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Optimally localized Wannier functions for quasi one-dimensional nonperiodic insulators

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Abstract

It is proved that for general, not necessarily periodic quasi one dimensional systems, the band position operator corresponding to an isolated part of the energy spectrum has discrete spectrum and its eigenfunctions have the same spatial localization as the corresponding spectral projection. As a consequence, an eigenbasis of the band position operator provides a basis of optimally localized (generalized) Wannier functions for quasi one dimensional systems. If the system has some translation symmetries (e.g. usual translations, screw transformations), they are "inherited" by the Wannier basis.

1 Introduction

Wannier functions (WF) were introduced by Wannier in 1937 [1] as bases in subspaces of states corresponding to energy bands in solids, bases consisting of exponentially localized functions (localized orbitals). For periodic crystals they are defined as Fourier transform of Bloch functions of the corresponding bands. Since then WF proved to be a key tool in quantum theory of solids as they provide a tight binding description of the electronic band structure of solids. At the conceptual level they lay at the foundation of all effective mass type theories e.g the famous Peierls-Onsager substitution describing the dynamics of Bloch electrons in the presence of an external magnetic field (see e.g.[2]and references therein). At the quantitative level, especially after the seminal paper by Marzari and Vanderbilt

[3], WF become an effective tool in *ab initio* computational studies of electronic properties of materials. Moreover during the last decades WF proved to be an essential ingredient in the study of low dimensional nanostructures such as linear chains of atoms, nanowires, nanotubes etc (see e.g. [4],[5]). In particular WF are essential for most formulations of transport phenomena using real space Green's function method based on Landauer-Büttiker formalism both at rigorous [6] and computational levels [7],[4].

A few remarks are in order here. The first one is that realistic low dimensional systems are not strictly one (two) dimensional but rather quasi one (two) dimensional and one has to take into account the (restricted) motion along perpendicular directions. This adds specific features as for example the screw symmetry in nanotubes and nanowires absent in strictly one dimensional systems. The second one is that realistic systems, due to the presence of defects, boundaries, randomness etc, do not have usually full translation symmetry and this ask for a theory of WF not based on Bloch formalism. Finally let us remind that contrary to a widespread opinion (see e.g. the discussion in [2]) that WF always exist for isolated band in solids this is not true. More precisely, in more than one dimension there are subtle topological obstructions and these are related to the QHE [8], [9], [10]: a band for which WF are known to exist gives no contribution to the quantum Hall current. It is then crucial to have rigorous proofs of the existence of exponentially localized WF.

For one dimensional periodic systems the existence of exponentially localized WF has been proved by Kohn in his classic paper [11] about analytic structure of Bloch functions. An extension of Kohn analysis to qusi one dimensional systems has been done recently by Prodan [12]. As for higher dimensions it was known since the work by des Cloizeaux [13] [14] that there are obstructions to the existence of exponentially localized WF and that these obstructions are of topological origin (more precisely as explicitly stated in [15] these obstructions are connected to the topology of a vector bundle of orthogonal projections). The fact that for simple bands of time reversal invariant systems the obstructions are absent was proved by des Cloizeaux [13] [14] under the additional condition of the existence of center of inversion and by Nenciu [15] in the general case. While the proofs in [13] [14], [15] did not use the vector bundle theory it was suggested in [2],[16] that the characteristic classes theory in combination with some deep results in the theory of analytic functions of several complex variables (Oka principle) can be used to give alternative proof of the above results and to extend them to composite bands of time reversal symmetric systems. This has been substantiated recently in [17], [10] where the existence of exponentially localized Wannier functions has been proved for composite bands of time reversal symmetric systems in two and three dimensions settling in the affirmative a long standing conjecture. In conclusion the situation is satisfactory as far as periodic time reversal symmetric hamiltonians are considered (as already mentioned for hamiltonians which are not time reversal symmetric exponentially localized Wannier functions might not exists).

Motivated by the great interest in nonperiodic structures much effort has been devoted to extend the results about existence of exponentially localized bases for isolated bands in nonperiodic systems. The basic difficulty stems from the fact that for nonperiodic systems one cannot define Wannier functions as Fourier transforms of the Bloch functions. One way out of the difficulty is to start from the periodic case or tight-binding limit where the

Wannier functions are known to exist and and use perturbation or "continuity" arguments. The basic idea is that since the obstructions are of topological origin the existence of exponentially localized WF is stable against perturbations. Indeed along these lines it has been possible to prove the existence of (generalized) WF for a variety of nonperiodic systems [18], [19], [20], [2], [16]. Since in the periodic case the obstructions to the existence of exponentially localized WF are absent [13],[14],[15] in one dimension it was naturally to conjecture [16],[21] that in one dimension WF exist for all isolated bands irrespective of periodicity properties.

The first problem to be solved was to find an alternative definition of WF. The basic idea goes back to Kivelson [22], who proposed to *define* the generalized WF as eigenfunctions of the "band position" operator. To substantiate the idea one has to prove that the band position operator is self-adjoint, has discrete spectrum and its eigenfunctions are exponentially localized. For the particular case of a periodic one dimensional crystal with one defect Kivelson proved that the eigenfunctions of the band position operator are indeed exponentially localized and asked for a general proof. In the general case, by a bootstrap argument, Niu [21] argued that the eigenfunctions of the band position operator (if they exist) are at least polynomially localized. In full generality the fact that for all isolated parts of the spectrum the band position operator is self-adjoint, has discrete spectrum and its eigenfunctions are exponentially localized has been proved in [23].

In this paper we extend the results in [23] to quasi one-dimensional systems i.e. three dimensional systems for which the motion extends to infinity only in one direction. In addition we add the result (which is new even in the strictly one dimensional case) that (see Theorem 2 below for details) the "density" of WF is uniformly bounded. While the main ideas of the proof are the same as in [23] there are major differences both at the technical and physical level. In particular for quasi one dimensional systems with screw symmetry the constructed WF inherits this symmetry a property which is very useful in computational applications. Finally let us remark that WF defined as eigenfunctions of the band position operator have very nice properties. They are maximally and exponential optimally localized in the sense of Marzari and Vanderbilt [3], are (up to uninteresting phases) uniquely defined and for real (i.e. time reversal invariant) Hamiltonians they can be chosen to be real functions and this solves for the general quasi one dimensional case the "strong conjecture" in Section V.A of [3].

2 The results

Consider in $L^2(\mathbb{R}^3)$ the following Hamiltonian describing a particle subjected to a scalar potential V:

$$H = \mathbf{P}^2 + V, \quad \mathbf{P} = -i\nabla, \quad \sup_{\mathbf{x}\in\mathbb{R}^3} \int_{|\mathbf{x}-\mathbf{y}|\leq 1} |V(\mathbf{y})|^2 d\mathbf{y} < \infty \tag{2.1}$$

which, as is well known (see [24]), is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. We have already said in the introduction that we are interested in potentials V which tend to zero as the distance from the Ox_1 axis tends to infinity. Let us now be more precise. The notation

$\mathbf{x} = (x_1, \mathbf{x}_\perp)$ will be used throughout the paper. For any $R > 0$, define:

$$I_V(R) := \sup_{x_1 \in \mathbb{R}, |\mathbf{x}_\perp| \geq R} \int_{|\mathbf{x}-\mathbf{y}| \leq 1} |V(\mathbf{y})|^2 d\mathbf{y}. \tag{2.2}$$

The decay assumption for V will be:

$$\lim_{R \to \infty} I_V(R) = 0. \tag{2.3}$$

It is easy to see that $[0, \infty) \subset \sigma(H)$ (using a Weyl sequence argument), thus the only region where H might have an isolated spectral island is below zero. Now suppose that σ_0 is such an isolated part of the spectrum and define:

$$-E_+ := \sup\{E : \ E \in \sigma_0\} < 0. \tag{2.4}$$

If Γ is a positively oriented contour of finite length enclosing σ_0, then the spectral subspace corresponding to σ_0 is:

$$\mathcal{K} \ := \mathrm{Ran}(P_0), \quad P_0 = \frac{i}{2\pi} \int_\Gamma (H - z)^{-1} dz. \tag{2.5}$$

At a heuristic level, due to the fact that the wave packets from $\mathcal{K}$ cannot propagate in the classically forbidden region (see (2.4) and (2.3)), at negative energies the motion is confined near the Ox_1 axis, i.e. the system has a quasi one dimensional behavior.

2.1 The technical results

The following proposition states the "localization" properties of P_0. On one hand, this give a precise meaning to the previously discussed quasi one dimensional character, and on the other hand it provides some key ingredients to the proof of exponential localization of eigenfunctions of the band position operator.

Let $a \in \mathbb{R}$, and let $\langle X_{\parallel,a} \rangle$ be the multiplication operator corresponding to:

$$g_a(\mathbf{x}) := \sqrt{(x_1 - a)^2 + 1}, \tag{2.6}$$

and $\langle X_\perp \rangle$ be multiplication operator given by:

$$g_\perp(\mathbf{x}) := \sqrt{|\mathbf{x}_\perp|^2 + 1}. \tag{2.7}$$

Proposition 1. *There exist $\alpha_\parallel > 0$, $\alpha_\perp > 0$, $M < \infty$ such that:*

$$\sup_{a \in \mathbb{R}} \| \, e^{\alpha_\parallel \langle X_{\parallel,a} \rangle} P_0 e^{-\alpha_\parallel \langle X_{\parallel,a} \rangle} \, \| \leq M, \quad \text{and} \tag{2.8}$$

$$\| \, e^{\alpha_\perp \langle X_\perp \rangle} P_0 e^{\alpha_\perp \langle X_\perp \rangle} \, \| \leq M. \tag{2.9}$$

The proof of Proposition 1 will also give values for $\alpha_\parallel$ and $\alpha_\perp$. In particular $\alpha_\perp$ can be any number strictly smaller than $\sqrt{E_+}$.

We now can formulate the main technical result of this paper. To emphasize its generality we stress that its proof only uses the decay condition (2.3) and the existence of an isolated part of the spectrum satisfying (2.4).

Theorem 2. *Let $X_\parallel$ be the operator of multiplication with x_1 in $L^2(\mathbb{R}^3)$ and consider in $\mathcal{K}$ the operator*

$$\hat{X}_\parallel := P_0 X_\parallel P_0 \tag{2.10}$$

defined on $\mathcal{D}(\hat{X}_\parallel) = \mathcal{D}(X_\parallel) \cap \mathcal{K}$. Then
i. *$\hat{X}_\parallel$ is self-adjoint on $\mathcal{D}(\hat{X})$;*
ii. *$\hat{X}_\parallel$ has purely discrete spectrum;*
iii. *Let $g \in G := \sigma(\hat{X}_\parallel)$ be an eigenvalue, m_g its multiplicity, and $\{W_{g,j}\}_{1\le j\le m_g}$ an orthonormal basis in the eigenspace of $\hat{X}$ corresponding to g. Then for all $\beta \in [0,1]$, there exists $M_1 < \infty$ independent of g, j and β such that:*

$$\int_{\mathbb{R}^3} e^{2(1-\beta)\alpha_\parallel |x_1 - g|} e^{2\beta\alpha_\perp |\mathbf{x}_\perp|} |W_{g,j}(\mathbf{x})|^2 d\mathbf{x} \le M_1, \tag{2.11}$$

where $\alpha_\parallel$ and $\alpha_\perp$ are the same exponents as for P_0;
iv. *Let $a \in \mathbb{R}$ and $L \ge 1$. Denote by $N(a,L)$ the total multiplicity of the spectrum of $\hat{X}_\parallel$ contained in $[a-L, a+L]$. Then there exists $M_2 < \infty$ such that*

$$N(a,L) \le M_2 \cdot L. \tag{2.12}$$

2.2 Further properties of the Wannier basis

We come now to the case when V (hence H) has additional symmetries. The point here is that although the Wannier functions are not eigenfunctions of H, one would like them to inherit in some sense the symmetries of H. The reason is that usually the Wannier basis is used in order to write down an effective Hamiltonian in $\mathcal{K}$, and one would like this effective Hamiltonian to inherit as much as possible the symmetries of H.

First we comment on time reversal invariance. Since $V(\mathbf{x})$ is real, H commutes with the anti-unitary operator induced by complex conjugation. It follows (see (2.5)) that P_0 and $\hat{X}_\parallel$ are also real, thus the eigenfunctions of $\hat{X}_\parallel$ can be chosen to be real. Hence Theorem 2 provides us with a Wannier basis which is time reversal invariant.

Second we consider the so called "screw-symmetry" along the Ox_1-axis, of much interest in the physics of carbon nanotubes. Namely, writing

$$\mathbf{x}_\perp = (r, \theta), \quad r \ge 0,\ \theta \in [0, 2\pi), \tag{2.13}$$

one assumes that for some $\theta_0 \in [0, 2\pi)$ we have:

$$V(x_1, r, \theta) = V(x_1 + 1, r, \theta + \theta_0). \tag{2.14}$$

Here $\theta + \theta_0$ has to be understood modulo 2π. Defining the screw-symmetry operators $T_n^{\theta_0}$ by:

$$(T_n^{\theta_0} f)(x_1, r, \theta) := f(x_1 - n, r, \theta - n\theta_0), \tag{2.15}$$

one has a (unitary!) representation of $\mathbb{Z}$ in $L^2(\mathbb{R}^3)$. Taking into account (2.14) and the fact that $[-\Delta, T_n^{\theta_0}] = 0$ (use cylindrical coordinates to prove this), one obtains:

$$[H, T_n^{\theta_0}] = 0, \tag{2.16}$$

and then from functional calculus and (2.5):

$$[P_0, T_n^{\theta_0}] = 0. \tag{2.17}$$

In particular, this implies that the family $\{T_n^{\theta_0}\}_{n\in\mathbb{Z}}$ induces a unitary representation of $\mathbb{Z}$ in $\mathcal{K}$. Moreover, from (2.10) and 2.17) one obtains:

$$[T_n^{\theta_0}, \hat{X}_\parallel] = n T_n^{\theta_0}. \tag{2.18}$$

Let $p < \infty$ be the number of eigenvalues of $\hat{X}_\parallel$ in the interval $[0, 1)$, and let $\{g_j\}_{j=1}^p$ be the distinct eigenvalues (each with multiplicity $m_j < \infty$). We have:

$$\hat{X}_\parallel W_{g_j,\alpha_j} = g_j W_{g_j,\alpha_j},\ \alpha_j = 1, 2, ..., m_{g_j}. \tag{2.19}$$

From (2.18) and (2.19) one obtains that for all $g_j,\ \alpha_j,\ n \in \mathbb{Z}$:

$$\hat{X}_\parallel T_n^{\theta_0} W_{g_j,\alpha_j} = (g_j + n) T_n^{\theta_0} W_{g_j,\alpha_j}. \tag{2.20}$$

Conversely, for every other $g \in \sigma(\hat{X}_\parallel)$, choose an eigenvector W_g. We can find $n \in \mathbb{Z}$ such that $g + n \in [0, 1)$. Since $\hat{X}_\parallel T_n^{\theta_0} W_g = (g + n) T_n^{\theta_0} W_g$, it means that $g + n$ must be one of the g_j's considered above. Therefore we proved the following corollary:

Corollary 3. *The spectrum of $\hat{X}_\parallel$ consists of a union of p ladders:*

$$G = \cup_{j=1}^p G_j, \quad G_j = \{g :\ g = g_j + n,\ n \in \mathbb{Z}\}, \quad j \in \{1, 2, ..., p\}, \tag{2.21}$$

and an orthonormal basis in $\mathcal{K}$ can be chosen as:

$$\begin{aligned} &W_{n,g_j,\alpha_j} := W_{g_j+n,\alpha_j} := T_n^{\theta_0} W_{g_j,\alpha_j}, \\ &n \in \mathbb{Z},\ j \in \{1, 2, ..., p\},\ \alpha_j \in \{1, 2, ..., m_{g_j}\}. \end{aligned} \tag{2.22}$$

It is interesting to express the effective Hamiltonian P_0HP_0 as an infinite matrix with the help of the Wannier basis. For notational simplicity we relabel the pair $(g_j,\ \alpha_j)$ as $l \in \{1, 2, ..., N_c = \sum_{j=1}^{p} m_{g_j}\}$ and write the Wannier basis as $\{W_{n,l}\}_{n\in\mathbb{Z},\, l\in\{1,2,...,N_c\}}$. Note that N_c is nothing that the number of Wannier functions per unit cell $[0, 1)$. Let

$$h^{\theta_0}_{l,k}(m, n) := \langle W_{m,l}, HW_{n,k}\rangle. \tag{2.23}$$

The important fact is that in spite of a rotation with an angle θ_0 for which it might happen that $\frac{\theta_0}{2\pi}$ to be irrational, from (2.16) and (2.22) one obtains (with the usual abuse of notation):

$$h^{\theta_0}_{l,k}(m, n) = h^{\theta_0}_{l,k}(m - n). \tag{2.24}$$

Then a standard computation gives the effective Hamiltonian as an operator in $(l^2)^{N_c}$ which is of *standard translation invariant* tight binding type:

$$(h^{\theta_0}_{eff}\phi)_l(m) := \sum_{k,n} h^{\theta_0}_{l,k}(m - n)\phi_k(n). \tag{2.25}$$

This is another consequence of the quasi one-dimensional character of the motion for negative energies. More precisely, it reflects the fact that for arbitrary values of θ_0, since $T^{\theta_0}_n$ is a unitary representation of $\mathbb{Z}$, one can still develop a Bloch type analysis but with a more complicated form of "Bloch" functions:

$$\Psi_k(\mathbf{x}) = e^{ikx_1}u_k(\mathbf{x}),\ u_k(\mathbf{x}) = T^{\theta_0}_n u_k(\mathbf{x}). \tag{2.26}$$

However, due to the complicated symmetry of the resulting Bloch functions (which does not allow to represent the fiber Hamiltonian as a differential operator on the unit cell with "simple" boundary conditions), the analysis gets much harder. The Bloch analysis reduces to the standard one (with a larger unit cell) for rational values of $\frac{\theta_0}{2\pi}$.

We end up this section with a remark about localization properties of Wannier functions as given by Theorem 2. As eigenfunctions of $\hat{X}_\parallel$ they are optimally localized in the sense of Marzari and Vanderbilt (see the discussion in [3]). More precisely, since the constants $\alpha_\parallel$ and $\alpha_\perp$ in (2.8), (2.9) and (2.11) are the same, the Wannier functions have maximal exponential localization in the sense that they have the same exponential decay as the integral kernel of P_0. This proves for general quasi one-dimensional systems the "strong conjecture" in Section VA of [3] concerning the exponential localization of the optimally localized Wannier functions.

3 Proofs

This section is devoted to the proof of Proposition 1 and Theorem 2. A certain number of unimportant finite positive constants appearing during the proof will be denoted by M.

One of the key ingredients in both proofs is the exponential decay of the integral kernel of the resolvent of Schrödinger operators. This is an elementary result in the Combes-Thomas-Agmon theory of weighted estimates. We summarize the needed result in:

Lemma 4. *Let W be a potential such that* $\sup_{\mathbf{x}\in\mathbf{R}^3}\int_{|\mathbf{x}-\mathbf{y}|\le 1}|W(\mathbf{y})|^2 d\mathbf{y}<\infty$. *Define* $K:=\mathbf{P}^2+W(\mathbf{x})$ *as an operator sum, and let h be a real function satisfying:*

$$h\in C^\infty(\mathbb{R}^3),\quad \sup_{\mathbf{x}\in\mathbb{R}^3}\{|\nabla h(\mathbf{x})|+|\Delta h(\mathbf{x})|\}=m<\infty. \tag{3.1}$$

Fix $z\in\rho(H)$. Then there exists $\alpha_z>0$ such that

$$\|e^{\alpha_z h}(K-z)^{-1}e^{-\alpha_z h}\|\le M, \tag{3.2}$$

$$\|e^{\alpha_z h}P_j(K-z)^{-1}e^{-\alpha_z h}\|\le M, \tag{3.3}$$

where $P_j=-i\frac{\partial}{\partial x_j}$, $j\in\{1,2,3\}$.

Without giving the details of the proof of Lemma 4, for later use we write down a key identity in (3.5): under the condition

$$1+\alpha_z(\pm i\mathbf{P}\cdot\nabla h\pm i\nabla h\cdot\mathbf{P}-\alpha_z|\nabla h|^2)(K-z)^{-1}\quad\text{invertible} \tag{3.4}$$

one has

$$\begin{aligned}&e^{\pm\alpha_z h}(K-z)^{-1}e^{\mp\alpha_z h}\\&=(K-z)^{-1}[1+\alpha_z(\pm i\mathbf{P}\cdot\nabla h\pm i\nabla h\cdot\mathbf{P}-\alpha_z|\nabla h|^2)(K-z)^{-1}]^{-1}.\end{aligned} \tag{3.5}$$

Then (3.4) holds true if for example $\alpha_z>0$ is small enough.

3.1 Proof of Proposition 1

Take Γ in (2.5) a contour of finite length enclosing σ_0 and satisfying

$$\operatorname{dist}(\Gamma,\sigma(H))=\frac{1}{2}\operatorname{dist}(\sigma_0,\sigma(H)\setminus\sigma_0). \tag{3.6}$$

Then since $|\nabla g_a|\le 1$, $|\Delta g_a|^2\le 2$, the estimate (2.8) follows directly from Lemma 4 by taking $\alpha_\parallel$ sufficiently small such that for all $z\in\Gamma$:

$$\|\alpha_\parallel(i\mathbf{P}\cdot\nabla g_a+i\nabla g_a\cdot\mathbf{P}-\alpha_\parallel|\nabla g_a|^2)(K-z)^{-1}\|\le b<1.$$

We now prove (2.9). If $R>0$, define:

$$H_R=-\Delta+(1-\chi_R)V, \tag{3.7}$$

where

$$\chi_R(\mathbf{x})=\begin{cases}1 & \text{for}\quad |\mathbf{x}_\perp|\le R\\ 0 & \text{for}\quad |\mathbf{x}_\perp|>R\end{cases}. \tag{3.8}$$

From (2.3) it follows that

$$\lim_{R\to\infty}\inf\sigma(H_R)=0.$$

In particular, for sufficiently large R, $(H_R - z)^{-1}$ is analytic inside Γ. Since $H - H_R = \chi_R V$, then using resolvent identities we obtain:

$$\begin{aligned}(H-z)^{-1} &= (H_R-z)^{-1} \\ &- (H_R-z)^{-1}\chi_R V (H_R-z)^{-1} + (H_R-z)^{-1}\chi_R V(H-z)^{-1}\chi_R V(H_R-z)^{-1}.\end{aligned} \tag{3.9}$$

From (2.5), (3.9) and the fact that $(H_R - z)^{-1}$ is analytic inside Γ one has

$$P_0 = \frac{i}{2\pi}\int_\Gamma (H_R-z)^{-1}\chi_R V(H-z)^{-1}\chi_R V(H_R-z)^{-1}. \tag{3.10}$$

Notice that for all $\alpha > 0$:

$$\sup_{\mathbf{x}\in\mathbf{R}^3}\int_{|\mathbf{x}-\mathbf{y}|\le 1} |(e^{\alpha g_\perp}\chi_R V)(\mathbf{y})|^2 d\mathbf{y} < \infty. \tag{3.11}$$

Take now $\alpha_\perp > 0$ such that 3.4 holds true for all $z \in \Gamma$, $K = H_R$, $h = g_\perp$ and $\alpha_z = \alpha_\perp$. That is let us suppose that

$$1 + \alpha_\perp(\pm i\mathbf{P}\cdot\nabla g_\perp \pm i\nabla g_\perp\cdot\mathbf{P} - \alpha_\perp|\nabla g_\perp|^2)(H_R-z)^{-1} \quad \text{is invertible} \tag{3.12}$$

uniformly on Γ. Then we can rewrite P_0 as:

$$\begin{aligned}P_0 = e^{-\alpha_\perp\langle X_\perp\rangle}&\left\{\frac{i}{2\pi}\int_\Gamma \left[e^{\alpha_\perp\langle X_\perp\rangle}(H_R-z)^{-1}e^{-\alpha_\perp\langle X_\perp\rangle}\right]\right. \\ &\left[e^{\alpha_\perp g_\perp}\chi_R V(H-z)^{-1}\right]\left[e^{\alpha_\perp g_\perp}\chi_R V(H_R-z)^{-1}\right] \\ &\left.\left[1+\alpha_\perp(-i\mathbf{P}\cdot\nabla g_\perp - i\nabla g_\perp\cdot\mathbf{P} - \alpha_\perp|\nabla g_\perp|^2)(H_R-z)^{-1}\right]^{-1} dz\right\} e^{-\alpha_\perp\langle X_\perp\rangle}.\end{aligned} \tag{3.13}$$

Due to (3.11) the operator under the integral sign is uniformly bounded in z and the proof of Proposition 1 is finished provided we can show why we can choose $\alpha_\perp$ as close to $\sqrt{E_+}$ as we want. The argument is as follows. Choose $0 \le \alpha_\perp < \sqrt{E_+}$. Choose a contour Γ which is very close to σ_0, at a distance $\delta > 0$, infinitesimally small. Using the spectral theorem (or in this case the Plancherel theorem), there exists δ small enough such that the following estimates hold true:

$$\sup_{z\in\Gamma}\left\|(\mathbf{P}^2-z)^{-1}\right\| \le \text{const}, \quad \sup_{z\in\Gamma}\max_{j\in\{1,2,3\}}\left\|P_j(\mathbf{P}^2-z)^{-1}\right\| \le \text{const}. \tag{3.14}$$

Hence we can find δ small enough and R large enough such that the operator in (3.12) is invertible if

$$1 + \alpha_\perp(\pm i\mathbf{P}\cdot\nabla g_\perp \pm i\nabla g_\perp\cdot\mathbf{P} - \alpha_\perp|\nabla g_\perp|^2)(\mathbf{P}^2 - \Re(z))^{-1} \quad \text{is invertible} \tag{3.15}$$

uniformly on Γ. Now the operator in (3.15) is invertible if

$$\begin{aligned}1 &\pm i\alpha_\perp(\mathbf{P}^2-\Re(z))^{-\frac12}(\mathbf{P}\cdot\nabla h + \nabla h\cdot\mathbf{P})(\mathbf{P}^2-\Re(z))^{-\frac12} \\ &- \alpha_\perp^2(\mathbf{P}^2-\Re(z))^{-\frac12}|\nabla h|^2(\mathbf{P}^2-\Re(z))^{-\frac12}\end{aligned} \tag{3.16}$$

is invertible (by a resummation of the Neumann series and analytic continuation). Now assume that uniformly on Γ we have:

$$0 < \alpha_\perp^2 (\mathbf{P}^2 - \Re(z))^{-\frac{1}{2}} |\nabla h|^2 (\mathbf{P}^2 - \Re(z))^{-\frac{1}{2}} \leq \frac{\alpha_\perp^2}{-\Re(z)} < 1,$$

which can be achieved if $\alpha_\perp^2 < E_+$ and δ is chosen to be small enough. Define

$$S := \left(1 - \alpha_\perp^2 (\mathbf{P}^2 - \Re(z))^{-\frac{1}{2}} |\nabla h|^2 (\mathbf{P}^2 - \Re(z))^{-\frac{1}{2}}\right)^{-\frac{1}{2}},$$

and

$$T = T^* := S(\mathbf{P}^2 - \Re(z))^{-\frac{1}{2}} (\mathbf{P} \cdot \nabla h + \nabla h \cdot \mathbf{P})(\mathbf{P}^2 - \Re(z))^{-\frac{1}{2}} S.$$

Then the operator in (3.16) is invertible if $1 \pm i\alpha_\perp T$ is invertible, which is always the case:

$$(1 \pm i\alpha_\perp T)^{-1} = (1 \mp i\alpha_\perp T)(1 + \alpha_\perp^2 T^2)^{-1}.$$

Therefore Proposition 1 is proved. □

3.2 Proof of Theorem 2

Proof of (i). First we recall an older result (see e.g. [25, 2, 26]), according to which the commutator $[X_\parallel, P_0]$ defined on $\mathcal{D}(X_\parallel)$ has a bounded closure on $L^2(\mathbb{R}^3)$. We seek an approximate resolvent of $\hat{X}_\parallel$ by defining for $\mu > 0$ the operator

$$\hat{R}_{\pm\mu} = P_0 (X_\parallel \pm i\mu)^{-1} P_0. \tag{3.17}$$

Since one can rewrite $\hat{R}_{\pm\mu}$ as

$$\hat{R}_{\pm\mu} = (X_\parallel \pm i\mu)^{-1} P_0 + (X_\parallel \pm i\mu)^{-1} [X_\parallel, P_0](X_\parallel \pm i\mu)^{-1} P_0$$

it follows that $\hat{R}_{\pm\mu}\mathcal{K} \subset D(\hat{X}_\parallel)$ and by a straightforward computation (as operators in $\mathcal{K}$)

$$(\hat{X}_\parallel \pm i\mu)\hat{R}_{\pm\mu} = P_0 (X_\parallel \pm i\mu) P_0 (X_\parallel \pm i\mu)^{-1} P_0 = 1_\mathcal{K} + \hat{A}_{\pm\mu} \tag{3.18}$$

with

$$\hat{A}_{\pm\mu} = P_0 [X_\parallel, P_0](X_\parallel \pm i\mu)^{-1} P_0. \tag{3.19}$$

Since $[X_\parallel, P_0]$ is bounded and $\|(X_\parallel \pm i\mu)^{-1}\| \leq \frac{1}{\mu}$, it follows that for sufficiently large μ:

$$\|\hat{A}_{\pm\mu}\| \leq \frac{1}{2}. \tag{3.20}$$

Then again as operators in $\mathcal{K}$:

$$(\hat{X} \pm i\mu)\hat{R}_{\pm\mu}(1_\mathcal{K} + \hat{A}_{\pm\mu})^{-1} = 1_\mathcal{K} \tag{3.21}$$

This implies that $\hat{X} \pm i\mu$ is surjective on $\hat{R}_{\pm\mu}(1_{\mathcal{K}} + \hat{A}_{\pm\mu})^{-1}\mathcal{K} \subset D(\hat{X})$. By the fundamental criterion of self-adjointness [24] $\hat{X}$ is self-adjoint in $\mathcal{K}$ on $\mathcal{D}(\hat{X})$. In addition, from (3.21) one obtains the following formula for the resolvent of $\hat{X}_{\|}$:

$$(\hat{X}_{\|} \pm i\mu)^{-1} = \hat{R}_{\pm\mu}(1_{\mathcal{K}} + \hat{A}_{\pm\mu})^{-1}. \tag{3.22}$$

Proof of (ii). We will show that $\hat{R}_{\pm\mu}$ is compact in $\mathcal{K}$ which implies (see (3.22)) that $\hat{X}_{\|}$ has compact resolvent, thus purely discrete spectrum. Consider a cut-off function ϕ_N which equals 1 if $|\mathbf{x}| \leq N$ and is zero if $|\mathbf{x}| \geq 2N$. For $N \geq 1$ we can decompose:

$$\hat{R}_{\pm\mu} = P_0(X_{\|} \pm i\mu)^{-1}\phi_N P_0 + P_0(X_{\|} \pm i\mu)^{-1}(1 - \phi_N)P_0. \tag{3.23}$$

Writing

$$\phi_N P_0 = \{\phi_N(\mathbf{P}^2 + 1)^{-1}\}\{(\mathbf{P}^2 + 1)P_0\}$$

we see that $\phi_N P_0$ is compact (even Hilbert-Schmidt) in $L^2(\mathbb{R}^3)$ (the first factor is Hilbert-Schmidt while the second one is bounded). Now if $0 < \alpha$ is small enough, we know that $e^{\alpha g_\perp}P_0$ is bounded (see (2.9)). Since

$$\lim_{N\to\infty} \left\|(X_{\|} \pm i\mu)^{-1}(1 - \phi_N)e^{-\alpha g_\perp}\right\| = 0,$$

we have shown:

$$\lim_{N\to\infty} \left\|\hat{R}_{\pm\mu} - P_0(X_{\|} \pm i\mu)^{-1}\phi_N P_0\right\| = 0,$$

thus $\hat{R}_{\pm\mu}$ equals the norm limit of a sequence of compact operators, therefore it is compact. Accordingly, since the self-adjoint operator $\hat{X}_{\|}$ has compact resolvent it has purely discrete spectrum [24]:

$$\sigma(\hat{X}_{\|}) = \sigma_{disc}(\hat{X}_{\|}) =: G, \tag{3.24}$$

and the proof of the second part of Theorem 2 is finished.

Proof of (iii). Now we will consider the exponential localization of eigenfunctions of $\hat{X}_{\|}$. Let $g \in G$ be an eigenvalue, m_g its multiplicity and $W_{g,j}$, $1 \leq j \leq m_g$ be an orthonormal basis in the eigenspace of $\hat{X}_{\|}$ corresponding to g. We shall prove that uniformly in g and j

$$\|e^{\alpha_{\|}\langle X_{\|},g\rangle}W_{g,j}\| \leq M \quad \text{and} \tag{3.25}$$

$$\|e^{\alpha_\perp\langle X_\perp\rangle}W_{g,j}\| \leq M. \tag{3.26}$$

Taking (3.25) and (3.26) as given, one can easily obtain (2.11) by a simple convexity argument: the function $f(x) = a^{1-x}b^x$; $a, b > 0$ is convex on $\mathbb{R}$, and for $0 \leq \beta \leq 1$ one has:

$$\beta e^{2\alpha_{\|}g_a(\mathbf{x})} + (1 - \beta)e^{2\alpha_\perp g_\perp} \geq e^{2(1-\beta)\alpha_{\|}g_a(\mathbf{x})}e^{2\beta\alpha_\perp g_\perp}, \tag{3.27}$$

which together with (3.25) and (3.26) it proves (2.11) with $M_1 = M^2$. Since (3.26) follows directly from (2.9) and $W_{g,j} = P_0 W_{g,j}$ we are left with the proof of (3.25).

Although the proof of (3.25) mimics closely the proof in the one dimensional case [23], we give it here for completeness. In order to emphasize the main idea of the proof let us remind one of the simplest proofs of the exponential decay of eigenfunctions of Schrödinger operators corresponding to discrete eigenvalues (assuming that the potential V is bounded and has compact support). Namely assume that for some $E > 0$ we have $(-\Delta + V + E)\Psi = 0$, which can be rewritten as

$$\Psi = -(-\Delta + E)^{-1} V \Psi. \tag{3.28}$$

Since for $|\alpha| < \sqrt{E}$, $e^{\alpha|\cdot|}(-\Delta + E)^{-1} e^{-\alpha|\cdot|}$ and $e^{\alpha|\cdot|}V$ are bounded:

$$\Psi = -e^{-\alpha|\cdot|} \left\{ e^{\alpha|\cdot|}(-\Delta + E)^{-1} e^{-\alpha|\cdot|} \right\} (e^{\alpha|\cdot|} V)\Psi$$

which proves the exponential localization of Ψ. The main idea in proving (3.25) is to rewrite the eigenvalue equation for $\hat{X}_{\|}$ in a form similar to (3.28) and and then to use (2.8).

Let us start with some notation. If $b > 0$ (sufficiently large) and $a \in \mathbb{R}$, define:

$$f_{a,b}(\mathbf{x}) := b\, f\left(\frac{x_1 - a}{b} \right) \tag{3.29}$$

where f is a real $C_0^\infty(\mathbb{R})$ cut-off function satisfying $0 \leq f(y) \leq 1$ and

$$f(y) = \begin{cases} 1 & \text{for} \quad |y| \leq \frac{1}{2} \\ 0 & \text{for} \quad |y| \geq 1 \end{cases} .$$

Define the function $h_{a,b}$ by:

$$h_{a,b}(\mathbf{x}) := x_1 - a + i f_{a,b}(\mathbf{x}). \tag{3.30}$$

Note that by construction, $h_{a,b}$ only depends on x_1, and obeys:

$$|h_{a,b}(\mathbf{x})| \geq \frac{b}{2}. \tag{3.31}$$

Moreover, its first two derivatives are uniformly bounded:

$$\sup_{\mathbf{x}\in\mathbb{R}^3} \sup_{a\in\mathbb{R}} \sup_{b\geq 1} \{ |\nabla h_{a,b}(\mathbf{x})| + |\Delta h_{a,b}(\mathbf{x})| \} = K < \infty. \tag{3.32}$$

The eigenvalue equation for $W_{g,j}$ reads as $P_0(\hat{X}_{\|} - g)P_0 W_{g,j} = 0$. Using (3.30) it can be rewritten as:

$$P_0 h_{g,b} P_0 W_{g,j} = i P_0 f_{g,b} P_0 W_{g,j}. \tag{3.33}$$

We now prove that $P_0 h_{g,b} P_0$ is invertible. Like in the proof self-adjointness of $\hat{X}_{\|}$ we compute

$$P_0 h_{g,b}^{-1} P_0 P_0 h_{g,b} P_0 = 1_{\mathcal{K}} + P_0 h_{g,b}^{-1} \left[P_0, h_{g,b} \right] P_0. \tag{3.34}$$

The key remark is that $[P_0, h_{g,b}]$ is bounded. Indeed we have the identity:

$$\begin{aligned}[P_0, h_{g,b}] &= -\frac{1}{2\pi}\int_\Gamma (H-z)^{-1}\left\{\mathbf{P}\cdot\nabla h_{g,b} + \nabla h_{g,b}\cdot\mathbf{P}\right\}(H-z)^{-1}dz \\ &= -\frac{1}{2\pi}\int_\Gamma (H-z)^{-1}\left\{-i\Delta h_{g,b} + 2\nabla h_{g,b}\cdot\mathbf{P}\right\}(H-z)^{-1}dz. \end{aligned} \tag{3.35}$$

It follows that $[P_0, h_{g,b}]$ is uniformly bounded in $g \in \mathbb{R}$ and $b \geq 1$ (see (3.32)). Taking into account (3.31) one obtains that the operator

$$\hat{B}_{g,b} = P_0 h_{g,b}^{-1}\left[P_0, h_{g,b}\right] P_0 \quad : \quad \mathcal{K} \to \mathcal{K} \tag{3.36}$$

satisfies

$$\|\hat{B}_{g,b}\| \leq \frac{1}{2} \tag{3.37}$$

if $b \geq b_0$ for some large enough $b_0 < \infty$. It follows that $1 + \hat{B}_{g,b}$ is invertible and then the eigenvalue equation (see (3.33), (3.34) and (3.36)) takes the form

$$W_{g,j} = i\left(1 + \hat{B}_{g,b}\right)^{-1} P_0 h_{g,b}^{-1} P_0 f_{g,b} P_0 W_{g,j} \tag{3.38}$$

which is the analog of (3.28). By construction (see the definition of $f_{g,b}$ in (3.29)):

$$\|e^{\alpha_\parallel \langle X_\parallel, g\rangle} f_{g,b}\| \leq b e^{\alpha_\parallel (b+1)}.$$

Moreover,

$$e^{\alpha_\parallel \langle X_\parallel, g\rangle} P_0 h_{g,b}^{-1} P_0 e^{-\alpha_\parallel \langle X_\parallel, g\rangle} = \left\{e^{\alpha_\parallel \langle X_\parallel, g\rangle} P_0 e^{-\alpha_\parallel \langle X_\parallel, g\rangle}\right\} h_{g,b}^{-1} \left\{e^{\alpha_\parallel \langle X_\parallel, g\rangle} P_0 e^{-\alpha_\parallel \langle X_\parallel, g\rangle}\right\}$$

is bounded due to (2.8). Thus the only thing it remains to be proved is the existence of a b large enough such that the following bound holds:

$$\sup_{g\in\mathbb{R}} \left\| e^{\alpha_\parallel \langle X_\parallel, g\rangle} \left(1 + \hat{B}_{g,b}\right)^{-1} e^{-\alpha_\parallel \langle X_\parallel, g\rangle} \right\| < \infty. \tag{3.39}$$

Using the Neumann series for $\left(1 + \hat{B}_{g,b}\right)^{-1}$, it follows that it suffices to prove that

$$\lim_{b\to\infty} \sup_{g\in\mathbb{R}} \left\| e^{\alpha_\parallel \langle X_\parallel, g\rangle} \hat{B}_{g,b} e^{-\alpha_\parallel \langle X_\parallel, g\rangle} \right\| = 0. \tag{3.40}$$

Since (see (3.31)) $\lim_{b\to\infty} \|h_{g,b}^{-1}\| = 0$ (uniformly in $g \in \mathbb{R}$), for (3.40) to holds true it is sufficient to show:

$$\sup_{g\in\mathbb{R}} \left\| e^{\alpha_\parallel \langle X_\parallel, g\rangle} \left[P_0, h_{g,b}\right] e^{-\alpha_\parallel \langle X_\parallel, g\rangle} \right\| \leq \text{const}. \tag{3.41}$$

But this easily follows from (3.35), (3.32), (3.2) and (3.3) where we take $K = H$, $\alpha_z = \alpha_\parallel$ and $h = g_g$. The proof of (iii) is concluded.

Proof of (iv). We start with a technical result:

Lemma 5. *Fix $0 \leq \alpha_\perp < \sqrt{E_+}$. Then there exists a bounded operator D such that*

$$P_0 = e^{-\alpha_\perp \langle X_\perp \rangle} (\mathbf{P}^2 + 1)^{-1} D \tag{3.42}$$

Proof. We use the notation and ideas of Proposition 1, and we rewrite P_0 in a convenient form. First, for $R > 0$ we have

$$(H - z)^{-1} = (H_R - z)^{-1} - (H_R - z)^{-1} \chi_R V (H - z)^{-1}.$$

Second, choose Γ close enough to σ_0 and R large enough, such that $(H_R - z)^{-1}$ becomes analytic inside Γ and (3.12) holds true for all $z \in \Gamma$. Then we can write:

$$P_0 = -e^{-\alpha_\perp \langle X_\perp \rangle} \frac{i}{2\pi} \int_\Gamma \tag{3.43}$$

$$(H_R - z)^{-1} [1 + \alpha_\perp (i\mathbf{P} \cdot \nabla g_\perp + i \nabla g_\perp \cdot \mathbf{P} - \alpha_\perp |\nabla g_\perp|^2)(H_R - z)^{-1}]^{-1} e^{\alpha_\perp g_\perp} \chi_R V (H - z)^{-1} dz.$$

Now by the closed graph theorem we have that $(\mathbf{P}^2 + 1)(H_R + 1)^{-1}$ is bounded (here R is large enough such that $(-\infty, -1/2) \subset \rho(H_R)$), and together with the spectral theorem:

$$\sup_{z \in \Gamma} \|(\mathbf{P}^2 + 1)(H_R - z)^{-1}\| < \infty.$$

Use this in (3.43) and we are done. □

We now have all the necessary ingredients for proving the last statement of our theorem. For every $L > 0$ and $a \in \mathbb{R}$, denote by $\chi_{L,a}$ the characteristic function of the slab $\{\mathbf{x} : |x_1 - a| \leq L\}$. Then define the operator $B := \chi_{L,a} P_0$. Using (3.42) let us show that B is Hilbert-Schmidt, and moreover, uniformly in $a \in \mathbb{R}$ we have:

$$\|B\|_2^2 \leq M \cdot L, \tag{3.44}$$

for some $M < \infty$. Indeed, since $B = \chi_{L,a} e^{-\alpha_\perp \langle X_\perp \rangle} (-\Delta + 1)^{-1} D$, a direct computation using the explicit formula for the integral kernel of the free Laplacian gives:

$$\|\chi_{L,a} e^{-\alpha_\perp \langle X_\perp \rangle} (\mathbf{P}^2 + 1)^{-1}\|_2^2 \leq \text{const} \cdot L.$$

It follows that the operator $\chi_{L,a} P_0 \chi_{L,a} = BB^*$ is trace class and

$$|\mathrm{Tr}(\chi_{L,a} P_0 \chi_{L,a})| \leq \|B\|_2^2 \leq M \cdot L \tag{3.45}$$

for some $M < \infty$ independent of L and a.

Now let $P_0^{L,a}$ be the orthogonal projection onto the subspace spanned by those $W_{g,j}$ for which $g \in [a - L, a + L]$:

$$P_0^{L,a} := \sum_{|g-a| \leq L} \sum_{j=1}^{m_g} \langle \cdot, W_{g,j} \rangle W_{g,j}. \tag{3.46}$$

We can choose A sufficiently large such that (3.25) implies:

$$\int_{|x_1-a|\geq A} |W_{g,j}(\mathbf{x})|^2 d\mathbf{x} \leq \frac{1}{2}, \tag{3.47}$$

uniformly in a and $g \in [a-L, a+L]$. Since $P_0 \geq P_0^{L,a}$, from (3.45) one obtains:

$$\begin{aligned} M\cdot(L+A) &\geq \mathrm{Tr}(\chi_{L+A,a} P_0 \chi_{L+A,a}) \geq \mathrm{Tr}(\chi_{L+A,a} P_0^{L,a} \chi_{L+A,a}) \\ &= \sum_{|g-a|\leq L} \sum_{j=1}^{m_g} \int_{\mathbb{R}^3} \chi_{L+A,a}(\mathbf{x}) |W_{g,j}(\mathbf{x})|^2 d\mathbf{x} \\ &\geq \sum_{|g-a|\leq L} \sum_{j=1}^{m_g} \frac{1}{2} = \frac{1}{2} N(a,L), \end{aligned} \tag{3.48}$$

where in the last inequality we used (3.47). In particular, if $L \geq 1$, then uniformly in $a \in \mathbb{R}$ we have

$$N(a,L) \leq 2M \cdot (1+A)L$$

and the proof is finished.

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