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Original Paper

Algebraic Localization of Wannier Functions Implies Chern Triviality in Non-periodic Insulators

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Abstract. For gapped periodic systems (insulators), it has been established that the insulator is topologically trivial (i.e., its Chern number is equal to 0) if and only if its Fermi projector admits an orthogonal basis with finite second moment (i.e., all basis elements satisfy $\int |\boldsymbol{x}|^2 |w(\boldsymbol{x})|^2 d\boldsymbol{x} < \infty$). In this paper, we extend one direction of this result to non-periodic gapped systems. In particular, we show that the existence of an orthogonal basis with slightly more decay $(\int |\boldsymbol{x}|^{2+\epsilon} |w(\boldsymbol{x})|^2 d\boldsymbol{x} < \infty$ for any $\epsilon > 0$) is a sufficient condition to conclude that the Chern marker, the natural generalization of the Chern number, vanishes.

1. Introduction

In electron structure theory, we are often interested in studying the subspace of low energy states spanned by the range of Fermi projector P. For numerical and theoretical purposes, we are in particular interested in finding a basis for the occupied space range (P) which is as well localized in space as possible. The elements of such a basis are known as Wannier functions or generalized Wannier functions (see review [8] and references therein). Typically for insulating materials (i.e., materials with a spectral gap), the existence of a spectral gap implies the Fermi projector P admits an integral kernel which is exponentially localized in the following sense (see, for example, [7]):

$$|P(\boldsymbol{x}, \boldsymbol{y})| \lesssim e^{-c_{gap}|\boldsymbol{x}-\boldsymbol{y}|}.$$
(1)

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Here, the constant c_{gap} depends on the size of the gap and vanishes as the gap closes. Therefore, we might expect that these insulators admit a basis which decays exponentially quickly in space. Somewhat surprisingly, even if P satisfies an estimate like Eq. (1), it is not necessarily true that range (P) admits a basis which decays exponentially quickly in space due to the existence of so-called topological obstructions.

In two-dimensional periodic insulators, it is now well understood [1,9,10] that the existence of a well-localized basis for range (P) is fully characterized by the Chern number which is defined as follows:

$$c(P) = \frac{1}{2\pi} \int_{\mathcal{B}} \operatorname{tr} \Big(P(\boldsymbol{k}) \big[\partial_{k_1} P(\boldsymbol{k}), \partial_{k_2} P(\boldsymbol{k}) \big] \Big) dk_1 \wedge dk_2,$$

where \mathcal{B} is the first Brillouin zone and $P(\mathbf{k})$ is the Bloch decomposition of P (see, e.g., [11]).

For periodic systems, P possesses a basis with finite second moment (known as Wannier functions) if and only if c(P) = 0, as established in [9]. Furthermore, c(P) = 0 if and only if there exists a basis of range (P) which is exponentially localized [1]. These results, which connect the existence of a basis with finite second moment to the vanishing of the Chern number and to the existence of an exponentially localized basis, are known as the localization dichotomy in periodic insulators.

Since the notion of the Chern number depends on the Bloch decomposition, the Chern number is no longer well defined for non-periodic systems. For generic systems, the Chern marker was proposed in [3,6] as an extension.

Definition 1 (*Chern Marker*). Let P be a projection on $L^2(\mathbb{R}^2)$ and χ_L be the indicator function of the set $[-L, L)^2$. The **Chern marker** of P is defined by

$$C(P) := \lim_{L \to \infty} \frac{2\pi i}{4L^2} \operatorname{tr} \left(\chi_L P \Big[[X, P], [Y, P] \Big] P \chi_L \right)$$

whenever the limit on the right-hand side exists.

Note that this generalizes the Chern number as for periodic systems the Chern number and the Chern marker agree [6,7]. Therefore, parallel to the periodic case, it is conjectured that the Chern marker characterizes the existence of localized Wannier basis for gapped systems [6,7]. Before continuing to state the conjecture more precisely and state the main result of this paper, which confirms the conjecture in one direction, let us start by making some definitions:

Definition 2. Suppose that A is a bounded linear operator on $L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$. We say that A admits an *exponentially localized kernel* with decay rate γ , if A admits an integral kernel $A(\cdot, \cdot) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$ and there exists a finite, positive constant C so that:

$$|A(\boldsymbol{x}, \boldsymbol{x}')| \le C e^{-\gamma |\boldsymbol{x} - \boldsymbol{x}'|} \quad a.e.$$

Definition 3 (s-localized generalized Wannier basis). Given an orthogonal projector P, we say an orthonormal basis $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}} \subseteq L^2(\mathbb{R}^2)$ is an s-localized generalized Wannier basis for P for some s > 0 if:

- (1) The collection $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ spans range (P),
- (2) There exists a finite, positive constant C and a collection of points $\{\mu_{\alpha}\}_{\alpha \in \mathcal{I}} \subseteq \mathbb{R}^2$ such that for all $\alpha \in \mathcal{I}$

$$\int_{\mathbb{R}^2} \langle \boldsymbol{x} - \boldsymbol{\mu}_{\alpha} \rangle^{2s} |\psi_{\alpha}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \le C,$$
(2)

where $\langle \pmb{x} - \pmb{\mu}_{\alpha} \rangle := (|\pmb{x} - \pmb{\mu}_{\alpha}|^2 + 1)^{1/2}$ is the Japanese bracket.

We refer to the collection $\{\mu_{\alpha}\}_{\alpha \in \mathcal{I}}$ as the *center points* of the basis $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$.

With these definitions, the localization dichotomy conjecture for non-periodic systems is as follows:

Conjecture (Localization dichotomy for non-periodic gapped systems). Let P be an orthogonal projector which admits an exponentially localized kernel. Then the following statements are equivalent:

- (a) P admits a generalized Wannier basis that is exponentially localized.
- (b) P admits a generalized Wannier basis that is s-localized for s = 1.
- (c) P is topologically trivial in the sense that its Chern marker C(P) exists and is equal to zero.

Note that obviously (a) implies (b). For the other equivalence, there have been a few works devoted to the study of non-periodic localization dichotomy. In particular, recent work [7] has shown that (b) \Rightarrow (c) with s > 4. Additionally, our previous work [4] has shown that (b) \Rightarrow (a) (and hence (b) \Rightarrow (c)) with s > 5/2. In this paper, we improve upon these previous works by showing that (b) \Rightarrow (c) for s > 1. Formally stated, the main result of this paper is the following:

Theorem 1. Suppose that P is an orthogonal projection on $L^2(\mathbb{R}^2)$ which admits an exponentially localized kernel. If P admits an $(1 + \delta)$ -localized generalized Wannier basis for some $\delta > 0$, then the Chern marker C(P) vanishes.

We note that Theorem 1 establishes only one part of the localization dichotomy, while the other direction, C(P) = 0 implies the existence of a localized generalized Wannier basis, is still quite open in the most general setting. We remark that for Hamiltonians with both rational and irrational magnetic flux it has been shown that C(P) = 0 implies exponential localization of a generalized Wannier basis [2].

Notations

Vectors in \mathbb{R}^d will be denoted by bold face with their components denoted by subscripts. For example, $\boldsymbol{v} = (v_1, v_2, v_3, \dots, v_d) \in \mathbb{R}^d$. For any $\boldsymbol{v} \in \mathbb{R}^d$, we use $|\cdot|$ to denote its ℓ^2 -norm and $|\cdot|_{\infty}$ to denote its ℓ^{∞} -norm; that is, $|\boldsymbol{v}| := (\sum_{i=1}^d v_i^2)^{1/2}$, $|\boldsymbol{v}|_{\infty} := \max_i |v_i|$. For any $\boldsymbol{x} \in \mathbb{R}^2$ and $a \in \mathbb{R}^+$, we define χ_a to be the indicator function of the set $[-a, a)^2$ and $B_a(\boldsymbol{x})$ be the ball of radius *a* centered at \boldsymbol{x} .

For any $f : \mathbb{R}^2 \to \mathbb{C}$, we will use ||f|| to denote the L^2 -norm. For any bounded linear operator A on $L^2(\mathbb{R}^2)$, we adopt the following conventions:

- Let ||A|| denote the spectral norm of A, $||A|| := \sup_{||f||=1} ||Af||$.
- If A is compact, let $\{\sigma_n(A)\}_{n=1}^{\infty}$ denote the singular values of A in decreasing order (i.e., if i < j then $\sigma_i(A) \ge \sigma_j(A)$).
- If A is compact, let $||A||_{\mathfrak{S}_p} = \left(\sum_{n=1}^{\infty} \sigma_n(A)^p\right)^{1/p}$ denote the Schatten *p*-norm for any $p \ge 1$.

Note that with this convention $||A|| = ||A||_{\mathfrak{S}_{\infty}}$.

In our estimates, C is used as a generic constants whose value may change from line to line. We also write $A \leq B$ if there exists a constant C such that $A \leq CB$.

Organization

The remainder of this paper is organized as follows. In Sect. 2, we outline the proof of Theorem 1 relying on a number of propositions (Proposition 2.4, 2.5, 2.6). Next, in Sect. 3 we state and prove three important technical estimates which are central to the proofs of these propositions. We provide proofs of Proposition 2.4 in Sect. 4, Proposition 2.5 in Sect. 5 and Proposition 2.6 in Sect. 6, respectively.

2. Proof of Main Theorem

We begin our proof by recalling the notion of bounded density which was introduced in [4] to simplify the analytic estimates. After recalling the consequences of bounded density (in particular, Lemma 2.2), we will use these results to prove the main theorem.

2.1. Bounded Density

We begin with the definition of bounded density

Definition 4. We say that a collection of points $\{\mu_{\alpha}\}_{\alpha \in \mathcal{I}}$ has **bounded density** if there exists a constant $M < \infty$ such that for all $\boldsymbol{x} \in \mathbb{R}^2$ we have

$$\#\{\alpha: \boldsymbol{\mu}_{\alpha} \in B_1(\boldsymbol{x})\} \le M$$

Importantly, if orthogonal projector P has an exponentially localized kernel, one can show that the center points of every well-localized basis must have bounded density.

Lemma 2.1. Let P be an orthogonal projector which admits an exponentially localized kernel. If $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ is an s-localized generalized Wannier basis for P for some s > 0, then the center points for $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ have bounded density.

Proof. For this proof, let $\chi_{B_r(a)}$ denote the characteristic function of the ball $B_r(a)$: $\chi_{B_r(a)}(x) = 1$ if $x \in B_r(a)$ and zero otherwise. We start by observing two important facts.

(i) If $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ is an s-localized basis for s > 0 with center points $\{\mu_{\alpha}\}_{\alpha \in \mathcal{I}}$, then we have that

$$\begin{split} \|(1-\chi_{B_r(\boldsymbol{\mu}_{\alpha})})\psi_{\alpha}\|^2 &= \int_{\mathbb{R}^2} (1-\chi_{B_r(\boldsymbol{\mu}_{\alpha})}(\boldsymbol{x})) \frac{\langle \boldsymbol{x}-\boldsymbol{\mu}_{\alpha} \rangle^{2s}}{\langle \boldsymbol{x}-\boldsymbol{\mu}_{\alpha} \rangle^{2s}} |\psi_{\alpha}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \\ &\lesssim r^{-2s} \int_{\mathbb{R}^2} \langle \boldsymbol{x}-\boldsymbol{\mu}_{\alpha} \rangle^{2s} |\psi_{\alpha}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \end{split}$$

Since the collection $\{\psi_{\alpha}\}_{\alpha\in\mathcal{I}}$ is s-localized, there exists a constant C, uniform in α , so that $\|(1-\chi_{B_r(\mu_{\alpha})})\psi_{\alpha}\|^2 \leq Cr^{-2s}$. Thus, we can find a radius R > 0 so that for all $\alpha \in \mathcal{I}$ and all $r \geq R$

$$\|(1 - \chi_{B_r(\mu_{\alpha})})\psi_{\alpha}\|^2 \le \frac{1}{2}.$$
(3)

Since $\|(1 - \chi_{B_r(\mu_{\alpha})})\psi_{\alpha}\|^2 + \|\chi_{B_r(\mu_{\alpha})}\psi_{\alpha}\|^2 = 1$, have that for all $r \ge R$, $\|\chi_{B_r(\mu_{\alpha})}\psi_{\alpha}\|^2 \ge \frac{1}{2}$.

(ii) Since P admits an exponentially localized kernel, one easily checks that there exists a constant K so that for all $a \in \mathbb{R}^2$:

$$\|\chi_{B_r(a)}P\|_{\mathfrak{S}_2}^2 = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \chi_{B_r(a)}(\boldsymbol{x}) |P(\boldsymbol{x}, \boldsymbol{y})|^2 \,\mathrm{d}\boldsymbol{x} \,\mathrm{d}\boldsymbol{y} \le Kr^2 \tag{4}$$

Now let $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ be an s-localized basis for some s > 0 and toward a contradiction suppose that the center points of this basis does not have bounded density.

Since the center points for this basis do not have bounded density, we can find a point $\boldsymbol{x}^* \in \mathbb{R}^2$ so that the ball $B_1(\boldsymbol{x}^*)$ has more than $4K(R+1)^2$ center points where the constant R is from Eq. (3) and the constant K is from Eq. (4). Let us denote the set of these center points by $\mathcal{A} := \{\alpha : \boldsymbol{\mu}_{\alpha} \in B_1(\boldsymbol{x}^*)\}$.

Due to Eq. (3) we have that

$$\|\chi_{B_{R+1}(x^*)}P\|_{\mathfrak{S}_2}^2 \le K(R+1)^2$$

but on the other hand we have that

$$\|\chi_{B_{R+1}(x^*)}P\|_{\mathfrak{S}_2}^2 \ge \sum_{\alpha \in \mathcal{A}} \|\chi_{B_{R+1}(x^*)}\psi_{\alpha}\|^2 \ge \frac{1}{2}(\#\mathcal{A}) \ge 2K(R+1)^2$$

where we have used that $\alpha \in \mathcal{A}$ implies that $B_R(\boldsymbol{\mu}_{\alpha}) \subseteq B_{R+1}(\boldsymbol{x}^*)$ and Eq. (3). This is a contradiction, and hence, the center points of $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ must have bounded density.

The usefulness of the notion of bounded density is that we can effectively treat any basis with bounded density to have its center points on the integer lattice.

Lemma 2.2. Let $\{\psi_{\alpha}\}_{\alpha \in \mathcal{I}}$ be an s-localized basis with center points $\{\mu_{\alpha}\}_{\alpha \in \mathcal{I}}$. For each $m \in \mathbb{Z}^2$ define

$$\mathcal{I}_{\boldsymbol{m}} := \left\{ \alpha \in \mathcal{I} : \boldsymbol{\mu}_{\alpha} \in \left[m_1 - \frac{1}{2}, m_1 + \frac{1}{2} \right] \times \left[m_2 - \frac{1}{2}, m_2 + \frac{1}{2} \right] \right\}$$
(5)

If the center points $\{\mu_{\alpha}\}_{\alpha \in \mathcal{I}}$ have bounded density, then:

• There exists a constant M, so that for all $m \in \mathbb{Z}^2$, $\#|\mathcal{I}_m| \leq M$

• If $\alpha \in \mathcal{I}_m$, then the center point of ψ_α can be treated as \boldsymbol{m} without loss of generality.

Proof of Lemma 2.2. Since the basis $\{\psi_{\alpha}\}_{\alpha\in\mathcal{I}}$ has center points with bounded density, we know that for each $\boldsymbol{m}\in\mathbb{Z}^2$ there are at most M center points contained in the square $[m_1-\frac{1}{2},m_1+\frac{1}{2})\times[m_2-\frac{1}{2},m_2+\frac{1}{2})$ as it is contained in $B_1(\boldsymbol{m})$. If ψ_{α} initially had center point $\boldsymbol{\mu}_{\alpha}\in\mathcal{I}_{\boldsymbol{m}}$, by construction $|\boldsymbol{m}-\boldsymbol{\mu}_{\alpha}|_2 \leq \frac{\sqrt{2}}{2}$. Therefore, using triangle inequality, it is easy to check that the collection $\{\psi_{\alpha}\}$ is s-localized if we choose \boldsymbol{m} as the center point of ψ_{α} instead of $\boldsymbol{\mu}_{\alpha}$ (perhaps with a slightly larger constant in Eq. (2)).

Remark 2.3. As a consequence Lemma 2.2, we can relabel the set of basis functions $\{\psi_{\alpha}\}_{\alpha\in\mathcal{I}}$ as $\psi_{m}^{(j)}$ where $j \in \{1,\ldots,\#|\mathcal{I}_{m}|\}$ whenever \mathcal{I}_{m} is non-empty (and $\psi_{m}^{(j)}$ is undefined if \mathcal{I}_{m} is empty).

Throughout our proof, we will assume that $\#|\mathcal{I}_m| = 1$ to simplify notation. Considering the case $\#|\mathcal{I}_m| \neq 1$ only has the effect of introducing a multiplicative factor of M to some of our upper bounds and does not change the overall argument or results.

2.2. Proof Outline

As discussed in the previous section, as a consequence of bounded density, any s-localized basis may be written as $\{\psi_m\}$ where ψ_m has its center point at m. Given a fixed choice of basis, we can now define the projector P_L which projects onto the basis functions centered within the box of size L:

$$P_L := \sum_{|\boldsymbol{m}|_{\infty} \le L} |\psi_{\boldsymbol{m}}\rangle \langle \psi_{\boldsymbol{m}}|.$$
(6)

Throughout the rest of this paper, we will assume that projector P_L is fixed and defined through a basis $\{\psi_m\}$ which is $(1 + \delta)$ -localized for some $\delta > 0$.

Unlike $\chi_L P$ which appears in the definition of the Chern marker, the projector P_L has finite rank and range $(P_L) \subseteq$ range (P). In some sense, the orthogonal projector P_L captures the local information of P in more controlled way than multiplying P by the cutoff χ_L as in the definition of the Chern marker. Importantly, thanks to the decay property of the basis functions $\{\psi_m\}$, approximating $\chi_L P$ with P_L incurs an error which is subleading compared to the area of χ_L :

Proposition 2.4. Suppose that P admits a $(1 + \delta)$ -localized basis where $\delta > 0$. There exists a constant C such that for all $L \ge 1$:

$$\|\chi_L P - P_L\|_{\mathfrak{S}_2} \le CL^{2/3}$$

Proof. Proved in Sect. 4.

As a consequence of this proposition, we can show that replacing $\chi_L P$ with P_L in the definition of the Chern marker does not change the overall limit:

Proposition 2.5. If P admits a $(1 + \delta)$ -localized generalized Wannier basis where $\delta > 0$, then

$$\lim_{L \to \infty} \frac{1}{L^2} \left\| \chi_L P[[X, P], [Y, P]] \right\| P \chi_L - P_L[[X, P], [Y, P]] P_L \right\|_{\mathfrak{S}_1} = 0.$$
(7)

Hence,

$$\lim_{L \to \infty} \frac{2\pi i}{4L^2} \operatorname{tr}\left(\chi_L P\Big[[X, P], [Y, P]\Big] P \chi_L\right) = \lim_{L \to \infty} \frac{2\pi i}{4L^2} \operatorname{tr}\left(P_L\Big[[X, P], [Y, P]\Big] P_L\right)$$
(8)

whenever at least one of the above limits exists.

Proof. Proved in Sect. 5

Hence, to prove Theorem 1 it suffices to show that if P admits an $(1+\delta)$ -localized generalized Wannier basis then

$$\lim_{L \to \infty} \frac{2\pi i}{4L^2} \operatorname{tr} \left(P_L \left[[X, P], [Y, P] \right] P_L \right) = 0.$$
(9)

Toward proving Eq. (9), we begin by observing that since P_L is defined through a $(1 + \delta)$ -localized basis, the position operator X is a bounded operator on range (P_L) for each L. In particular, we have that

$$\|XP_{L}\|^{2} \leq \sum_{\|\boldsymbol{m}\|_{\infty} \leq L} \|X\psi_{\boldsymbol{m}}\|^{2}$$

$$\leq \sum_{\|\boldsymbol{m}\|_{\infty} \leq L} \left(\|(X - m_{1})\psi_{\boldsymbol{m}}\| + |m_{1}|\|\psi_{\boldsymbol{m}}\|\right)^{2}$$

$$\leq \sum_{\|\boldsymbol{m}\|_{\infty} \leq L} \left(\|(X - m_{1})\psi_{\boldsymbol{m}}\| + L\right)^{2}$$

$$\lesssim L^{4}$$

Similarly, it is easily checked that Y is also a bounded operator on range (P_L) .

We will now use the fact that X and Y are both bounded operators on range (P_L) to perform some algebraic manipulations. Using the fact that $P^2 = P$ and [X, Y] = 0, one can verify that (see also [7], [5])

$$P\Big[[X,P],[Y,P]\Big]P = [PXP,PYP].$$

Therefore, since $P_L = P_L P = P P_L$, we have the following:

$$P_{L} [[X, P], [Y, P]] P_{L}$$

= $P_{L} [PXP, PYP] P_{L}$
= $P_{L} XPYP_{L} - P_{L} YPXP_{L}$
= $P_{L} X (P - P_{L} + P_{L}) YP_{L} - P_{L} Y (P - P_{L} + P_{L}) XP_{L}$
= $[P_{L} XP_{L}, P_{L} YP_{L}] + P_{L} X (P - P_{L}) YP_{L} - P_{L} Y (P - P_{L}) XP_{L}$.

These manipulations are justified since X and Y are bounded operators on range (P_L) . Since P_L is finite rank, $[P_L X P_L, P_L Y P_L]$ is traceless, and hence,

$$\operatorname{tr}\left(P_{L}\left[[X,P],[Y,P]\right]P_{L}\right) = \operatorname{tr}\left(P_{L}X(P-P_{L})YP_{L}-P_{L}Y(P-P_{L})XP_{L}\right).$$
(10)

Hence, using Hölder's inequality and $(P - P_L) = (P - P_L)^2$, we have that

$$|\operatorname{tr}\left(P_{L}\left[[X,P],[Y,P]\right]P_{L}\right)|$$

$$\leq \|P_{L}X(P-P_{L})YP_{L}\|_{\mathfrak{S}_{1}} + \|P_{L}Y(P-P_{L})XP_{L}\|_{\mathfrak{S}_{1}}$$

$$\leq 2\|(P-P_{L})XP_{L}\|_{\mathfrak{S}_{2}}\|(P-P_{L})YP_{L}\|_{\mathfrak{S}_{2}}.$$
(11)

Proposition 2.6. If P admits a $(1 + \delta)$ -localized generalized Wannier basis where $\delta > 0$ then

$$\lim_{L \to \infty} \frac{1}{L^2} \| (P - P_L) X P_L \|_{\mathfrak{S}_2}^2 = 0$$
 (12)

$$\lim_{L \to \infty} \frac{1}{L^2} \| (P - P_L) Y P_L \|_{\mathfrak{S}_2}^2 = 0.$$
 (13)

Proof. Proved in Sect. 6.

Since the mapping $x \mapsto \sqrt{x}$ is continuous for x > 0, Proposition 2.6 and Eq. (11) imply that

$$\lim_{L \to \infty} \frac{1}{L^2} \left| \operatorname{tr} \left(P_L \left[[X, P], [Y, P] \right] P_L \right) \right| = 0$$

which proves Eq. (9), completing the proof of Theorem 1.

3. Technical Estimates

In this section, we prove two technical estimates (Propositions 3.1 and 3.2) which are fundamental in our proofs of Propositions 2.4 and 2.6.

Proposition 3.1. If P admits a $(1+\delta)$ -localized generalized Wannier basis, then for all $a, b \geq 1$:

$$\|(1-\chi_{a+b})P_a\|_{\mathfrak{S}_2}^2 \lesssim a^2 b^{-2(1+\delta)}$$

Proof. We can expand the Hilbert–Schmidt norm we want to bound as follows:

$$\|(1-\chi_{a+b})P_a\|_{\mathfrak{S}_2}^2 = \sum_{|m|_{\infty} \le a} \|(1-\chi_{a+b})\psi_m\|^2.$$
(14)

Because of the separation between the sets $\{m \in \mathbb{Z}^2 : |m|_{\infty} \leq a\}$ and $\sup (1 - \chi_{a+b})$, we can show that each of the terms in the above sum are

small. In particular,

$$\begin{split} \|(1-\chi_{a+b})\psi_{m}\|^{2} \\ &= \int_{\mathbb{R}^{2}} (1-\chi_{a+b}(\boldsymbol{x})) |\psi_{m}(\boldsymbol{x})|^{2} \,\mathrm{d}\boldsymbol{x} \\ &= \int_{\mathbb{R}^{2}} (1-\chi_{a+b}(\boldsymbol{x})) \frac{(1+|x_{1}-m_{1}|+|x_{2}-m_{2}|)^{2(1+\delta)}}{(1+|x_{1}-m_{1}|+|x_{2}-m_{2}|)^{2(1+\delta)}} |\psi_{m}(\boldsymbol{x})|^{2} \,\mathrm{d}\boldsymbol{x} \end{split}$$

Since $|\boldsymbol{m}|_{\infty} \leq a$, we have the pointwise bound

$$\frac{(1-\chi_{a+b}(\boldsymbol{x}))}{(1+|x_1-m_1|+|x_2-m_2|)} \le \frac{1}{1+(a+b)-|\boldsymbol{m}|_{\infty}} \le \frac{1}{1+b}$$

Therefore, for each since ψ_m is $(1 + \delta)$ -localized we have that:

$$\|(1-\chi_{a+b})\psi_{\boldsymbol{m}}\|^{2} \leq (1+b)^{-2(1+\delta)} \int_{\mathbb{R}^{2}} (1+|x_{1}-m_{1}|+|x_{2}-m_{2}|)^{2(1+\delta)} |\psi_{\boldsymbol{m}}(\boldsymbol{x})|^{2} \,\mathrm{d}\boldsymbol{x}$$
$$\leq Cb^{-2(1+\delta)}$$

for some absolute constant C. Using this bound in Eq. (14), we conclude that

$$\|(1 - \chi_{a+b})P_a\|_{\mathfrak{S}_2}^2 \le \sum_{\substack{|m|_{\infty} \le a \\ \le a^2b^{-2(1+\delta)}}} Cb^{-2(1+\delta)}$$

which completes the proof.

Proposition 3.2. If P admits a $(1+\delta)$ -localized generalized Wannier basis, then for all $a, b \geq 1$:

$$\|\chi_a(P - P_{a+b})\|_{\mathfrak{S}_2}^2 \lesssim b^{-\delta} + ab^{-(1+\delta)}$$

We start by stating a lemma which we prove at the end of the section.

Lemma 3.3. Suppose that $\{\psi_{\mathbf{m}}\}$ is a $(1 + \delta)$ -localized basis. For any $a \ge 1$, we have the following bounds depending on the location of \mathbf{m} in relation to $\operatorname{supp}(\chi_a)$:

(i) If $|m_1| > a$ and $|m_2| > a$, then

$$\|\chi_a\psi_m\|^2 \lesssim \langle |m_1| - a \rangle^{-(1+\delta)} \langle |m_2| - a \rangle^{-(1+\delta)}.$$

(ii) If $|m_1| > a$ and $|m_2| \le a$, then

$$\|\chi_a\psi_m\|^2 \lesssim \langle |m_1| - a \rangle^{-2(1+\delta)}$$

(iii) If $|m_1| \le a \text{ and } |m_2| > a$, then

$$\|\chi_a\psi_m\|^2 \lesssim \langle |m_2| - a \rangle^{-2(1+\delta)}$$

With this lemma in hand, we can now prove Proposition 3.2.

Proof of Proposition 3.2. By the properties of the Hilbert–Schmidt norm, we see that

$$\|\chi_a(P - P_{a+b})\|_{\mathfrak{S}_2}^2 = \sum_{\|m\| > a+b} \|\chi_a \psi_m\|^2$$

We now split the set $\{m \in \mathbb{Z}^2 : |m|_{\infty} > a + b\}$ into three parts and bound each part separately

$$S_1 := \left\{ oldsymbol{m} : |m_1| > a + b ext{ and } |m_2| > a + b
ight\}$$

 $S_2 := \left\{ oldsymbol{m} : |m_1| > a + b ext{ and } |m_2| \le a + b
ight\}$
 $S_3 := \left\{ oldsymbol{m} : |m_1| \le a + b ext{ and } |m_2| > a + b
ight\}$

We start with controlling S_1 ; by applying Lemma 3.3(1), we have that

$$\begin{split} \sum_{m \in S_1} \|\chi_a \psi_m\|^2 &\leq \sum_{m \in S_1} \frac{C}{\langle |m_1| - a \rangle^{-(1+\delta)} \langle |m_2| - a \rangle^{-(1+\delta)}} \\ &\leq C b^{-\delta} \sum_{m \in S_1} \frac{1}{\langle |m_1| - a \rangle^{(1+\delta/2)} \langle |m_2| - a \rangle^{(1+\delta/2)}} \\ &\leq C b^{-\delta} \sum_{m \in \mathbb{Z}^2} \frac{1}{\langle |m_1| - a \rangle^{(1+\delta/2)} \langle |m_2| - a \rangle^{(1+\delta/2)}} \end{split}$$

where in the second to last line we have used that since $\mathbf{m} \in S_1$, $\min\{\langle |m_1| - a \rangle, \langle |m_2| - a \rangle\} > b$. Therefore,

$$\sum_{\boldsymbol{m}\in S_1} \|\chi_a\psi_{\boldsymbol{m}}\|^2 \lesssim b^{-\delta}$$

We now turn to bound the sum for $m \in S_2$. Applying Lemma 3.3(2), we have that there exists a constant C such that

$$\sum_{m \in S_2} \|\chi_a \psi_m\|^2 \le \sum_{|m_1| > a+b} \sum_{|m_2| \le a+b} \frac{C}{\langle |m_1| - a \rangle^{2(1+\delta)}} \\ \le Cb^{-(1+\delta)} \sum_{|m_1| > a+b} \sum_{|m_2| \le a+b} \frac{1}{\langle |m_1| - a \rangle^{(1+\delta)}} \\ \le 2C(a+b)b^{-(1+\delta)} \sum_{m_1 \in \mathbb{Z}} \frac{1}{\langle |m_1| - a \rangle^{(1+\delta)}}$$

where in the second to last line we have used that $\langle |m_1| - a \rangle > b$. Therefore,

$$\sum_{\boldsymbol{m}\in S_2} \|\chi_a\psi_{\boldsymbol{m}}\|^2 \lesssim (a+b)b^{-(1+\delta)}$$

Repeating the same calculation for S_3 making the obvious changes, we have that

$$\sum_{\boldsymbol{m}\in S_3} \|\chi_a\psi_{\boldsymbol{m}}\|^2 \lesssim (a+b)b^{-(1+\delta)}$$

Hence,

$$\|\chi_a(P - P_{a+b})\|_{\mathfrak{S}_2}^2 \le C_1 b^{-\delta} + C_2(a+b)b^{-(1+\delta)} + C_3(a+b)b^{-(1+\delta)}$$

which proves the result.

It remains to prove Lemma 3.3 to finish the proof.

Proof of Lemma 3.3. We will focus on the case when $|m_1| > a$ and $|m_2| > a$ and note the changes which must be made for the other cases. For these estimates, we will introduce the strip characteristic functions $\chi_D^{\text{strip},X}$ and $\chi_D^{\text{strip},Y}$ defined as follows

$$\chi_D^{\text{strip},X}(\boldsymbol{x}) = \begin{cases} 1 & |x_1| \le D \\ 0 & \text{otherwise} \end{cases} \qquad \qquad \chi_D^{\text{strip},Y}(\boldsymbol{x}) = \begin{cases} 1 & |x_2| \le D \\ 0 & \text{otherwise} \end{cases}$$

Next, let us define the distances $D_x := |m_1| - a$ and $D_y := |m_2| - a$. With these definitions, it is clear that up to a set of measure zero:

$$\chi_{D_x}^{\operatorname{strip},X}(\boldsymbol{x}-\boldsymbol{m})\chi_a(\boldsymbol{x}) = 0 \quad \text{and} \quad \chi_{D_y}^{\operatorname{strip},Y}(\boldsymbol{x}-\boldsymbol{m})\chi_a(\boldsymbol{x}) = 0$$

Therefore,

$$\begin{split} \|\chi_L \psi_{\boldsymbol{m}} \|^2 &= \int_{\mathbb{R}^2} \chi_a(\boldsymbol{x}) |\psi_{\boldsymbol{m}}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \\ &= \int_{\mathbb{R}^2} \chi_a(\boldsymbol{x}) \Big(1 - \chi_{D_x}^{\mathrm{strip},X}(\boldsymbol{x} - \boldsymbol{m}) \Big) |\psi_{\boldsymbol{m}}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \\ &= \int_{\mathbb{R}^2} \chi_a(\boldsymbol{x}) \Big(1 - \chi_{D_x}^{\mathrm{strip},X}(\boldsymbol{x} - \boldsymbol{m}) \Big) \frac{\langle x_1 - m_1 \rangle^{(1+\delta)}}{\langle x_1 - m_1 \rangle^{(1+\delta)}} |\psi_{\boldsymbol{m}}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \end{split}$$

By definition of $\chi_{D_x}^{\text{strip},X}$, we have the pointwise bound:

$$\frac{1 - \chi_{D_x}^{\text{strip}, X} (\boldsymbol{x} - \boldsymbol{m})}{\langle x_1 - m_1 \rangle} \le \frac{1}{\langle |m_1| - a \rangle}$$

Therefore,

$$\|\chi_L \psi_{\boldsymbol{m}}\|^2 \leq \frac{1}{\langle |m_1| - a \rangle^{(1+\delta)}} \int_{\mathbb{R}^2} \chi_a(\boldsymbol{x}) \langle x_1 - m_1 \rangle^{(1+\delta)} |\psi_{\boldsymbol{m}}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x}.$$

By similar logic,

$$\begin{split} \int_{\mathbb{R}^2} \chi_a(\boldsymbol{x}) \langle x_1 - m_1 \rangle |\psi_{\boldsymbol{m}}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \\ &= \int_{\mathbb{R}^2} \chi_a(\boldsymbol{x}) \Big(1 - \chi_{D_y}^{\mathrm{strip},Y}(\boldsymbol{x} - \boldsymbol{m}) \Big) \frac{\langle x_2 - m_2 \rangle^{(1+\delta)}}{\langle x_2 - m_2 \rangle^{(1+\delta)}} \langle x_1 - m_1 \rangle |\psi_{\boldsymbol{m}}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \\ &\leq \frac{1}{\langle |m_2| - a \rangle^{(1+\delta)}} \int_{\mathbb{R}^2} \chi_a(\boldsymbol{x}) \langle x_1 - m_1 \rangle^{(1+\delta)} \langle x_2 - m_2 \rangle^{(1+\delta)} |\psi_{\boldsymbol{m}}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x}. \end{split}$$

Hence,

$$\|\chi_a \psi_{\boldsymbol{m}}\|^2 \leq \frac{1}{\langle |m_1| - a \rangle^{(1+\delta)} \langle |m_2| - a \rangle^{(1+\delta)}} \\ \int_{\mathbb{R}^2} \chi_a(\boldsymbol{x}) \langle x_1 - m_1 \rangle^{(1+\delta)} \langle x_2 - m_2 \rangle^{(1+\delta)} |\psi_{\boldsymbol{m}}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x}.$$

Now recall that the geometric mean is bounded by the arithmetic mean so

$$\langle x_1 - m_1 \rangle^{(1+\delta)} \langle x_2 - m_2 \rangle^{(1+\delta)} \le \frac{1}{2} \Big(\langle x_1 - m_1 \rangle^{2(1+\delta)} + \langle x_2 - m_2 \rangle^{2(1+\delta)} \Big)$$

Therefore,

$$\|\chi_a \psi_m\|^2 \le \frac{\|\langle X - m_1 \rangle^{(1+\delta)} \psi_m \|^2 + \|\langle Y - m_2 \rangle^{(1+\delta)} \psi_m \|^2}{2\langle |m_1| - a \rangle^{(1+\delta)} \langle |m_1| - a \rangle^{(1+\delta)}}.$$

which implies the result since ψ_m is $(1 + \delta)$ -localized.

The case $|m_1| > a$ and $|m_2| \le a$ follows by inserting $\langle x_1 - m_1 \rangle^{2(1+\delta)} \langle x_1 - m_1 \rangle^{-2(1+\delta)}$ instead of $\langle x_1 - m_1 \rangle^{(1+\delta)} \langle x_2 - m_2 \rangle^{(1+\delta)} \langle x_1 - m_1 \rangle^{-(1+\delta)} \langle x_2 - m_2 \rangle^{-(1+\delta)}$; the case $|m_1| \le a$ and $|m_2| > a$ follows similarly. \Box

4. Proof of Proposition 2.4

Let us start by fixing some ℓ where $\ell \in [1, L)$ to be chosen later. We can split the quantity we would like to bound into four parts:

$$\begin{aligned} \|\chi_L P - P_L\|_{\mathfrak{S}_2} &\leq \|\chi_L (P - P_L)\|_{\mathfrak{S}_2} + \|(1 - \chi_L) P_L\|_{\mathfrak{S}_2} \\ &\leq \|\chi_L (P - P_{L+\ell})\|_{\mathfrak{S}_2} + \|\chi_L (P_{L+\ell} - P_L)\|_{\mathfrak{S}_2} \\ &+ \|(1 - \chi_L) (P_L - P_{L-\ell})\|_{\mathfrak{S}_2} + \|(1 - \chi_L) P_{L-\ell}\|_{\mathfrak{S}_2} \end{aligned}$$

The first term is bounded by Proposition 3.2; by letting a = L, $b = \ell$, there exists a constant C_1 so that:

$$\|\chi_L(P - P_{L+\ell})\|_{\mathfrak{S}_2} \le C_1(\ell^{-\delta} + L\ell^{-(1+\delta)})^{1/2}.$$
(15)

The next two terms are bounded by observing that

$$\operatorname{rank} (P_{L+\ell} - P_L) \le 4((L+\ell)^2 - L^2) \le 12L\ell$$
$$\operatorname{rank} (P_L - P_{L-\ell}) \le 4(L^2 - (L-\ell)^2) \le 12L\ell$$

where we have used that $\ell < L$. Hence, there exists a constant C_2 so that

$$\|\chi_L(P_{L+\ell} - P_L)\|_{\mathfrak{S}_2} + \|(1 - \chi_L)(P_L - P_{L-\ell})\|_{\mathfrak{S}_2} \le C_2(L\ell)^{1/2}.$$
 (16)

As for the final term, we can apply Proposition 3.1 with $a = L - \ell$, $b = \ell$ to conclude that there exists a constant C_3 so that

$$\|(1-\chi_L)P_{L-\ell}\|_{\mathfrak{S}_2} \le C_3 (L^2 \ell^{-2(1+\delta)})^{1/2}$$
(17)

Combining the bounds in Eqs. (15), (16), (17), we have that

$$\|\chi_L P - P_L\|_{\mathfrak{S}_2} \le C_1 (\ell^{-\delta} + L\ell^{-(1+\delta)})^{1/2} + C_2 (L\ell)^{1/2} + C_3 (L^2 \ell^{-2(1+\delta)})^{1/2}.$$

Now in the above equation, we have four different terms each which have different big–O as $L \to \infty$:

$$O(\ell^{-\delta})$$
 $O(L\ell^{-(1+\delta)})$ $O(L\ell)$ $O(L^2\ell^{-2(1+\delta)})$

Since $\ell > 1$, it is clear that the two dominating terms are $O(L\ell)$ and $O(L^2\ell^{-2(1+\delta)})$. Since we are free to choose ℓ , we will make a choice of ℓ so that these two terms balance. A simple calculation shows that choosing $\ell = L^{1/(3+2\delta)}$ gives

$$L\ell = L^{2(2+\delta)/(3+2\delta)}$$
$$L^{2}\ell^{-2(1+\delta)} = L^{2(2+\delta)/(3+2\delta)}$$
$$L\ell^{-(1+\delta)} = L^{(2+\delta)/(3+2\delta)}$$

This valid choice for ℓ since $\delta > 0$ so $\frac{1}{3+2\delta} < 1$. With this choice of ℓ , we have that

 $\|\chi_L(P-P_L)\|_2 \le C_1 (L^{-\delta/(3+2\delta)} + 2L^{(2+\delta)/(3+2\delta)})^{1/2} + C_2 L^{(2+\delta)/(3+2\delta)} + C_3 L^{(2+\delta)/(3+2\delta)}$ Hence, for $L \ge 1$

$$\|\chi_L P - P_L\|_{\mathfrak{S}_2} \lesssim L^{(2+\delta)/(3+2\delta)}.$$

The proof is completed by observing that for all $\delta \geq 0$:

$$\frac{2+\delta}{3+2\delta} \le \frac{2}{3}.$$

5. Proof of Proposition 2.5

For this proof, let us abbreviate the commutator in the definition of the Chern marker as C, that is:

$$\mathcal{C} := \left[[X, P], [Y, P] \right].$$

With this notation, we have that:

$$\chi_L P C P \chi_L - P_L C P_L = (\chi_L P - P_L) C P \chi_L + P_L C (P \chi_L - P_L)$$

Applying Hölder's inequality to the trace norm we want to bound, we have that

$$\begin{aligned} \|\chi_L P \mathcal{C} P \chi_L - P_L \mathcal{C} P_L \|_{\mathfrak{S}_1} \\ &\leq \|(\chi_L P - P_L) \mathcal{C} P \chi_L \|_{\mathfrak{S}_1} + \|P_L \mathcal{C} (P \chi_L - P_L)\|_{\mathfrak{S}_1} \\ &\leq \|\chi_L P - P_L \|_{\mathfrak{S}_2} \|\mathcal{C}\|_{\mathfrak{S}_\infty} \|P \chi_L \|_{\mathfrak{S}_2} + \|P_L \|_{\mathfrak{S}_2} \|\mathcal{C}\|_{\mathfrak{S}_\infty} \|P \chi_L - P_L \|_{\mathfrak{S}_2}. \end{aligned}$$

The right-hand side can be upper bounded by observing that

(i) Since P admits an exponentially localized kernel,

 $\|\mathcal{C}\|_{\mathfrak{S}_{\infty}} = \|\mathcal{C}\| = \|[[X, P], [Y, P]]\| \le 2\|[X, P]\|\| \|[Y, P]\| \lesssim 1.$

(ii) Additionally, since ${\cal P}$ admits an exponentially localized kernel, one easily checks that

$$\|P\chi_L\|_{\mathfrak{S}_2} \lesssim L.$$

(iii) Since rank $(P_L) \leq 4L^2$ and $||P_L|| \leq 1$, we have that

$$\|P_L\|_{\mathfrak{S}_2} \le 2L.$$

(iv) Proposition 2.4 implies that

$$\|\chi_L P - P_L\|_{\mathfrak{S}_2} \lesssim L^{2/3}$$

Combining these four bounds, we conclude that

$$\|\chi_L P \mathcal{C} P \chi_L - P_L \mathcal{C} P_L\|_{\mathfrak{S}_1} \lesssim L^{5/3}$$

Hence,

$$\lim_{L \to \infty} \frac{1}{L^2} \| \chi_L P \mathcal{C} P \chi_L - P_L \mathcal{C} P_L \|_{\mathfrak{S}_1} = 0$$

and the proposition is proved.

6. Proof of Proposition 2.6

Our main goal in this section is to show that the following quantity is $o(L^2)$:

$$\|(P-P_L)XP_L\|_{\mathfrak{S}_2}^2$$

The corresponding bound for Y follows by an analogous argument.

Similar to the proof of Proposition 2.5, our first step will be to introduce a length parameter $\ell \in [1, \frac{1}{2}L)$ to be fixed later. For any such choice of ℓ , by the properties of the Hilbert–Schmidt norm we have that:

$$\|(P - P_L)XP_L\|_{\mathfrak{S}_2}^2 = \|(P - P_L)XP_{L-2\ell}\|_{\mathfrak{S}_2}^2 + \|(P - P_L)X(P_L - P_{L-2\ell})\|_{\mathfrak{S}_2}^2$$
(18)

The second of these terms can be shown to be $O(L\ell)$ using that $(P - P_L)(P_L - P_{L-2\ell}) = 0$. In particular:

$$\begin{aligned} \|(P - P_L)X(P_L - P_{L-\ell})\|_{\mathfrak{S}_2}^2 &= \sum_{L-2\ell < |m|_{\infty} \le L} \|(P - P_L)X\psi_m\|^2 \\ &= \sum_{L-2\ell < |m|_{\infty} \le L} \|(P - P_L)(X - m_1)\psi_m\|^2 \\ &\le \left(\sup_m \|(X - m_1)\psi_m\|^2\right) \sum_{L-2\ell < |m|_{\infty} \le L} 1 \\ &\lesssim L\ell. \end{aligned}$$

Therefore, this term is $o(L^2)$ so long as we choose $\ell = o(L)$.

Returning to the first term in Eq. (18), using that $(P - P_L)P_{L-2\ell} = 0$ we have that

$$\|(P - P_L)XP_{L-2\ell}\|_{\mathfrak{S}_2}^2 = \sum_{\|m\|_{\infty} \le L-2\ell} \|(P - P_L)(X - m_1)\psi_m\|^2$$

We will now show that each of the terms in the above sum are small using Proposition 3.2. In particular, we have the following easy lemma

Lemma 6.1. If ψ_m is $(1+\delta)$ -localized with center point m where $|m|_{\infty} \leq L-2\ell$, then

$$\|(P - P_L)(X - m_1)\psi_{\boldsymbol{m}}\| \lesssim \ell^{-\delta} + L\ell^{-(1+\delta)}$$

Proof. We start by inserting $\chi_{L-\ell} + (1-\chi_{L-\ell})$ and applying triangle inequality

$$\|(P - P_L)(X - m_1)\psi_{\mathbf{m}}\| \le \|(P - P_L)\chi_{L-\ell}(X - m_1)\psi_{\mathbf{m}}\| + \|(P - P_L)(1 - \chi_{L-\ell})(X - m_1)\psi_{\mathbf{m}}\|$$

By Proposition 3.2, we have that

$$\|(P - P_L)\chi_{L-\ell}(X - m_1)\psi_m\| \le \|(P - P_L)\chi_{L-\ell}\|\|(X - m_1)\psi_m\| \le \ell^{-\delta} + L\ell^{-(1+\delta)}.$$

By repeating a similar argument as used in the proof of Proposition 3.1, it is easily verified that

$$\|(P - P_L)(1 - \chi_{L-\ell})(X - m_1)\psi_m\| \le \|(1 - \chi_{L-\ell})(X - m_1)\psi_m\| \le \ell^{-\delta}$$

high proves the lemma

which proves the lemma.

Using Lemma 6.1, it follows that:

$$|(P - P_L)XP_{L-\ell}||_{\mathfrak{S}_2}^2 \lesssim L^2(\ell^{-\delta} + L\ell^{-(1+\delta)})^2$$

For our final step, we will choose $\ell = L^{2/(2+\delta)}$. Since $\delta > 0$, note that this choice of ℓ is o(L) consistent with our previous requirement. Furthermore, we have that

$$||(P - P_L)XP_{L-\ell}||_{\mathfrak{S}_2}^2 \lesssim L^2 (L^{-2\delta/(2+\delta)} + L^{-\delta/(2+\delta)})^2.$$

Since $\delta > 0$, we conclude that

$$\lim_{L \to \infty} \frac{1}{L^2} \| (P - P_L) X P_{L-\ell} \|_{\mathfrak{S}_2}^2 = 0$$

which completes the proof.

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