$  such that  $T_\psi \geq C \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} dx$ . 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

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

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

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

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

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

Combining this with (1.8) we find that

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

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

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

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

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

with some constants  $C_1, C_2 > 0$  independent of  $\psi$  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

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

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

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

from which the claim follows:

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

$\square$

(d)

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

$$\rho_\psi(x) = d \left( \frac{1}{\mathfrak{D}(x)} - b \right)^{3/2} \chi_{\{\frac{1}{\mathfrak{D}(x)} - b \geq 0\}}(x) \quad (1.18)$$

for some  $d > 0$  independent of  $\psi$  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

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

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

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

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

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

with  $K_1(Z) = \max \{0, -(C_1 d^{5/3} - Zd)\} \frac{8\pi}{\sqrt{b}}$ ,  $K_2(Z) = (Zb + C_2)$ , 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  $d$  we would have to minimize w.r.t to  $d$ . Thus we find  $d = \left( \frac{3Z}{5C_1} \right)^{3/2}$ .

## 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  $\mathcal{E}(\psi) = T_\psi + (V_C)_\psi \geq -CN$  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

$$(1 - \lambda)T_\psi + (V_C)_\psi \geq -\frac{CN}{1 - \lambda}, \quad (2.1)$$

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

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

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

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

from which it follows that

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

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

From this we may conclude that

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

*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  $\lambda$ :

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

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

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

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  $\lambda_-$  solution is consistent with  $0 < \lambda < 1$  (it is consistent since  $\mathcal{E}(\psi) \geq -CN$ ). We now insert this  $\lambda_-$  back into (2.2). First notice that by combining (2.2) and (2.6) we have

$$T_\psi/\lambda_- \leq \frac{\mathcal{E}(\psi) + CN}{\lambda_-^2} + \frac{CN}{(1 - \lambda_-)\lambda_-} = \frac{CN}{(1 - \lambda_-)^2} + \frac{CN}{(1 - \lambda_-)\lambda_-} = \frac{CN}{(1 - \lambda_-)^2\lambda_-}. \quad (2.8)$$

Thus, we find

$$\begin{aligned}
 T_\psi &\leq \frac{CN}{(1-\lambda_-)^2} = \frac{\mathcal{E}(\psi)^2 CN}{(-CN + \sqrt{\mathcal{E}(\psi)CN + C^2 N^2})^2} = \frac{\mathcal{E}(\psi)^2}{(-\sqrt{CN} + \sqrt{\mathcal{E}(\psi) + CN})^2} \\
 &= \frac{(\sqrt{\mathcal{E}(\psi) + CN} + \sqrt{CN})^2 (\sqrt{\mathcal{E}(\psi) + CN} - \sqrt{CN})^2}{(-\sqrt{CN} + \sqrt{\mathcal{E}(\psi) + CN})^2} \\
 &= (\sqrt{\mathcal{E}(\psi) + CN} + \sqrt{CN})^2,
 \end{aligned} \tag{2.9}$$

such that we have

$$T_\psi \leq (\sqrt{\mathcal{E}(\psi) + CN} + \sqrt{CN})^2, \tag{2.10}$$

as desired.  $\square$

(c)

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

$$\left( \int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} dx \right)^{p/2} \int_{\mathbb{R}^3} |x|^p \rho_\psi(x) dx \geq C_p \left( \int_{\mathbb{R}^3} \rho_\psi(x) dx \right)^{1+\frac{5p}{6}}, \tag{2.11}$$

Thus from the previous sections it follows that

$$\left( \frac{1}{N} \int_{\mathbb{R}^3} \rho_\psi(x) |x|^p dx \right)^{1/p} \geq C'_p \left( \sqrt{\mathcal{E}(\psi)/N + C} + \sqrt{C} \right)^{-1} N^{1/3}. \tag{2.12}$$

*Proof.* By the proof of problem 1.(b) we know that there exist  $C'$  independent of  $\rho_\psi$  such that

$$\int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} dx \leq C' T_\psi. \tag{2.13}$$

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

$$\int_{\mathbb{R}^3} \rho_\psi(x)^{5/3} dx \leq C' (\sqrt{\mathcal{E}(\psi) + CN} + \sqrt{CN})^2. \tag{2.14}$$

Now using that  $\int_{\mathbb{R}^3} \rho_\psi(x) dx = N$  we get from (2.11) the inequality

$$\left( \sqrt{C'} (\sqrt{\mathcal{E}(\psi) + CN} + \sqrt{CN}) \right)^p \int_{\mathbb{R}^3} |x|^p \rho_\psi(x) dx \geq C_p N^{1+5p/6}. \tag{2.15}$$

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

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

which is equivalent to (since all quantities are positive)

$$\begin{aligned} \left( \frac{1}{N} \int_{\mathbb{R}^3} |x|^p \rho_\psi(x) dx \right)^{1/p} &\geq \left( \sqrt{C'} (\sqrt{\mathcal{E}(\psi) + CN} + \sqrt{CN}) \right)^{-1} C_p N^{5/6} \\ &= C'_p \left( (\sqrt{\mathcal{E}(\psi)/N + C} + \sqrt{C}) \right)^{-1} N^{1/3}, \end{aligned} \quad (2.17)$$

where we defined  $C'_p = C_p / \sqrt{C'}$  which is clearly independent of  $\rho_\psi$ . 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  $H_{yx} = P_y H P_x$  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  $l^2(\mathbb{Z}^d, \mathbb{C}^N)$  (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

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

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

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

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

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

Since we require the Hamiltonian to be self-adjoint we have  $H_{yx}^* = (P_y H P_x)^* = (P_x H P_y) = H_{xy}$ . Hence, we find

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

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

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

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

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

*i.e.* the ball of radius  $R$  in the Manhattan metric. The first inequality is simply the triangle inequality of the sums followed by Cauchy-Schwartz and use of bound  $\|H_{yx}\| < c$ . To understand the second inequality notice that  $\sum_{y \in \mathbb{Z}^d} \chi_{\{\|y - x_l\|_1 < R\}} \chi_{\{\|y - x_{l'}\|_1 < R\}} \leq \sum_{y \in \mathbb{Z}^d} \chi_{\{\|y - x_l\|_1 < R\}} = \text{Num}(R)$ . Furthermore, we used the following bound of the finite sum

$$\sum_{l=1}^K \sum_{\substack{l'=1 \\ \|x_l - x_{l'}\|_1 \leq 2(R-1)}}^K |c_l| |c_{l'}| \leq (2\text{Num}(2R-1) - 1) \sum_{l=1}^K |c_l|^2. \quad (3.7)$$

To understand this bound, take the  $\beta \in \{1, \dots, K\}$  such that  $|c_\beta| \geq |c_l|$  for all  $l \in \{1, \dots, K\}$ . Then we observe

$$\sum_{l=1}^K \sum_{\substack{l'=1 \\ \|x_l - x_{l'}\|_1 \leq 2(R-1)}}^K |c_l| |c_{l'}| \leq (2\text{Num}(2R-1) - 1) |c_\beta|^2 + \sum_{\substack{l=1 \\ l \neq \beta}}^K \sum_{\substack{l'=1 \\ l' \neq \beta \\ \|x_l - x_{l'}\|_1 \leq 2(R-1)}}^K |c_l| |c_{l'}|, \quad (3.8)$$



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  $(2\text{Num}(2R-1)-1)$  such terms. Here  $2\text{Num}(2R-1)-1$  comes from the bound on the distance between  $x_l$  and  $x_{l'}$ . By induction of (3.8) we find (3.7).

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

$$\left\| H \left( \sum_{l=1}^K c_l |l\rangle \right) \right\|_2^2 \leq \text{Num}(R)(2\text{Num}(2R-1)-1)c^2 \left\| \sum_{l=1}^K c_l |l\rangle \right\|_2^2, \quad (3.9)$$

which implies  $\|H\| \leq c\sqrt{\text{Num}(R)(2\text{Num}(2R-1)-1)}$ . Therefore, we only need to bound  $\text{Num}(R)$ . 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 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  $\text{Vol}(\mathcal{K}) = (2R)^d d^{-d/2}$ . 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

$$\text{Num}(R) \leq (2R)^d d^{-d/2}. \quad (3.10)$$

Thereby, we arrive at the bound

$$\|H\| \leq c\sqrt{d^{-d/2}(2R)^d (2d^{-d/2}(2R-1)^d - 1)} \leq c\sqrt{2} \left( \frac{2R}{\sqrt{d}} \right)^d, \quad (3.11)$$

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

$\langle |x, \sigma_i\rangle \rangle_{(x,i) \in \mathbb{Z}^d \times \{1, \dots, N\}}$ , 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  $\langle |x, \sigma_i\rangle \rangle_{(x,i) \in \mathbb{Z}^d \times \{1, \dots, N\}}$  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  $\mathbb{T} \rightarrow \text{Proj}_1(\mathbb{C}^N) : k \mapsto \tilde{P}(k)$ , 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

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

(a)

We show first that the Wannier states  $\{w_x : x \in \mathbb{Z}\}$  form an orthonormal basis of  $\text{Ran}(P)$  where  $(P_{yx})_{j,i} = \langle y, \sigma_j | P | x, \sigma_i \rangle = \int_{\mathbb{T}} dk e^{ik(y-x)} \langle \sigma_j | \tilde{P}(k) | \sigma_i \rangle$ . Let  $|v\rangle \in \text{Ran}(P)$  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

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

and using

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

Now notice that (Fourier inversion theorem)

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

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

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

where  $\tilde{c}_{x'} = \sum_{x \in \mathbb{Z}} \sum_{i=1}^N c_{x,i} \int_{\mathbb{T}} dk e^{ik(x-x')} \langle v(k) | \sigma_i \rangle$ . Since  $|y, \sigma'_j\rangle$  was arbitrary we conclude that  $P|u\rangle = \sum_{x' \in \mathbb{Z}} \tilde{c}_{x'} w_{x'}$ . 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  $l^2(\mathbb{Z}; \mathbb{C}^N)$ . It Remains to show that they are orthonormal and thus form an orthonormal basis.

To see this consider the inner product

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

To calculate this we notice that  $w_x(y)$  are the Fourier coefficients of  $e^{-ikx} v(k)$ , and  $w'_x(y)$  are similarly the Fourier coefficients of  $e^{-ikx'} v(k)$ . Thus by analyticity of  $v(k)$  and Parseval's

identity we immediately conclude

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

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

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

(c)

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

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

This may be seen directly from the definition

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

(d)

We now show the converse, namely that if  $\text{Ran}(P)$  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  $\sum_{x \in \mathbb{Z}} w_x(y) e^{ik(x-y)}$  is a finite sum due to the exponential localization. Furthermore, it is independent of  $y$  since

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

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

$$(P_{yx})_{j,i} = \sum_{x' \in \mathbb{Z}} \langle \sigma_j | w_{x'}(y) \rangle \langle w_{x'}(x) | \sigma_i \rangle = \frac{1}{2\pi} \int_{\mathbb{T}} dk e^{ik(y-x)} \langle \sigma_j | v(k) \rangle \langle v(k) | \sigma_i \rangle \quad (4.12)$$

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  $e^{iky} \langle \sigma_j | v(k) \rangle$  and that  $(\langle w_{x'}(x) | \sigma_i \rangle)_{x' \in \mathbb{Z}}$  are the Fourier coefficients of

$e^{-ikx} \langle v(k), \sigma_i \rangle$ . However, knowing that

$$(P_{yx})_{j,i} = \frac{1}{2\pi} \int_{\mathbb{T}} dk e^{ik(y-x)} \langle \sigma_j | \tilde{P}(k) | \sigma_i \rangle, \quad (4.13)$$

we conclude 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 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.