Advanced Mathematical Physics, Assignment 1

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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

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

□

(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. □

(c)

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

$$\mathcal{E}(\psi) \geq C_1\int_{\mathbb{R}^3} \rho_\psi(x)^{5/3}\,\mathrm{d}x - Z\int_{\mathbb{R}^3} \rho_\psi(x)\left(\frac{1}{\mathfrak{D}(x)} - b\right)\mathrm{d}x - ZbN - C_2N. \tag{1.14}$$

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

$$\mathcal{E}(\psi) \geq C_1\int_{\mathbb{R}^3} \rho_\psi(x)^{5/3}\,\mathrm{d}x - Z\int_{\mathbb{R}^3} \rho_\psi(x)\frac{1}{\mathfrak{D}(x)}\,\mathrm{d}x - C_2N. \tag{1.15}$$

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:

$$\mathcal{E}(\psi) \geq C_1\int_{\mathbb{R}^3} \rho_\psi(x)^{5/3}\,\mathrm{d}x - Z\int_{\mathbb{R}^3} \rho_\psi(x)\left(\frac{1}{\mathfrak{D}(x)} - b\right)\mathrm{d}x - ZbN - C_2N. \tag{1.17}$$

□

(d)

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

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

for some $d > 0$ 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

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

Now defining $\alpha := b^{-1}$ 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 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 $K_1(Z) = \max\left\{0, -(C_1 d^{5/3} - Zd)\right\} \frac{8\pi}{\sqrt{b}}$, $K_2(Z) = (Zb + C_2)$, 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 $\mathcal{E}(\psi) = T_\psi + (V_\mathrm{C})_\psi \geq -CN$ 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 to

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

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 $\mathcal{E}(\psi) \geq -CN$). We now insert this λ_- back into (2.2). First notice that by combining (2.2) and (2.6) we have

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

Thus, we find

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

such that we have

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

as desired. □

(c)

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

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

Thus from the previous sections it follows that

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

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

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

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

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

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

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

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

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

which is equivalent to (since all quantities are positive)

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

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 $N^{1/3}$. □

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

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

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: First for notational convenience we introduce the notation $A=\{(l,i):l\in\{1,\dots,K\},\ i\in\{1,\dots,M\}\}$ such that $\sum_{(l,i)=(1,1)}^{(K,M)}=\sum_{\alpha\in A}$, and $c_\alpha=c_{l,i}$, and $|\alpha\rangle=|x_l,\sigma_i\rangle$, and $x_\alpha=x_l$ for $\alpha=(l,i)$.

$$\left\|H\left(\sum_{\alpha\in A}c_\alpha|\alpha\rangle\right)\right\|_2^2=\sum_{\alpha\in A}\sum_{\alpha'\in A}\sum_{y\in Z^d}\sum_{y'\in Z^d}\langle\alpha'|\,\overline{c_{\alpha'}}H^*_{y'x_{\alpha'}}H_{yx_\alpha}c_\alpha|\alpha\rangle. \tag{3.3}$$

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

$$\left\| H\left(\sum_{\alpha\in A} c_\alpha |\alpha\rangle\right)\right\|_2^2 = \sum_{\alpha\in A}\sum_{\alpha'\in A}\sum_{y\in Z^d} \langle\alpha'|\, \overline{c_{\alpha'}} H_{x_{\alpha'}y} H_{yx_\alpha} c_\alpha |\alpha\rangle \tag{3.4}$$

Notice that $H_{x_{\alpha'}y}H_{yx_\alpha}$ is only non-zero if $\|x_\alpha - x_{\alpha'}\|_1 \leq \|x_\alpha - y\|_1 + \|y - x_{\alpha'}\|_1 \leq 2(R-1)$. Thereby we have

$$\begin{aligned}\left\| H\left(\sum_{\alpha\in A} c_\alpha |\alpha\rangle\right)\right\|_2^2 &= \sum_{\alpha\in A}\sum_{\alpha'\in A}\sum_{y\in Z^d} \langle\alpha'|\, \overline{c_{\alpha'}} H_{x_{\alpha'}y} H_{yx_\alpha} c_\alpha |\alpha\rangle \\ &\leq \sum_{\alpha\in A}\sum_{\substack{\alpha'\in A\\ \|x_\alpha - x_{\alpha'}\|_1\leq 2(R-1)}}\sum_{y\in Z^d} \chi_{\{\|y-\alpha\|_1<R\}}\chi_{\{\|y-\alpha'\|_1<R\}} |c_\alpha|\,|c_{\alpha'}|\, c^2 \\ &\leq \mathrm{Num}(R)\sum_{\alpha\in A} N\cdot(2\mathrm{Num}(2R-1)-1)|c_\alpha|^2 c^2\end{aligned} \tag{3.5}$$

where $\mathrm{Num}(R)$ is number of points in $B_{\mathbb{Z}^d}(0,R)^{\|\cdot\|_1} = \{x\in\mathbb{Z}^d : \|x\|_1 < R\}$ (the ball of radius R in the Manhattan metric). The first inequality is simply triangle inequality of the sums followed by Cauchy-Schwartz and use of bound $\|H_{yx}\| < c$. To understand the second inequality notice that $\sum_{y\in\mathbb{Z}^d}\chi_{\{\|y-\alpha\|_1<R\}}\chi_{\{\|y-\alpha'\|_1<R\}} \leq \sum_{y\in\mathbb{Z}^d}\chi_{\{\|y-\alpha\|_1<R\}} = \mathrm{Num}(R)$. Furthermore, we used the following bound of the finite sum

$$\sum_{\alpha\in A}\sum_{\substack{\alpha'\in A\\ \|x_\alpha - x_{\alpha'}\|_1\leq 2(R-1)}} |c_\alpha|\,|c'_\alpha| \leq N(2\mathrm{Num}(2R-1)-1)\sum_{\alpha\in A}|c_\alpha|^2. \tag{3.6}$$

To understand this bound, take the $\beta\in A$ such that $|c_\beta| \geq |c_\alpha|$ for all $\alpha\in A$. Then we observe

$$\sum_{\alpha\in A}\sum_{\substack{\alpha'\in A\\ \|x_\alpha - x_{\alpha'}\|_1\leq 2(R-1)}} |c_\alpha|\,|c'_\alpha| \leq N(2\mathrm{Num}(2R-1)-1)\,|c_\beta|^2 + \sum_{\alpha\in A\setminus\{\beta\}}\sum_{\substack{\alpha'\in A\setminus\{\beta\}\\ \|x_\alpha - x_{\alpha'}\|_1\leq 2(R-1)}} |c_\alpha|\,|c'_\alpha|, \tag{3.7}$$

where we have simply taken all terms in the sum of the form $|c_\beta||c_\alpha|$ and replaced with the larger term $|c_\beta|^2$, and used that there is a maximal of $N(2\mathrm{Num}(2R-1)-1)$ such terms. Here N comes from the sum over the $\mathbb{C}^N$ index, and $2\mathrm{Num}(2R-1)-1$ comes from the bound on the distance between x_α and $x_{\alpha'}$. By induction of (3.7) we find (3.6).
Notice now that $\sum_{\alpha\in A}|c_\alpha|^2 = \left\|\sum_{\alpha\in A} c_\alpha|\alpha\rangle\right\|_2^2$. Thus, we have shown that

$$\left\| H\left(\sum_{\alpha\in A} c_\alpha |\alpha\rangle\right)\right\|_2^2 \leq N\cdot\mathrm{Num}(R)(2\mathrm{Num}(2R-1)-1)c^2\left\|\sum_{\alpha\in A} c_\alpha|\alpha\rangle\right\|_2^2, \tag{3.8}$$

which implies $\|H\| \leq c\sqrt{N\cdot\mathrm{Num}(R)(2\mathrm{Num}(2R-1)-1)}$. 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 small unit cubes symmetrically around each lattice point in $B_{\mathbb{Z}^d}(0,R)^{\|\cdot\|_1}$. Then non of the cubes overlap and this collection of cubes is contained in a d-dimensional cube, K, with diagonal $D = 2R$. Since D can be related to the side lengths, a, by $D = \sqrt{d}a$, we have $\mathrm{Vol}(K) = (2R)^d d^{-d/2}$. Thus the number of of lattice point in $B_{\mathbb{Z}^d}(0,R)^{\|\cdot\|_1}$ can be bounded by

$$\mathrm{Num}(R) \leq (2R)^d d^{-d/2}. \tag{3.9}$$

Thereby, we arrive at the bound

$$\|H\| \leq c\sqrt{N}\sqrt{d^{-d/2}(2R)^d\left(2d^{-d/2}(2R-1)^d - 1\right)} \leq c\sqrt{2N}\left(\frac{2R}{\sqrt{d}}\right)^d, \tag{3.10}$$

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