Constructing globally optimal Wannier functions for isolated composite bands in one dimension: Analysis

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Research Report YALEU/DCS/TR-1575
November 12, 2025

This paper generalizes the framework of [3] for obtaining exponentially localized and globally optimal Wannier functions in one dimension from isolated single bands to composite bands. The method builds on Kato's analytic perturbation theory, extending it from a local theory to a global one on the Brillouin circle: analytic Bloch frames are first constructed via parallel transport, and their boundary discontinuities are removed through a gauge transformation determined by a unitary Zak matrix. A subsequent diagonalization of this transformation identifies the gauge that achieves the most localized Wannier functions. In this sense, the framework provides a constructive proof of the existence of exponentially localized, real, and globally optimal Wannier functions, clarifying the analytic and topological structure underlying their localization.

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Contents

1 Introduction

This paper presents a framework for constructing real and globally optimal Wannier functions in one dimension for an isolated group of bands. It extends the single-band theory introduced in [3] to the composite-band setting—where degeneracies and non-Abelian gauge freedoms appear—by providing an explicit analytic construction that guarantees exponential localization while minimizing the total spatial spread.

The construction proceeds by first solving the parallel-transport equation across the Brillouin zone to obtain an analytic family of Bloch frames. The resulting discontinuities at the zone boundaries are removed (to all derivative orders) through a gauge transformation determined by a single unitary matrix, yielding exponentially localized states. Diagonalizing this transformation produces the globally optimal gauge that minimizes the total spread. This framework offers a global formulation of Kato's analytic perturbation theory on the circle, in which the Zak phase naturally emerges as the only relevant topological quantity.

The remainder of the paper is organized as follows. Section 3 contains the preliminaries, including the definitions of Bloch functions and frames, composite-band Wannier functions, and key results from analytic perturbation theory. Section 4 develops the analytic apparatus: Section 4.1 applies the analytic perturbation theory to construct an analytic family of Bloch frames, while Section 4.3 introduces the Fourier representation of Wannier functions and its connection to localization. Sections 4.5–4.7 present the gauge transformations that remove zone-boundary discontinuities, establish exponential localization, and identify the unique globally optimal gauge. Finally, Section 5 summarizes the complete constructive procedure for obtaining real and globally optimal Wannier functions.

2 Notations and conventions

We denote by δ_{mn} the Kronecker delta. Let $\ell^2(\mathbb{Z})$ denote the Hilbert space for square-summable complex sequences $\boldsymbol{x} = (x_i)_{i\in\mathbb{Z}}$ with the standard inner product. The right-shift operator in $\ell^2(\mathbb{Z})$ is denoted by R, defined by

$$R(\boldsymbol{x}) = (x_{i-1})_{i\in\mathbb{Z}} \tag{1}$$

We use bold symbols, such as $\boldsymbol{P}$ and $\boldsymbol{\mathcal{U}}$, for infinite matrices and operators on $\ell^2(\mathbb{Z})$ with the exception of the right-shift R in (1) and the time-reversal operator T in Section 4.7. Finite-dimensional matrices are denoted by non-bold symbols, such as A and U.

For a vector $\boldsymbol{x} \in \ell^2(\mathbb{Z})$ or $\mathbb{C}^N$, we denote by $\boldsymbol{x}^*$ the conjugate transpose and $\boldsymbol{x}^T$ the *unconjugated* transpose. We denote the Frobenius norm of a finite matrix by $\|A\|_F = \sqrt{\mathrm{Tr}(A^*A)}$. We also use the same notation for infinite matrices whenever the series defining it converges.

We use $\mathrm{U}(n)$ to denote the group of $n \times n$ unitary matrices. The Lie algebra of $U(n)$ is given by the real vector space of skew-Hermitian matrices, $\mathfrak{u}(n) = \{A \in C^{n\times n} \mid A^* = -A\}$.

We choose the principal branch of the logarithm so that the real phase φ in $e^{\mathrm{i}\varphi}$ takes values in $(-\pi, \pi]$.

3 Physical and Mathematical Preliminaries

3.1 Bloch functions

In this section, we introduce standard notions from the Bloch theory of one-dimensional periodic systems. These are standard results in band structure and spectral theory (see [5], [6] and [10]).

We first define a periodic lattice $\Lambda = \{na : n \in \mathbb{Z}\}$ with lattice constant a. The primitive unit cell is defined by the interval

$$I_{\mathrm{uc}} = [-a/2, a/2). \tag{2}$$

We define $\Omega = \frac{2\pi}{a}$ as the period for the reciprocal lattice $\Lambda^* = \{n\Omega : n \in \mathbb{Z}\}$. We denote the first Brillouin zone by the following interval I_{bz}:

$$I_{\mathrm{bz}} = [-\Omega/2, \Omega/2). \tag{3}$$

We regard both I_{uc} and I_{bz} as a circle obtained by identifying their end points, but we also treat I_{bz} as an interval when convenient.

Let $V : \mathbb{R} \to \mathbb{R}$ be a piecewise continuous function of period a:

$$V(x + y) = V(x), \quad x \in \mathbb{R},\, y \in \Lambda. \tag{4}$$

By Bloch's theorem [6], the Schrödinger eigenvalue problem with a periodic potential given by V is equivalent to solving the family of self-adjoint operators $H(k) : H^2_{\mathrm{per}}(I_{\mathrm{uc}}) \to L^2(I_{\mathrm{uc}})$ for $k \in I_{\mathrm{bz}}$, defined by the formula

$$H(k) = -\left(\frac{\mathrm{d}}{\mathrm{d}x} + \mathrm{i}k\right)^2 + V\,, \tag{5}$$

where the domain H^2_{per} is given by

$$H^2_{\mathrm{per}}(I_{\mathrm{uc}}) = \left\{u \in H^2(I_{\mathrm{uc}}) \mid u(-a/2) = u(a/2)\,, u'(-a/2) = u'(a/2)\right\}\,. \tag{6}$$

In other words, if $u : I_{\mathrm{uc}} \to \mathbb{C}$ is an eigenfunction of $H(k)$, then u and u' are continuous and periodic with $u'' \in L^2(I_{\mathrm{uc}})$. (We observe that the domain of $H(k)$ is independent of k.) It satisfies the so-called time-reversal symmetry:

$$H(k) = \overline{H}(-k)\,, \quad k \in I_{\mathrm{bz}}\,. \tag{7}$$

The following lemma contains basic results concerning the spectrum of $H(k)$; they are part of Theorem XIII.89 in [10] and stated in a slightly different form.

Lemma 3.1. Suppose the potential V in (5) is a piecewise continuous periodic function on I_{bz}. Then the following holds:
1. The operator $H(k)$ for $k \in I_{\mathrm{bz}}$ has purely discrete spectrum.
2. Eigenvalues of $H(k)$ are simple for $k \in I_{\mathrm{bz}}$ except at $k = 0, \pm\frac{\Omega}{2}$ with multiplicity at most 2.

It is the starting point for the construction of Wannier functions. The second shows that complete information about degeneracy can be obtained from the spectra of $H(k)$ at $k = 0, \pm\frac{\Omega}{2}$. Since the spectrum of $H(k)$ is discrete, we express the eigenvalue problem of $H(k)$ for $k \in I_{\mathrm{bz}}$ in the following form:

$$H(k)u_k^{(j)} = E_k^{(j)}u_k^{(j)}, \qquad j \in \mathbb{N}, \quad \text{with } u_k^{(j)} \in H^2_{\mathrm{per}}(I_{\mathrm{uc}})\,. \tag{8}$$

The Bloch functions $\psi_k^{(j)} : I_{\mathrm{uc}} \to \mathbb{C}$ are defined by multiplying the eigenfunctions by a phase factor:

$$\psi_k^{(j)} = e^{\mathrm{i}kx}u_k^{(j)}\,. \tag{9}$$

The value k is often referred to as the quasimomentum. The eigenvalues $\{E_k^{(j)}\}_{j=1}^{\infty}$ are called the energy of the states represented by the Bloch functions $\{\psi_k^{(j)}\}_{j=1}^{\infty}$ defined in (9). Throughout this paper, we do not assume simple eigenvalues; in general, we have

$$E_k^{(1)} \le E_k^{(2)} \le \ldots \le E_k^{(j)} \le \ldots\,, \quad k \in I_{\mathrm{bz}}\,. \tag{10}$$

We also assume that $\{\psi_k^{(j)}\}_{j=1}^{\infty}$ are chosen to be orthogonal (if degeneracy is present) with the standard normalization convention such that they become orthonormal:

$$\int_{-a/2}^{a/2} \overline{\psi}_k^{(i)}(x)\psi_k^{(j)}(x)\,\mathrm{d}x = \int_{-a/2}^{a/2} \overline{u}_k^{(i)}(x)u_k^{(j)}(x)\,\mathrm{d}x = \delta_{ij}, \quad k \in I_{\mathrm{bz}}, \quad j = 1, 2, \ldots. \tag{11}$$

The domain assumption in (6) implies that the eigenfunctions $u_k^{(j)}$ are spatially periodic:

$$u_k^{(j)}(x+y) = u_k^{(j)}(x)\,, \quad x \in I_{\mathrm{uc}}\,, \quad y \in \Lambda\,. \tag{12}$$

This in turn implies that the Bloch functions are quasi-periodic in x:

$$\psi_k^{(j)}(x+y) = e^{\mathrm{i}ky}\psi_k^{(j)}(x), \quad x \in I_{\mathrm{uc}}\,, \quad y \in \Lambda. \tag{13}$$

In the context of Wannier functions, it is natural to use the so-called periodic zone scheme, where the Bloch functions and eigenvalues are copies of those in the first Brillouin zone [12]. In other words, we extend the Bloch functions and eigenvalues to be periodic functions of k with period Ω. More explicitly, we have

$$\psi_{k+g}^{(j)} = \psi_k^{(j)} \tag{14}$$

for any $k \in I_{\mathrm{bz}}, g \in \Lambda^*$ and $j = 1, 2, \ldots$. Combining (14) and (9) shows that

$$u_{k+g}^{(j)}(x) = e^{-\mathrm{i}gx}u_k^{(j)}(x). \tag{15}$$

3.2 Bloch frames

In this section, we first introduce the so-called Bloch frames derived from the Bloch functions $\psi_k^{(j)}$ introduced in Section 3.1.

When a single band $E_k^{(j)}$ remains non-degenerate for all $k \in I_{\mathrm{bz}}$, the associated Wannier function can be defined directly as the Fourier series of $\psi_k^{(j)}$; the periodicity condition (14) is sufficient to ensure exponential localization [3]. When degeneracies occur, however, a single-band description is no longer globally valid for constructing exponentially localized functions. A natural generalization is to consider a finite *isolated* group of bands [2, 8, 12]—also known as composite bands—defined as follows.

We consider a group of n_b bands with eigenvalues $\mathcal{E}_k = \{E_k^{(j_i)}\}_{i=1}^{n_b}$ in (8) and Bloch functions given by

$$\Psi_k = \left(\psi_k^{(j_1)}, \psi_k^{(j_2)}, \ldots, \psi_k^{(j_{n_b})}\right) . \tag{16}$$

We call the group above *isolated* if they do not coincide (i.e. become degenerate) with any eigenvalues not in the group. More precisely, it is the so-called gapped condition:

$$\operatorname{dist}(\mathcal{E}(k), \sigma(H(k)) \backslash \mathcal{E}(k)) > 0 , \qquad \text{for all } k \in I_{\mathrm{bz}} , \tag{17}$$

where $\sigma(H(k))$ denotes the spectrum of $H(k)$. It should be observed that the eigenvalues within the group are *allowed* to become degenerate. Moreover, we can view Ψ_k as a map $\mathbb{C}^{n_b} \mapsto L^2(I_{\mathrm{uc}})$, thus treating it as a "matrix" whose columns are the Bloch functions $\psi_k^{(j)}$.

Furthermore, we define a family of subspaces $\mathcal{S}_k \subset L^2(I_{\mathrm{uc}})$ of dimension n_b spanned by the functions in Ψ_k :

$$\mathcal{S}_k = \operatorname{Range}(\Psi_k) , \quad k \in I_{\mathrm{bz}} . \tag{18}$$

At each $k \in I_{\mathrm{bz}}$, we define an orthonormal basis of S_k via

$$\Phi_k = \left(\varphi_k^{(1)}, \varphi_k^{(2)}, \ldots, \varphi_k^{(n_b)}\right) , \tag{19}$$

where the orthonormality is given by the formula

$$\int_{-a/2}^{a/2} \overline{\varphi}_k^{(i)}(x) \varphi_k^{(j)}(x) \, \mathrm{d}x = \delta_{ij} , \quad i, j = 1, 2, \ldots, n_b , \quad k \in I_{\mathrm{bz}} . \tag{20}$$

We refer to the collection of functions Φ_k as the Bloch frame at k .

By viewing Ψ_k and Φ_k as columns of functions, the orthonormality of Ψ_k in (11) is compactly written in the following form

$$\int_{-a/2}^{a/2} \Psi_k^*(x) \Psi_k(x) \, \mathrm{d}x = I_{n_b} , \quad k \in I_{\mathrm{bz}} , \tag{21}$$

where the integral in (21) is taken entry-wise and I_{n_b} is an $n_b \times n_b$ identity matrix. Similarly, the orthonormality requirement of the Bloch frame Φ_k in (20) is expressed via

$$\int_{-a/2}^{a/2} \Phi_k^*(x) \Phi_k(x) \, \mathrm{d}x = I_{n_b} , \quad k \in I_{\mathrm{bz}} . \tag{22}$$

Obviously, the collection of Bloch functions Ψ_k constitutes a very special Bloch frame.

Remark 3.1. It is often convenient to regard Ψ_k in (16) as the fundamental object and write the Bloch frame Φ_k in (19) by the formula

$$\Phi_k = \Psi_k U(k)\,, \quad k \in I_{\mathrm{bz}}\,, \tag{23}$$

where $U(k) \in \mathrm{U}(n_b)$ is a family of unitary matrices on I_{bz}. This representation automatically indicates the orthonormality (22) of Φ_k. However, there is generally no *a priori* (smooth) choice of Ψ_k. Hence, we refrain from using (23) and treat Φ_k as the primary object instead of Ψ_k in this paper.

We define a new family of frames consisting of the eigenfunctions in (9):

$$\mathcal{U}_k = \left(u_k^{(j_1)}, u_k^{(j_2)}, \dots, u_k^{(j_{n_b})}\right) = e^{-\mathrm{i}kx}\Psi_k\,, \quad k \in I_{\mathrm{bz}}\,. \tag{24}$$

Similarly, for each $\varphi_k^{(i)}$ in Φ_k, we define its spatially periodic $v_k^{(i)} \in L^2(I_{\mathrm{uc}})$ by the formula

$$v_k^{(i)} = e^{-\mathrm{i}kx}\varphi_k^{(i)}\,, \quad i = 1, 2, \dots, n_b\,, k \in I_{\mathrm{bz}}\,, \tag{25}$$

by which we introduce

$$\mathcal{V}_k = \left(v_k^{(1)}, v_k^{(2)}, \dots, v_k^{(n_b)}\right) = e^{-\mathrm{i}kx}\Phi_k\,, \quad k \in I_{\mathrm{bz}}\,. \tag{26}$$

The orthonormality in (21) is inherited by $\mathcal{U}_k$ and $\mathcal{V}_k$:

$$\int_{-a/2}^{a/2} \mathcal{U}_k^*(x)\,\mathcal{U}_k(x)\,\mathrm{d}x = I_{n_b}\,, \quad \int_{-a/2}^{a/2} \mathcal{V}_k^*(x)\mathcal{V}_k(x)\,\mathrm{d}x = I_{n_b}\,, \quad k \in I_{\mathrm{bz}}\,. \tag{27}$$

Furthermore, since functions in Φ_k and $\mathcal{V}_k$ are linear combinations of those in Ψ_k and $\mathcal{U}_k$ respectively, the quasi-periodic condition in (13) implies

$$\Phi_k(x+y) = e^{\mathrm{i}ky}\Phi_k(x)\,, \quad k \in I_{\mathrm{bz}}\,, \quad x \in I_{\mathrm{uc}}\,, \quad y \in \Lambda\,, \tag{28}$$

and (14)–(15) imply

$$\Phi_{k+g} = \Phi_k\,, \quad \mathcal{V}_{k+g} = e^{-\mathrm{i}gx}\mathcal{V}_k\,, \quad k \in I_{\mathrm{bz}}\,, \quad g \in \Lambda^*\,. \tag{29}$$

By the same reasoning, (12) becomes

$$\mathcal{V}_k(x+y) = \mathcal{V}_k(x)\,, \qquad k \in I_{\mathrm{bz}}\,, \quad x \in I_{\mathrm{uc}}\,, \quad y \in \Lambda\,. \tag{30}$$

The frames Φ_k and $\mathcal{V}_k$ will play a central role in the construction of composite-band Wannier functions.

3.3 Definition of composite-band Wannier functions

In this section, we introduce the definition of composite-band Wannier functions.

In the single-band case, Wannier functions $W_n^{(j)} : \mathbb{R} \to \mathbb{C}$ associated with band j centered at the n-th lattice point are given by the Fourier series of the Bloch function $\psi_k^{(j)}$:

$$W_n^{(j)}(x) = \frac{1}{\Omega}\int_{-\Omega/2}^{\Omega/2} e^{-\mathrm{i}nak}\psi_k^{(j)}(x)\,\mathrm{d}k\,. \tag{31}$$

In the composite-band case, the definition is unchanged but with the Bloch function $\psi_k^{(j)}(x)$ replaced by the Bloch-frame functions $\varphi_k^{(i)}$ in (19). Due to periodicity (29) of the Bloch frame

Φ_k, the composite-band (or multiband) Wannier functions $W_n^{(i)} : \mathbb{R} \to \mathbb{C}$ with index $i = 1, 2, \ldots, n_b$ centered at the n-th lattice point are defined as the Fourier series of the Bloch-frame functions via

$$W_n^{(i)}(x) = \frac{1}{\Omega} \int_{-\Omega/2}^{\Omega/2} e^{-\mathrm{i}nak} \varphi_k^{(i)}(x) \, \mathrm{d}k \,, \quad i = 1, 2, \ldots, n_b \,. \tag{32}$$

As in the single-band case, the condition in (28) and the definition (32) imply the Wannier functions in (32) centered at different lattice points are translated copies of one another. More explicitly, we have

$$W_n^{(i)}(x) = W_0^{(i)}(x - na) \,, \qquad i = 1, 2, \ldots, n_b \,, \quad n \in \mathbb{Z} \,, \tag{33}$$

where a is the lattice constant in (2). As a result, it suffices to consider Wannier functions centered around the origin (i.e. $n = 0$) in the following

$$W_0^{(i)}(x) = \frac{1}{\Omega} \int_{-\Omega/2}^{\Omega/2} \varphi_k^{(i)}(x) \, \mathrm{d}k = \frac{1}{\Omega} \int_{-\Omega/2}^{\Omega/2} e^{\mathrm{i}kx} v_k^{(i)}(x) \, \mathrm{d}k \,, \quad i = 1, 2, \ldots, n_b \,, \tag{34}$$

where we have used the definition in (25) for the second equality.

The Wannier functions defined above are highly non-unique. In the single-band case, the eigenfunction $\psi_k^{(j)}(x)$ in (31) is only defined up to a phase factor at every $k \in I_{\mathrm{bz}}$. In the composite-band case, such degrees of freedom are even larger. Given any choice of the Bloch frame Φ_k for defining (32), one can always modify Φ_k at any $k \in I_{\mathrm{bz}}$ by some unitary matrix $U(k) \in \mathrm{U}(n_b)$ via the transformation

$$\Phi_k \mapsto \Phi_k U(k) \,, \tag{35}$$

which results in new Wannier functions whenever (32) is well-defined. In the physics literature, this degree of freedom, described by some unitary matrix U, is often referred to as the non-Abelian gauge freedom (in contrast to scalar phase factors $e^{\mathrm{i}\varphi(k)}$ in the single-band case).

For both physical and numerical purposes, one seeks gauges yielding exponentially localized Wannier functions. More explicitly, for some $C > 0$ and $D > 0$, we have

$$|W_0^{(i)}(x)| \leq C \, e^{-D|x|} \,, \quad x \in \mathbb{R} \,, \quad i = 1, 2, \ldots, n_b. \tag{36}$$

The existence of exponentially localized Wannier functions in the composite-band case is well established, and proofs can be found, for example, in [2, 9]. Furthermore, among all exponentially localized Wannier functions, it is also desirable to choose the optimal ones, where they are as localized as possible. To quantify optimality, we define the first and second moments:

$$\langle x \rangle_i = \int_{-\infty}^{\infty} x |W_0^{(i)}(x)|^2 \, \mathrm{d}x \,, \quad i = 1, 2, \ldots, n_b \,, \tag{37}$$

often referred to as the Wannier centers, and

$$\langle x^2 \rangle_i = \int_{-\infty}^{\infty} x^2 |W_0^{(i)}(x)|^2 \, \mathrm{d}x \,, \quad i = 1, 2, \ldots, n_b \,. \tag{38}$$

The standard measure of optimality is the total spread $\mathcal{S}$, the sum of the variance of all Wannier functions:

$$\mathcal{S} = \sum_{i=1}^{n_b} \left(\langle x^2 \rangle_i - \langle x \rangle_i^2 \right) \,. \tag{39}$$

We observe that the total spread $\mathcal{S}$ coincides with the Marzari–Vanderbilt spread functional [8], here expressed directly in terms of the Wannier functions without projection onto other bases. A Bloch frame Φ_k is said to be globally optimal if it minimizes $\mathcal{S}$ over all admissible Bloch frames.

3.4 Analytic perturbation theory

This section summarizes results from Kato's classical analytic perturbation theory [4], which provide the analytic foundation for constructing Bloch frames introduced in Section 3.2.

First, we introduce standard definitions of an analytic family of unbounded operators (see [4, 10]). Let $\mathcal{H}$ be a Hilbert space and $\mathcal{D} \subset \mathcal{H}$ a dense subspace. Consider a simply connected $D_0 \subset \mathbb{C}$ and a family of closed operators $\{T(k)\}_{k \in D_0}$ defined on the common domain $\mathcal{D}$. The family is called an analytic family of type A if, for every $u \in \mathcal{D}$, the map $k \mapsto T(k)u$ is analytic as a vector-valued function from D_0 to $\mathcal{H}$. This ensures analyticity in the sense of Kato; namely, if z is in the resolvent set $\rho(T(k_0))$, then $(T(k)-z)^{-1}$ depends analytically on k as a bounded-operator-valued function on $\mathcal{H}$ for k near k_0. The type A assumption significantly simplifies the discussion on analytic perturbation theory.

Suppose further that D_0 is symmetric with respect to the real line and $T(k)$ satisfies $T(k)^* = T(\overline{k})$ for $k \in D_0$. The family is then referred to as a self-adjoint analytic family of type A. In particular, $T(k)$ is self-adjoint for all real k.

We restrict attention to a finite group of isolated eigenvalues of a self-adjoint analytic family $\{T(k)\}_{k \in D_0}$. In other words, it is possible for the subset of eigenvalues of $T(k)$ to be enclosed by a simple contour $\mathcal{C} \subset \rho(T(k))$ separated from the rest of the spectrum for all $k \in D_0$. This implies that the orthogonal projector given by

$$P(k) = -\frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} (T(k)-z)^{-1} \,\mathrm{d}z \,, \tag{40}$$

projects onto the invariant subspace associated with the eigenvalues enclosed by the contour $\mathcal{C}$. For real k, where $T(k)$ is self-adjoint, $\mathrm{Range}(P(k))$ coincides with the span of the corresponding eigenvectors. The type A assumption and the subspace being finite dimensional imply that most finite-dimensional results in Section II of [4] can be taken without modification, including analyticity of the projectors and perturbation formulas. We summarize these results below.

Theorem 3.2. Let $\{T(k)\}_{k \in D_0}$ be a self-adjoint analytic family defined above. Consider a group of n isolated eigenvalues (counted with multiplicity) of $T(k)$ enclosed by a simple contour $\mathcal{C} \subset \rho(T(k))$ for $k \in D_0$. Then the projector $P(k)$ defined in (40) depends analytically on k for real $k \in D_0$, where $\mathrm{Range}(P(k))$ is spanned by the corresponding n eigenvectors.

Having established the analyticity of $P(k)$, we now seek to construct an analytic family of orthonormal bases for $\mathrm{Range}(P(k))$ for real k. Kato showed that such a family of bases can be obtained by solving the following first-order differential equation.

Theorem 3.3. Let $\{P(k)\}_{k \in D_0}$ be the analytic family of projectors in Theorem 3.2. Fix a real $k_0 \in D_0$ and choose an orthonormal basis $\{q_j\}_{j=1}^n$ for $\mathrm{Range}(P(k_0))$. Then there exists an analytic family of orthonormal vectors $\{q_j(k)\}_{j=1}^n$ satisfying

$$\frac{\mathrm{d}q_j(k)}{\mathrm{d}k} = \frac{\mathrm{d}P(k)}{\mathrm{d}k} q_j(k) \,, \qquad q_j(k_0) = q_j \,, \quad j = 1, \ldots, n \,, \tag{41}$$

for all real $k \in D_0$ with $\mathrm{Range}(P(k)) = \mathrm{Span}\,\{q_j(k)\}_{j=1}^n$.

It should be observed that the orthonormal bases $\{q_j(k)\}_{j=1}^n$ might not be the eigenvectors. The orthonormality of $\{q_j(k)\}_{j=1}^n$ follows from the orthonormality of the initial basis set and the fact that

$$P(k)P'(k)P(k) = 0 \,. \tag{42}$$

Indeed, the identity (42) implies that

$$\langle q_i(k), q_j'(k) \rangle = 0 \,, \quad i, j = 1, \ldots, n \,, \tag{43}$$

which in turn implies $\frac{\mathrm{d}}{\mathrm{d}k}\langle q_i(k), q_j(k)\rangle = 0$. Hence we have

$$\langle q_i(k), q_j(k)\rangle = \langle q_i(k_0), q_j(k_0)\rangle = \delta_{ij} \quad i, j = 1, 2, \ldots, n\,. \tag{44}$$

The condition in (43) means that all variations of the basis vectors as k changes are orthogonal to the subspace $\mathrm{Range}(P(k))$. Hence (41) is often referred to as the parallel-transport equation.

The general derivative formulas for the projector in (40) in terms of the resolvent $(T(k) - z)^{-1}$ and derivatives $T^{(n)}(k)$ of the operator family can be found in Section II.1 of [4]. These derivatives $T^{(n)}(k)$ are well-defined linear operators on the same domain $\mathcal{D}$ as $T(k)$ due to the type A assumption. As only the first-order derivative is explicitly required in this paper, we omit explicit formulas for higher-order derivatives.

Theorem 3.4. Let the family of projectors $\{P(k)\}_{k\in D_0}$ be given in Theorem 3.2. Then the first-order derivative is given by the formula

$$\frac{\mathrm{d}P(k)}{\mathrm{d}k} = \frac{1}{2\pi \mathrm{i}}\int_{\mathcal{C}} (T(k) - z)^{-1}\frac{\mathrm{d}T(k)}{\mathrm{d}k}(T(k) - z)^{-1}\,\mathrm{d}z\,. \tag{45}$$

where the contour $\mathcal{C}$ is the same as that in (40). Furthermore, the higher-order derivatives $P^{(n)}(k)$ $(n \geq 2)$ are of a similar structure as (45) and are combinations of the resolvent $(T(k) - z)^{-1}$ and derivatives of $T^{(n_j)}(k)$ with $n_j \leq n$.

4 Analytic apparatus

In this section, we develop the analytic framework underlying the construction of composite-band Wannier functions defined in Section 3.3. Our goal is a constructive formulation ensuring exponential localization and global optimality. The presentation follows the logical sequence of the single-band setting [3], while emphasizing the additional analytic ingredients required in the composite-band case.

Section 4.1 applies the analytic perturbation theory from Section 3.4 to construct an analytic family (but not necessarily periodic) of Bloch frames on I_{bz} and to derive the analyticity of their Fourier coefficients. In Section 4.2, we introduce the Fourier transform of the Wannier functions and relate their regularity to the spatial decay of the Wannier functions. Section 4.3 reformulates the problem in the $\ell^2(\mathbb{Z})$ representation, where the Bloch frames are constructed via a parallel-transport equation. Section 4.4 analyzes the discontinuities of the frames at the Brillouin-zone boundaries, which are then removed by the gauge transformations introduced in Section 4.5, yielding exponentially localized Wannier functions. Finally, Section 4.6 characterizes the globally optimal Wannier functions, and Section 4.7 establishes their reality due to the time-reversal symmetry in (7).

4.1 Analytic properties of Bloch functions and frames

This section establishes analytic properties of the Bloch functions and frames introduced earlier and develops their Fourier representation. Unlike the single-band case, we treat the Bloch frames—not the Bloch functions—as the primary analytic objects.

Consider a group of n_b isolated bands. Following (16), the associated Bloch functions are collected in the column matrix $\Psi_k : \mathbb{C}^{n_b} \to L^2(I_{\mathrm{uc}})$ given by the formula

$$\Psi_k = \left(\psi_k^{(j_1)}, \psi_k^{(j_2)}, \ldots, \psi_k^{(j_{n_b})}\right)\,. \tag{46}$$

We use (24) to write $\Psi_k = e^{\mathrm{i}kx}\,\mathcal{U}_k$ with $\mathcal{U}_k$ given by

$$\mathcal{U}_k = \left(u_k^{(j_1)}, u_k^{(j_2)}, \ldots, u_k^{(j_{n_b})}\right)\,, \tag{47}$$

where each column is the eigenfunction $u_k^{(j_i)}$ associated with eigenvalue $E_k^{(j_i)}$:

$$H(k)u_k^{(j_i)} = \left[-\left(\frac{\mathrm{d}}{\mathrm{d}x} + \mathrm{i}k\right)^2 + V\right] u_k^{(j_i)} = E_k^{(j_i)} u_k^{(j_i)}\,, \quad i = 1, 2, \ldots, n_b\,, \tag{48}$$

for $k \in I_{\mathrm{bz}}$. As in Section 3.1, we assume that V is piecewise continuous on I_{uc}.

We observe that the operator family $\{H(k)\}_{k\in I_{\mathrm{bz}}}$ with the domain given in (6) is a self-adjoint analytic family of type A [11] as defined in Section 3.4; in particular, the analyticity follows from the fact that $H(k)$ is a polynomial in k. Furthermore, combined with the isolated eigenvalue assumption in (17), all results in Section 3.4 are applicable. Thus we apply Theorem 3.3 to construct a frame

$$\mathcal{V}_k = \left(v_k^{(1)}, v_k^{(2)}, \ldots, v_k^{(n_b)}\right) \tag{49}$$

where all $v_k^{(i)}$ depend on k analytically for $k \in I_{\mathrm{bz}}$. We thus obtain an analytic family of Bloch frames given by the formula

$$\Phi_k = \left(\varphi_k^{(1)}, \varphi_k^{(2)}, \ldots, \varphi_k^{(n_b)}\right) = e^{\mathrm{i}kx}\mathcal{V}_k\,, \tag{50}$$

with $\mathrm{Range}(\Psi_k) = \mathrm{Range}(\Phi_k)$ for all $k \in I_{\mathrm{bz}}$.

Lemma 4.1. Assume the potential V is piecewise continuous on I_{uc} so that $\{H(k)\}_{k\in I_{\mathrm{bz}}}$ forms a self-adjoint analytic family of type A. Let Ψ_k denote the family of Bloch functions associated with an isolated group of n_b bands as in (46). Then there exists a family of frames $k \mapsto \mathcal{V}_k$ defined in (49) that is analytic on I_{bz}, from which we obtain an analytic family of Bloch frames $\Phi_k = e^{\mathrm{i}kx}\mathcal{V}_k$ on I_{bz}.

We observe that Lemma 4.1 guarantees analyticity of Φ_k within $I_{\mathrm{bz}} = [-\Omega/2, \Omega/2)$ but does not ensure the periodicity condition in (29) across the zone boundaries $k = \pm\Omega/2$.

To analyze their spatial structure, we use the periodicity in (12) and take the Fourier series expansion of functions in $\mathcal{U}_k$ with respect to x:

$$u_k^{(j_i)}(x) = \sum_{m=-\infty}^{\infty} b_m^{(i)}(k)\, e^{\mathrm{i}m\Omega x}\,, \tag{51}$$

where the coefficients $b_m^{(i)} : I_{\mathrm{bz}} \to \mathbb{C}$ are given by the formula

$$b_m^{(i)}(k) = \frac{1}{a}\int_{-a/2}^{a/2} u_k^{(j_i)}(x)\, e^{-\mathrm{i}m\Omega x}\,\mathrm{d}x\,, \quad m \in \mathbb{Z}\,, \quad i = 1, 2, \ldots, n_b\,. \tag{52}$$

Similarly, using (30), we take the Fourier series expansion of those in $\mathcal{V}_k$ with respect to x:

$$v_k^{(i)}(x) = \sum_{m=-\infty}^{\infty} a_m^{(i)}(k)\, e^{\mathrm{i}m\Omega x}\,, \tag{53}$$

where the coefficients $a_m^{(i)} : I_{\mathrm{bz}} \to \mathbb{C}$ are given by the formula

$$a_m^{(i)}(k) = \frac{1}{a}\int_{-a/2}^{a/2} v_k^{(i)}(x)\, e^{-\mathrm{i}m\Omega x}\,\mathrm{d}x\,, \quad m \in \mathbb{Z}\,, \quad i = 1, 2, \ldots, n_b\,. \tag{54}$$

The generalized Parseval's identity implies that the orthonormality for $\mathcal{U}_k$ and $\mathcal{V}_k$ in (27) is equivalent to

$$\sum_{m=-\infty}^{\infty} \overline{b}_m^{(i)}(k) b_m^{(j)}(k) = \frac{1}{a}\delta_{ij}\,, \qquad \sum_{m=-\infty}^{\infty} \overline{a}_m^{(i)}(k) a_m^{(j)}(k) = \frac{1}{a}\delta_{ij} \tag{55}$$

for any $k \in I_{\mathrm{bz}}$ and any $i, j = 1, 2, \ldots, n_b$. Although (51)–(52) contain the eigenfunctions, we will primarily use (53)–(54) since the analyticity result in Lemma 4.1 is for $v_k^{(i)}$. Furthermore, the analyticity of $v_k^{(i)}$ in k implies that all coefficients $a_m^{(i)}$ are analytic functions on I_{bz}.

Lemma 4.2. Suppose that functions $v_k^{(i)}$ in $\mathcal{V}_k$ are chosen in Lemma 4.1. Then their corresponding Fourier coefficients $a_m^{(i)} : I_{\mathrm{bz}} \to \mathbb{C}$ defined in (54) are analytic (not necessarily periodic) on I_{bz}.

We next characterize how $v_k^{(i)}$ transforms under reciprocal-lattice shifts in k. We observe that the relation in (29) can be more explicitly written as

$$v_{k+g}^{(i)} = e^{-\mathrm{i}gx}\, v_k^{(i)}, \quad g \in \Lambda^*, \quad k \in I_{\mathrm{bz}}, \quad i = 1, 2, \ldots, n_b. \tag{56}$$

For $g = n\Omega \in \Lambda^*$, applying (56) to (54) yields the following relation:

$$v_{k+g}^{(i)}(x) = \sum_{m=-\infty}^{\infty} a_m^{(i)}(k+g)\, e^{\mathrm{i}m\Omega x} = e^{-\mathrm{i}gx}\, v_k^{(i)} = \sum_{m=-\infty}^{\infty} a_m^{(i)}(k)\, e^{\mathrm{i}(m-n)\Omega x} \tag{57}$$

$$= \sum_{m=-\infty}^{\infty} a_{m+n}^{(i)}(k)\, e^{\mathrm{i}m\Omega x}, \tag{58}$$

where the last equality is obtained by relabeling the summation index. Hence, we must have

$$a_m^{(i)}(k+n\Omega) = a_{m+n}^{(i)}(k), \quad k \in I_{\mathrm{bz}}, \quad m, n \in \mathbb{Z}, \quad i = 1, 2, \ldots, n_b, \tag{59}$$

in order to satisfy (56). To express the relation in (59) more compactly, we introduce for each $v_k^{(i)}$ a function $\alpha^{(i)} : \mathbb{R} \to \mathbb{C}$ defined via

$$\alpha^{(i)}(k + m\Omega) = a_m^{(i)}(k), \quad k \in I_{\mathrm{bz}}, \quad m \in \mathbb{Z}, \quad i = 1, 2, \ldots, n_b. \tag{60}$$

The functions $\alpha^{(i)}$ can be viewed as *unfolded* versions of the Fourier coefficients $a_m^{(i)}(k)$ defined on I_{bz} for $m \in \mathbb{Z}$ such that $a_m^{(i)}(k)$ takes up the interval $[-\Omega/2 + m\Omega, \Omega/2 + m\Omega)$. The unfolded functions $\alpha^{(i)}$ provide the key analytic representation in the construction of exponentially localized Wannier functions.

The decay of Fourier coefficients follows from the domain assumption in (6). For any $u \in H^2_{\mathrm{per}}$, the Fourier coefficients of u decay as $|m|^{-2}$ for large $|m|$ (see [18]). Hence, the eigenfunctions in $\mathcal{U}_k$ and all their linear combinations in $\mathcal{V}_k$ obey the same decay. In particular, there exists $D > 0$ independent of k and index i, such that

$$|a_m^{(i)}(k)| \le \frac{D}{|m|^2}, \quad \text{as } |m| \to \infty. \tag{61}$$

The next lemma collects these relations into a single analytic representation useful for constructing exponentially localized Wannier functions.

Lemma 4.3. Let $\alpha^{(i)} : \mathbb{R} \to \mathbb{C}$ be functions defined in (60). Then the Fourier series in (54) can be expressed by the formula

$$v_k^{(i)}(x) = \sum_{m=-\infty}^{\infty} \alpha^{(i)}(k + m\Omega)\, e^{\mathrm{i}m\Omega x}, \quad k \in I_{\mathrm{bz}}, \quad i = 1, 2, \ldots, n_b. \tag{62}$$

By Lemma 4.2, the functions $\alpha^{(i)}$ are analytic on the intervals $[-\Omega/2 + m\Omega, \Omega/2 + m\Omega)$ for $m \in \mathbb{Z}$. Furthermore, $|\alpha^{(i)}(k)|$ decays no slower than $|k|^{-2}$ as $|k| \to \infty$.

Although each $\alpha^{(i)}$ is analytic on every interval $[-\Omega/2 + m\Omega, \Omega/2 + m\Omega)$, discontinuities may arise at $k = \Omega/2 + m\Omega$ since $v_k^{(i)}$ need not satisfy (56). Consequently, $\alpha^{(i)}$ is generally non-analytic on $\mathbb{R}$. In Section 4.2, we show that analyticity of $\alpha^{(i)}$ on the entire real line is precisely the condition guaranteeing exponential localization of the associated Wannier function.

Remark 4.1. We note that the $\alpha^{(i)}$ functions in Lemma 4.3 are obtained from a very special choice of Bloch frames in Lemma 4.1 to ensure analyticity on $[-\Omega/2+m\Omega, \Omega/2+m\Omega)$ for $m \in \mathbb{Z}$. In general, such regularity does not hold if one forms the Bloch frames independently at each k, in which case the corresponding $\alpha^{(i)}$ can be an arbitrarily irregular function in k.

4.2 Properties of Wannier functions

We next use the analytic representation of the Bloch frames from Section 4.1 to derive Fourier formulas for the corresponding Wannier functions defined in Section 3.3 and quantify their localization. Throughout this section, we fix an isolated group of n_b bands Ψ_k in (46) with some Bloch frame denoted by Φ_k in (50).

To analyze the spatial localization of the Wannier functions, we first introduce their Fourier transforms. From (34), the Wannier function associated with component i of the Bloch frame is

$$W_0^{(i)}(x) = \frac{1}{\Omega}\int_{-\Omega/2}^{\Omega/2} v_k^{(i)}(x)\, e^{\mathrm{i}kx}\, \mathrm{d}x\,, \quad i = 1, 2, \ldots, n_b\,. \tag{63}$$

Substituting the Fourier expansion of $v_k^{(i)}$ obtained in Lemma 4.3, we obtain

$$W_0^{(i)}(x) = \frac{1}{\Omega}\int_{-\Omega/2}^{\Omega/2} \sum_{m=-\infty}^{\infty} \alpha^{(i)}(k + m\Omega) e^{\mathrm{i}(k+m\Omega)x}\, \mathrm{d}x\,. \tag{64}$$

Because the intervals $[-\Omega/2 + m\Omega, \Omega/2 + m\Omega)$ form a partition of $\mathbb{R}$, the change of variable $\xi = k + m\Omega$ turns the sum-integral into a single integral over the real line:

$$W_0^{(i)}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{2\pi}{\Omega}\alpha^{(i)}(\xi)\, e^{\mathrm{i}\xi x}\, \mathrm{d}\xi\,, \quad i = 1, 2, \ldots, n_b\,. \tag{65}$$

Hence each $W_0^{(i)}$ is, up to normalization, the inverse Fourier transform of $\alpha^{(i)}$ defined in (60).

We observe that the manipulation above is purely formal: the Bloch frame Φ_k may in general possess poor regularity in k, making $\alpha^{(i)}$ non-integrable (see Remark 4.1). However, if $\alpha^{(i)}$ is obtained from the analytic Bloch frame in Lemma 4.3, it is integrable and the expressions above are justified.

In order to apply the Fourier inversion theorem, we assume that the first and second derivatives $\alpha^{(i)\prime}$ and $\alpha^{(i)\prime\prime}$ are integrable. This leads to the following theorem for Fourier transforms of the Wannier functions.

Theorem 4.4. Suppose the Bloch frame Φ_k is chosen so that the functions $\alpha^{(i)} : \mathbb{R} \to \mathbb{C}$ are integrable. Then the corresponding composite-band Wannier functions are given by the formula

$$W_0^{(i)}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{2\pi}{\Omega}\alpha^{(i)}(\xi)\, e^{\mathrm{i}\xi x}\, \mathrm{d}\xi\,, \quad i = 1, 2, \ldots, n_b\,. \tag{66}$$

In addition, if the first and second derivatives $\alpha^{(i)\prime}$ and $\alpha^{(i)\prime\prime}$ are also integrable, then the Fourier transform of $W_0^{(i)}$ is given by

$$\widehat{W}_0^{(i)}(\xi) = \int_{-\infty}^{\infty} W_0^{(i)}(x) e^{-\mathrm{i}\xi x}\, \mathrm{d}x = \frac{2\pi}{\Omega}\alpha^{(i)}(\xi)\,, \quad i = 1, 2, \ldots, n_b\,. \tag{67}$$

We observe that the Riemann-Lebesgue lemma implies $|W_0^{(i)}(x)| \to 0$ as $|x| \to \infty$. Thus poor regularity of $\alpha^{(i)}$ yields slowly decaying Wannier functions, whereas analyticity of $\alpha^{(i)}$ on $\mathbb{R}$ guarantees exponential localization via the Paley-Wiener theorem [18]. This observation forms the analytic foundation for constructing exponentially localized Wannier functions.

To ensure the moments in (39) exist, we require that $|W_0^{(i)}(x)|$ for all $i = 1, 2, \dots, n_b$ go to zero faster than $1/|x|$ as $|x| \to \infty$; it suffices to assume that both derivatives $\alpha^{(i)\prime}$ and $\alpha^{(i)\prime\prime}$ are integrable. The following lemma contains the formulas for the first and second moment defined in (37) and (38) for all $W_0^{(i)}$ in terms of $\alpha^{(i)}$. They follow directly from the differentiation and the Plancherel theorem for the Fourier transform. The formulas can be viewed as a different form of the one-dimensional case of (7) and (8) in [8], first derived in [1].

Lemma 4.5. Suppose the Bloch frame Φ_k is chosen so that the functions $\alpha^{(i)} : \mathbb{R} \to \mathbb{C}$ for $i = 1, 2, \dots, n_b$ are integrable. Suppose further that the derivatives $\alpha^{(i)\prime}$ and $\alpha^{(i)\prime\prime}$ are also integrable. Then we have the following formulas for the first and second moments of $W_0^{(i)}(x)$:

$$\langle x \rangle_i = \int_{-\infty}^{\infty} x |W_0^{(i)}(x)|^2 \, \mathrm{d}x = \frac{2\pi}{\Omega^2} \mathrm{i} \int_{-\infty}^{\infty} \bar{\alpha}^{(i)}(\xi) \alpha^{(i)\prime}(\xi) \, \mathrm{d}\xi \,, \quad i = 1, 2, \dots, n_b \,, \tag{68}$$

and

$$\langle x^2 \rangle_i = \int_{-\infty}^{\infty} x^2 |W_0^{(i)}(x)|^2 \, \mathrm{d}x = \frac{2\pi}{\Omega^2} \int_{-\infty}^{\infty} |\alpha^{(i)\prime}(\xi)|^2 \, \mathrm{d}\xi \,, \quad i = 1, 2, \dots, n_b \,. \tag{69}$$

Hence, the total spread defined in (39) is given by the formula

$$\begin{aligned} \mathcal{S} &= \sum_{i=1}^{n_b} \left(\langle x^2 \rangle_i - \langle x \rangle_i^2 \right) \\ &= \sum_{i=1}^{n_b} \left[\frac{2\pi}{\Omega^2} \int_{-\infty}^{\infty} |\alpha^{(i)\prime}(\xi)|^2 \, \mathrm{d}\xi + \frac{4\pi^2}{\Omega^4} \left(\int_{-\infty}^{\infty} \bar{\alpha}^{(i)}(\xi) \alpha^{(i)\prime}(\xi) \, \mathrm{d}\xi \right)^2 \right] . \end{aligned} \tag{70}$$

Next, we develop a constructive procedure for obtaining the analytic Bloch frame underlying these results, through an explicit parallel-transport equation in the Fourier $\ell^2(\mathbb{Z})$ domain.

4.3 Perturbation analysis in the Fourier domain

In this section, we explicitly construct the analytic Bloch frame (Lemma 4.2) by solving the parallel-transport equation introduced in Section 3.4. Working in the Fourier domain provides a natural setting in which the k-dependence of the Fourier series in (54) and their analytic continuation become explicit. The strategy here closely parallels the single-band construction in [3] but requires substantial generalization in the composite-band setting, where all perturbation formulas must be expressed in terms of Bloch-frame projectors. We follow the notations in Section 4.1–4.2: we use Ψ_k to represent an isolated group of n_b bands and Φ_k to represent the Bloch frame to be constructed on I_{bz}.

Before applying analytic perturbation theory, we first rewrite the L^2 quantities in Section 4.1 in $\ell^2(\mathbb{Z})$ form. We recall that $u_k^{(j_i)}$ and $v_k^{(i)}$ were expanded in the Fourier series in (51)–(54). We collect all the Fourier coefficients of $u_k^{(j_i)}$ in (51) to define a family of vectors $\boldsymbol{u}^{(j_i)}(k)$ as follows:

$$\boldsymbol{u}_m^{(j_i)}(k) = b_m^{(i)}(k) \,, \quad m \in \mathbb{Z} \,, \quad k \in I_{\mathrm{bz}} \,, \quad i = 1, 2, \dots, n_b \,. \tag{71}$$

It is obvious that $\boldsymbol{u}^{(j_i)}(k) \in \ell^2(\mathbb{Z})$ for any $u_k^{(j_i)}$ that satisfies the assumptions in Lemma 4.3. Analogous to the definition (47), we collect all $\boldsymbol{u}^{(j_i)}(k)$ to form the frame $\boldsymbol{\mathcal{U}}(k) : \mathbb{C}^{n_b} \to \ell^2(\mathbb{Z})$ given by the formula

$$\boldsymbol{\mathcal{U}}(k) = \left(\boldsymbol{u}^{(j_1)}(k) \,, \boldsymbol{u}^{(j_2)}(k) \,, \cdots \,, \boldsymbol{u}^{(j_{n_b})}(k) \right) . \tag{72}$$

For the Bloch frame Φ_k in (50), we define a family of vectors $\boldsymbol{v}^{(i)}(k) \in \ell^2(\mathbb{Z})$ containing the Fourier coefficients of $v_k^{(i)}$ in (53):

$$\boldsymbol{v}_m^{(i)}(k) = a_m^{(i)}(k) = \alpha^{(i)}(k + m\Omega), \qquad m \in \mathbb{Z}, \quad k \in I_{\text{bz}}, \quad i = 1, \ldots, n_b, \tag{73}$$

where the second equality is due to (60). Similarly, we collect all $\boldsymbol{v}^{(i)}(k)$ to define another frame $\boldsymbol{\mathcal{V}}(k) : \mathbb{C}^{n_b} \to \ell^2(\mathbb{Z})$ via the formula

$$\boldsymbol{\mathcal{V}}(k) = \left(\boldsymbol{v}^{(1)}(k)\,, \boldsymbol{v}^{(2)}(k)\,, \cdots, \boldsymbol{v}^{(n_b)}(k)\right)\,, \quad k \in I_{\text{bz}}\,. \tag{74}$$

Then the orthogonality condition in (55) is compactly expressed as

$$\boldsymbol{\mathcal{U}}^*(k)\boldsymbol{\mathcal{U}}(k) = \frac{1}{a}I_{n_b}\,, \quad \boldsymbol{\mathcal{V}}^*(k)\,\boldsymbol{\mathcal{V}}(k) = \frac{1}{a}I_{n_b}\,. \tag{75}$$

We observe that (71)–(75) are merely the $\ell^2(\mathbb{Z})$ representation of (47), (49) and (55).

Next, we transform the eigenvalue equation (48) into its $\ell^2(\mathbb{Z})$ version. We introduce the Fourier series of the potential V in (48):

$$V(x) = \sum_{m=-\infty}^{\infty} \widehat{V}_m e^{\mathrm{i}m\Omega x}, \tag{76}$$

where the coefficients form a sequence $(\widehat{V}_m)_{m=-\infty}^{\infty}$ in $\ell^2(\mathbb{Z})$ for piecewise continuous potential V on I_{uc}. Inserting (76) and (71) into (48) produces an infinite linear system given by the formula

$$\left(\boldsymbol{D}(k) + \boldsymbol{V}\right)\boldsymbol{u}^{(j_i)}(k) = E_k^{(j_i)}\boldsymbol{u}^{(j_i)}(k)\,, \tag{77}$$

where $E_k^{(j_i)}$ is the eigenvalue as in (48), and infinite matrices $\boldsymbol{D}(k)$ and $\boldsymbol{V}$ are defined by the formulas

$$\boldsymbol{D}_{mn}(k) = (k + m\Omega)^2\delta_{mn}\,, \qquad \boldsymbol{V}_{mn} = \widehat{V}_{m-n}\,, \quad m, n \in \mathbb{Z}\,. \tag{78}$$

Hence, for any $k \in I_{\text{bz}}$, the operator $H(k)$ densely defined on $L^2(I_{\text{uc}})$ in (5) is transformed into the infinite matrix

$$\boldsymbol{H}(k) = \boldsymbol{D}(k) + \boldsymbol{V}\,, \tag{79}$$

densely defined on $\ell^2(\mathbb{Z})$.

In the following, we construct the analytic Bloch frames in Lemma 4.2 via Kato's theory introduced in Section 3.4. First, we consider the invariant subspace spanned by the chosen bands using the projector $\boldsymbol{P}(k) : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ with $\text{Range}(\boldsymbol{P}(k)) = \text{Range}(\boldsymbol{\mathcal{U}}(k))$ for $k \in I_{\text{bz}}$; the projector is expressed via the contour integral formula as in (40):

$$\boldsymbol{P}(k) = -\frac{1}{2\pi\mathrm{i}}\int_{\mathcal{C}} \left(\boldsymbol{H}(k) - z\right)^{-1}\,\mathrm{d}z \tag{80}$$

with its derivative similarly given by the formula (see Theorem 3.4)

$$\frac{\mathrm{d}\boldsymbol{P}(k)}{\mathrm{d}k} = \frac{1}{2\pi\mathrm{i}}\int_{\mathcal{C}} \left(\boldsymbol{H}(k) - z\right)^{-1}\frac{\mathrm{d}\boldsymbol{H}(k)}{\mathrm{d}k}\left(\boldsymbol{H}(k) - z\right)^{-1}\,\mathrm{d}z\,, \tag{81}$$

where the contour $\mathcal{C} \subset \mathbb{C}$ only encloses the eigenvalues of the selected group of bands for any $k \in I_{\text{bz}}$. Such a contour is possible due to the isolated band assumption in (17). Moreover, by simple calculation, the derivative $\frac{\mathrm{d}}{\mathrm{d}k}\boldsymbol{H}(k)$ is an infinite diagonal matrix given by

$$\frac{\mathrm{d}\boldsymbol{H}_{mn}(k)}{\mathrm{d}k} = 2(k + m\Omega)\delta_{mn}\,, \quad m, n \in \mathbb{Z}\,. \tag{82}$$

To construct a family of frames $k \mapsto \boldsymbol{\mathcal{V}}(k)$ analytic on $I_{\rm bz}$ (thus obtaining an analytic Bloch frame Φ_k as in Lemma 4.1), we apply Kato's construction in Theorem 3.3 by solving the following initial value problem on $I_{\rm bz}$:

$$\frac{\mathrm{d}\boldsymbol{\mathcal{V}}(k)}{\mathrm{d}k} = \frac{\mathrm{d}\boldsymbol{P}(k)}{\mathrm{d}k}\boldsymbol{\mathcal{V}}(k) \tag{83}$$

subject to the initial condition

$$\boldsymbol{\mathcal{V}}(-\Omega/2) = \boldsymbol{\mathcal{U}}(-\Omega/2)\,. \tag{84}$$

We observe that (83) is the composite-band version of (61) in [3] for the single-band case. Similar reasoning in (42)–(44) shows that the constructed frames have the same orthogonality and normalization as the initial frame $\boldsymbol{\mathcal{U}}(-\Omega/2)$ while satisfying

$$\boldsymbol{\mathcal{V}}^*(k)\frac{\mathrm{d}\boldsymbol{\mathcal{V}}(k)}{\mathrm{d}k} = 0\,, \quad k \in I_{\rm bz}\,. \tag{85}$$

The following lemma summarizes this explicit construction for an analytic family of Bloch frames in Lemma 4.1.

Lemma 4.6. Let Ψ_k in (46) and the corresponding $\mathcal{U}_k$ in (47) represent an isolated group of n_b bands. Let the matrix $\boldsymbol{\mathcal{U}}(k)$ in (72) denote the collection of Fourier coefficients of functions in $\mathcal{U}_k$. Then there exists an analytic family of projectors $\boldsymbol{P}(k)$ in (80) with $\mathrm{Range}(\boldsymbol{P}(k)) = \mathrm{Range}(\boldsymbol{\mathcal{U}}(k))$ and an analytic family of frames $\boldsymbol{\mathcal{V}}(k)$ satisfying

$$\frac{\mathrm{d}\boldsymbol{\mathcal{V}}(k)}{\mathrm{d}k} = \frac{\mathrm{d}\boldsymbol{P}(k)}{\mathrm{d}k}\boldsymbol{\mathcal{V}}(k)\,, \quad \boldsymbol{\mathcal{V}}(-\Omega/2) = \boldsymbol{\mathcal{U}}(-\Omega/2)\,, \tag{86}$$

with the orthogonality condition given by

$$\boldsymbol{\mathcal{V}}^*(k)\boldsymbol{\mathcal{V}}(k) = \frac{1}{a}I_{n_b}\,, \quad k \in I_{\rm bz}\,. \tag{87}$$

Consequently, the Bloch frame $\Phi_k = e^{\mathrm{i}kx}\mathcal{V}_k$ determined by $\boldsymbol{\mathcal{V}}(k)$ is analytic on $I_{\rm bz}$.

This analytic family $\boldsymbol{\mathcal{V}}(k)$ will next be examined at the Brillouin-zone boundaries to understand the discontinuities of the associated $\alpha^{(i)}$ defined in (60).

Remark 4.2. The choice of the initial frame $\boldsymbol{\mathcal{V}}(-\Omega/2)$ in (86) is arbitrary up to a right multiplication by a unitary matrix. In other words, for any $U_0 \in \mathrm{U}(n_b)$, the initial condition $\boldsymbol{\mathcal{U}}(-\Omega/2)U_0$ yields a valid Bloch frame. This arbitrariness will be fixed by imposing that the constructed Wannier functions are real.

4.4 Discontinuities at zone boundaries

Let $\boldsymbol{\mathcal{V}}(k)$ denote the analytic family constructed in Lemma 4.6. The i-th column of $\boldsymbol{\mathcal{V}}$ contains the coefficients of $v^{(i)}(k)$ defined in (54), which gives rise to $\alpha^{(i)}$ in (60):

$$\alpha^{(i)}(k + m\Omega) = a_m^{(i)}(k) = \boldsymbol{\mathcal{V}}_{mi}(k)\,, \quad k \in I_{\rm bz}\,, \quad i = 1, 2, \ldots, n_b\,, \quad m \in \mathbb{Z}\,. \tag{88}$$

In this section, we show that the discontinuities of $\alpha^{(i)}$ and all of their derivatives at the points $k = \Omega/2 + m\Omega$ are governed by a common unitary matrix.

To analyze the discontinuities, we extend the construction of $\boldsymbol{\mathcal{V}}$ on $I_{\rm bz}$ to cover the right boundary $k = \Omega/2$. The expression in (88) suggests that moving from $-\Omega/2$ to $\Omega/2$ corresponds to shifting the Fourier index by one. Thus we apply conjugation by R, the right-shifting operator defined in (1), to connect quantities at $-\Omega/2$ and $\Omega/2$. By index manipulation and unitarity of R, we first obtain

$$R\,\boldsymbol{H}(\Omega/2)R^* = \boldsymbol{H}(-\Omega/2)\,. \tag{89}$$

Similarly, we also have

$$R\,\left(\boldsymbol{H}(\Omega/2)-z\right)^{-1}R^* = \left(\boldsymbol{H}(-\Omega/2)-z\right)^{-1}\,, \tag{90}$$

for any $z \in \mathbb{C}$ not in the spectrum of $\boldsymbol{H}(k)$ at $k = \pm\Omega/2$. Applying (89)–(90) to (80) gives

$$R\,\boldsymbol{P}(\Omega/2)R^* = \boldsymbol{P}(-\Omega/2)\,. \tag{91}$$

Combining (91) with the following fact from Theorem 3.3,

$$\mathrm{Range}(\boldsymbol{\mathcal{V}}(k)) = \mathrm{Range}(\boldsymbol{P}(k))\,, \quad k \in I_{\mathrm{bz}}\,, \tag{92}$$

we conclude that

$$\mathrm{Range}\left(R\left(\boldsymbol{\mathcal{V}}(\Omega/2)\right)\right) = \mathrm{Range}(\boldsymbol{\mathcal{V}}(-\Omega/2))\,, \tag{93}$$

where R acts column-wise on $\boldsymbol{\mathcal{V}}(-\Omega/2)$. Since all columns of $\boldsymbol{\mathcal{V}}$ are orthogonal and of the same norm (see (87)), the identical range in (93) implies that there exists a unitary matrix, denoted by $U_{\mathrm{zak}} \in \mathrm{U}(n_b)$, such that

$$R\left(\boldsymbol{\mathcal{V}}(\Omega/2)\right) = \boldsymbol{\mathcal{V}}(-\Omega/2)U_{\mathrm{zak}}\,. \tag{94}$$

By the orthogonality in (87), we obtain

$$U_{\mathrm{zak}} = a\boldsymbol{\mathcal{V}}^*(-\Omega/2)R\left(\boldsymbol{\mathcal{V}}(\Omega/2)\right)\,. \tag{95}$$

We apply (88) to convert (94) into component form:

$$a_m^{(i)}(\Omega/2) = \sum_{j=1}^{n_b} U_{\mathrm{zak},ij}\,a_{m+1}^{(j)}(-\Omega/2)\,, \quad i = 1,2,\ldots,n_b, \quad m \in \mathbb{Z}\,, \tag{96}$$

which gives explicitly the jumps of $\alpha^{(i)}$ in (88) at $k = \Omega/2 + m\Omega$.

Remark 4.3. The unitary matrix U_{zak} is the multiband generalization of the scalar Zak phase factor [15], which is denoted by $e^{\mathrm{i}\varphi_{\mathrm{zak}}}$ in [3].

Next, we show that the derivatives of $\boldsymbol{\mathcal{V}}$ obey the same relation as in (94) using (86) and $\frac{\mathrm{d}\boldsymbol{P}}{\mathrm{d}k}$ from (81). A simple calculation involving $\frac{\mathrm{d}\boldsymbol{H}}{\mathrm{d}k}$ in (82) also shows that

$$R\,\frac{\mathrm{d}\boldsymbol{H}(\Omega/2)}{\mathrm{d}k}R^* = \frac{\mathrm{d}\boldsymbol{H}(-\Omega/2)}{\mathrm{d}k}\,. \tag{97}$$

Combining (90), (97) with (81) yields

$$R\,\frac{\mathrm{d}\boldsymbol{P}(\Omega/2)}{\mathrm{d}k}R^* = \frac{\mathrm{d}\boldsymbol{P}(-\Omega/2)}{\mathrm{d}k}\,. \tag{98}$$

Thus applying the right-shift operator to the differential equation in (86) at $k = \Omega/2$ produces

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}k}R\left(\boldsymbol{\mathcal{V}}(\Omega/2)\right) &= \frac{\mathrm{d}\boldsymbol{P}(-\Omega/2)}{\mathrm{d}k}R\left(\boldsymbol{\mathcal{V}}(\Omega/2)\right)\\ &= \frac{\mathrm{d}\boldsymbol{P}(-\Omega/2)}{\mathrm{d}k}\boldsymbol{\mathcal{V}}(-\Omega/2)U_{\mathrm{zak}}\\ &= \frac{\mathrm{d}\boldsymbol{\mathcal{V}}(-\Omega/2)}{\mathrm{d}k}U_{\mathrm{zak}}\,,\end{aligned} \tag{99}$$

where the second equality is from (94). Just like that (96) is the component form of (94), the relation in (99) is equivalent to

$$\frac{\mathrm{d}}{\mathrm{d}k} a_m^{(i)}(\Omega/2) = \sum_{j=1}^{n_b} U_{\mathrm{zak},ij} \frac{\mathrm{d}}{\mathrm{d}k} a_{m+1}^{(j)}(-\Omega/2)\,, \quad i = 1, 2, \ldots, n_b, \quad m \in \mathbb{Z}\,, \tag{100}$$

which specifies the jumps of the first derivative of $\alpha^{(i)}$ in (88) at the boundary points.

Furthermore, the same reasoning extends to derivatives of any order n. By repeatedly differentiating (86), one obtains expressions for $\boldsymbol{\mathcal{V}}^{(n)}$ with $n = 2, 3, \ldots$, each involving higher-order derivatives of $\boldsymbol{P}$. According to Theorem 3.4, the contour-integral representation of the derivatives of $\boldsymbol{P}$ depends only on $(\boldsymbol{H} - z)^{-1}$ and derivatives of $\boldsymbol{H}$. Since $\boldsymbol{H}$ is a quadratic polynomial in k, only $\frac{\mathrm{d}\boldsymbol{H}}{\mathrm{d}k}$ from (82) and $\frac{\mathrm{d}^2\boldsymbol{H}}{\mathrm{d}k^2}$—the latter being a constant multiple of the identity—appear in these expressions. This allows the extension of (98) to higher-order derivatives of $\boldsymbol{P}$. The extension of (100) to higher-order derivatives then follows by induction.

Lemma 4.7. Let $\boldsymbol{\mathcal{V}}$ of the form (74) be the analytic family of matrices constructed in Lemma 4.6. Then there exists a unitary matrix $U_{\mathrm{zak}} \in \mathrm{U}(n_b)$ such that

$$R\left(\boldsymbol{\mathcal{V}}(\Omega/2)\right) = \boldsymbol{\mathcal{V}}(-\Omega/2)U_{\mathrm{zak}}\,, \tag{101}$$

where R is the right-shift operator on $\ell^2(\mathbb{Z})$. Moreover, all derivatives of $\boldsymbol{\mathcal{V}}(k)$ at the zone boundaries $k = \pm\Omega/2$ satisfy the same relation:

$$R\left(\boldsymbol{\mathcal{V}}^{(n)}(\Omega/2)\right) = \boldsymbol{\mathcal{V}}^{(n)}(-\Omega/2)U_{\mathrm{zak}}\,, \quad n \in \mathbb{N}\,. \tag{102}$$

Consequently, the functions $\alpha^{(i)}$ in (88) and all their derivatives have identical jump relations at $k = \Omega/2 + m\Omega$ for $m \in \mathbb{Z}$, given by U_{zak}.

We now construct a gauge transformation that removes these discontinuities, ensuring the analyticity of $\alpha^{(i)}$ on $\mathbb{R}$.

Remark 4.4. We observe that results in Lemma 4.7 all stem from the simple algebraic identity (89), which is due to the fact that the original Schrödinger operator in (5) is a combination of differentiation and multiplication by a function. Although this paper focuses on the Schrödinger operator, the same reasoning applies to other periodic differential operators—such as Maxwell or Dirac—where relations analogous to (89) hold.

4.5 Gauge transformation

In this section, we introduce the notion of a gauge transformation and show that a simple class of gauge choices removes all discontinuities of $\alpha^{(i)}$ in Lemma 4.7, therefore obtaining exponentially localized Wannier functions. This class does not exhaust all possible gauges; Section 4.6 treats the general case for obtaining the optimal solution.

Let $U : I_{\mathrm{bz}} \to \mathrm{U}(n_b)$ be a continuously differentiable (not necessarily periodic) family of unitary matrices. Applying $U(k)$ to $\boldsymbol{\mathcal{V}}(k)$ constructed in Lemma 4.6 produces a new family

$$\widetilde{\boldsymbol{\mathcal{V}}}(k) = \boldsymbol{\mathcal{V}}(k)U(k)\,, \quad k \in I_{\mathrm{bz}}\,. \tag{103}$$

We refer to the operation in (103) as a gauge transformation. It clearly preserves the orthogonality in (75):

$$\widetilde{\boldsymbol{\mathcal{V}}}^*(k)\widetilde{\boldsymbol{\mathcal{V}}}(k) = \frac{1}{a} I_{n_b}\,, \quad k \in I_{\mathrm{bz}}\,. \tag{104}$$

The transformed $\widetilde{\boldsymbol{\mathcal{V}}}(k)$ induces a new set of functions $\widetilde{\alpha}^{(i)}:\mathbb{R}\to\mathbb{C}$ for $i=1,2,\dots,n_b$; using the definition of $\alpha^{(i)}$ in (60), the new functions $\widetilde{\alpha}^{(i)}$ are given by the formula

$$\widetilde{\alpha}^{(i)}(k+m\Omega)=\sum_{j=1}^{n_b} U_{ij}(k)\,\alpha^{(j)}(k+m\Omega)\,,\quad k\in I_{\mathrm{bz}}\,,\quad m\in\mathbb{Z}\,. \tag{105}$$

Since $\boldsymbol{\mathcal{V}}$ satisfies (86), we differentiate (103) to obtain

$$\frac{\mathrm{d}\widetilde{\boldsymbol{\mathcal{V}}}(k)}{\mathrm{d}k}=\frac{\mathrm{d}\boldsymbol{P}(k)}{\mathrm{d}k}\widetilde{\boldsymbol{\mathcal{V}}}(k)+\widetilde{\boldsymbol{\mathcal{V}}}(k)U^*(k)\frac{\mathrm{d}U(k)}{\mathrm{d}k}\,. \tag{106}$$

Since $U(k)$ is unitary, the matrix $U^*(k)U'(k)$ is skew-Hermitian:

$$\left(U^*(k)\frac{\mathrm{d}U(k)}{\mathrm{d}k}\right)^*=-U^*(k)\frac{\mathrm{d}U(k)}{\mathrm{d}k}\,,\quad k\in I_{\mathrm{bz}}\,, \tag{107}$$

which implies that the matrix $U^*(k)\frac{\mathrm{d}U(k)}{\mathrm{d}k}$ is an element in $\mathfrak{u}(n_b)$, the Lie algebra of $\mathrm{U}(n_b)$. (This quantity is also often referred to as the right-invariant vector field on $\mathrm{U}(n_b)$.) We define a family of matrices $A:I_{\mathrm{bz}}\to\mathbb{C}^{n_b\times n_b}$ via the formula

$$A(k)=\mathrm{i}U^*(k)\frac{\mathrm{d}U(k)}{\mathrm{d}k}\,, \tag{108}$$

so that $A(k)$ is a Hermitian matrix. Thus, the new notation turns (106) into

$$\frac{\mathrm{d}\widetilde{\boldsymbol{\mathcal{V}}}(k)}{\mathrm{d}k}=\frac{\mathrm{d}\boldsymbol{P}(k)}{\mathrm{d}k}\widetilde{\boldsymbol{\mathcal{V}}}(k)-\mathrm{i}\widetilde{\boldsymbol{\mathcal{V}}}(k)A(k)\,. \tag{109}$$

In the physics literature, the quantity A is often referred to as the (non-Abelian) Berry connection [13, 14]. Left-multiplying (109) by $\mathrm{i}\widetilde{\boldsymbol{\mathcal{V}}}^*(k)$ and using (104) gives

$$\mathrm{i}\widetilde{\boldsymbol{\mathcal{V}}}^*(k)\frac{\mathrm{d}\widetilde{\boldsymbol{\mathcal{V}}}(k)}{\mathrm{d}k}=\frac{1}{a}A(k)\,, \tag{110}$$

where the term containing $\frac{\mathrm{d}\boldsymbol{P}}{\mathrm{d}k}$ vanishes due to (85) and the prefactor $\frac{1}{a}$ is due to the normalization in (104). The Berry connection is typically defined in the form of (110).

Next, we determine a class of gauge transformations that yields exponentially localized Wannier functions. We take U_{zak} in (95) and apply the standard matrix $\log:\mathrm{U}(n_b)\to\mathfrak{u}(n_b)$ and divide it by Ω for normalization to obtain

$$A_{\mathrm{zak}}=\frac{\mathrm{i}}{\Omega}\log(U_{\mathrm{zak}})\,, \tag{111}$$

by which we define the following family of unitary matrices

$$U_\star(k)=\exp\left(-\mathrm{i}A_{\mathrm{zak}}\left(k+\frac{\Omega}{2}\right)\right)\,,\quad k\in I_{\mathrm{bz}}\,, \tag{112}$$

whose boundary values are

$$U_\star(-\Omega/2)=I_{n_b}\,,\quad U_\star(\Omega/2)=U_{\mathrm{zak}}\,. \tag{113}$$

We then apply the gauge transformation defined in (112) with $U(k)=U_\star(k)$ in (112); Combining the identity $\widetilde{\boldsymbol{\mathcal{V}}}(\Omega/2)=\boldsymbol{\mathcal{V}}(\Omega/2)U_{\mathrm{zak}}$ with Lemma 4.7, it is obvious that this removes the discontinuity in (101) and we now have

$$R\left(\widetilde{\boldsymbol{\mathcal{V}}}(\Omega/2)\right)=\widetilde{\boldsymbol{\mathcal{V}}}(-\Omega/2)\,. \tag{114}$$

Moreover, all derivative discontinuities are also removed since Lemma 4.7 shows that they are identical. Thus every $\widetilde{\alpha}^{(i)}$ defined in (105) with the gauge transformation by (112) is an analytic function on $\mathbb{R}$. By Theorem 4.4, all composite-band Wannier functions $W_0^{(i)}$, given by the inverse Fourier transform of $\widetilde{\alpha}^{(i)}$ via (66), are exponentially localized. This observation completes the construction of exponentially localized Wannier functions.

Theorem 4.8. Let $\boldsymbol{\mathcal{V}}(k)$ be the parallel-transport solution on I_{bz} from Lemma 4.6 and define the unitary matrix U_{zak} by (95) and the Hermitian matrix A_{zak} by (111). Consider the gauge transformation on I_{bz} given by the formulas

$$\widetilde{\boldsymbol{\mathcal{V}}}(k) = \boldsymbol{\mathcal{V}}(k) U_\star(k)\,, \quad \text{with} \quad U_\star(k) = \exp\left(-\mathrm{i} A_{\text{zak}}\left(k + \frac{\Omega}{2}\right)\right)\,, \tag{115}$$

so that $\widetilde{\boldsymbol{\mathcal{V}}}(k)$ satisfies

$$\frac{\mathrm{d}\widetilde{\boldsymbol{\mathcal{V}}}(k)}{\mathrm{d}k} = \frac{\mathrm{d}\boldsymbol{P}(k)}{\mathrm{d}k}\widetilde{\boldsymbol{\mathcal{V}}}(k) - \mathrm{i}\widetilde{\boldsymbol{\mathcal{V}}}(k) A_{\text{zak}}\,. \tag{116}$$

Then the Wannier functions $W_0^{(i)}$ associated with the transformed $\widetilde{\alpha}^{(i)}$ in (105) given by the formula

$$W_0^{(i)}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{2\pi}{\Omega}\widetilde{\alpha}^{(i)}(\xi)\, e^{\mathrm{i}\xi x}\,\mathrm{d}\xi\,, \quad i = 1, 2, \ldots, n_b\,. \tag{117}$$

are exponentially localized.

It is worth noting that the unitary matrix U_{zak} (95) that determines the jump condition may in general be non-diagonal. To expose its internal structure, we diagonalize it via the spectral theorem,

$$U_{\text{zak}} = W_0 D W_0^*, \quad D = \operatorname{diag}\left(e^{-\mathrm{i}\varphi_1}, e^{-\mathrm{i}\varphi_2}, \ldots, e^{-\mathrm{i}\varphi_{n_b}}\right)\,, \tag{118}$$

from which we use (111) to obtain the diagonal form of A_{zak}:

$$A_{\text{zak}} = W_0 D_{\text{zak}} W_0^*, \quad D_{\text{zak}} = \frac{1}{\Omega}\operatorname{diag}\left(\varphi_1, \varphi_2, \ldots, \varphi_{n_b}\right)\,. \tag{119}$$

Remark 4.5. We have implicitly assumed the matrix log is taken on the principal branch such that $\varphi_1, \varphi_2, \ldots, \varphi_{n_b} \in (-\pi, \pi]$ in (118). More generally, we may as well choose

$$\log(D) = -\mathrm{i}\operatorname{diag}\left(\varphi_1 + 2\pi m_1, \varphi_2 + 2\pi m_2, \ldots, \varphi_{n_b} + 2\pi m_{n_b}\right) \tag{120}$$

for any $m_1, m_2, \ldots, m_{n_b} \in \mathbb{Z}$ when computing

$$A_{\text{zak}} = \frac{\mathrm{i}}{\Omega}\log(U_{\text{zak}}) = \frac{\mathrm{i}}{\Omega} W_0 \log(D) W_0^*\,. \tag{121}$$

All these choices will not affect the exponential localization result of Theorem 4.8 since the matrix exponential in (112) removes all the 2π-phase differences.

4.6 Globally optimal gauge choice

Section 4.5 established that gauge transformations in the form of (115) yield exponentially localized Wannier functions. In this section, we show that (115) *nearly* yields the globally optimal gauge that minimizes the total spread in Lemma 4.5 among all possible exponentially localized Wannier functions; the truly optimal choice is the diagonal form of (115).

Given the solution in Theorem 4.8, we next examine whether any additional analytic gauge transformation $W(k)$, defined by the formula

$$\widetilde{\boldsymbol{\mathcal{V}}}(k) = \boldsymbol{\mathcal{V}}(k)U_\star(k)W(k)\,, \quad k \in I_{\rm bz}\,, \tag{122}$$

can further reduce the total spread. This representation encompasses all gauge choices that lead to exponential localization, since for any permissible $U(k)$ in (103) we simply set $W(k) = U_\star^*(k)U(k)$. Furthermore, to ensure continuity across the Brillouin zone as in (114), it is necessary that W is periodic:

$$W(-\Omega/2) = W(\Omega/2)\,. \tag{123}$$

The transformed $\widetilde{\boldsymbol{\mathcal{V}}}$ still satisfies (109):

$$\frac{\mathrm{d}\widetilde{\boldsymbol{\mathcal{V}}}(k)}{\mathrm{d}k} = \frac{\mathrm{d}\boldsymbol{P}(k)}{\mathrm{d}k}\widetilde{\boldsymbol{\mathcal{V}}}(k) - \mathrm{i}\widetilde{\boldsymbol{\mathcal{V}}}(k)A(k)\,, \tag{124}$$

with a different Berry connection given by the formula (see (108))

$$A(k) = W^*(k)A_{\rm zak}W(k) + \mathrm{i}W^*(k)\frac{\mathrm{d}W(k)}{\mathrm{d}k}\,. \tag{125}$$

To make the gauge dependence of the total spread $\mathcal{S}$ transparent, we rewrite the formulas of Lemma 4.5 in terms of the quantities in (124). By combining (68) and (69) in Lemma 4.5 with (105) applied to $\widetilde{\boldsymbol{\mathcal{V}}}$ in (122), we obtain the following expression for the individual Wannier center

$$\langle x\rangle_i = \frac{a}{2\pi}\int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} A_{ii}(k)\,\mathrm{d}k\,, \quad i = 1, 2, \ldots, n_b\,, \tag{126}$$

from which we obtain the sum of all centers

$$\sum_{i=1}^{n_b}\langle x\rangle_i = \frac{a}{2\pi}\int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} \mathrm{Tr}(A(k))\,\mathrm{d}k\,, \tag{127}$$

and the sum of the second moments is given by the formula

$$\sum_{i=1}^{n_b}\langle x^2\rangle_i = \frac{a^2}{2\pi}\int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} \left\|\frac{\mathrm{d}}{\mathrm{d}k}\boldsymbol{P}(k)\widetilde{\boldsymbol{\mathcal{V}}}(k)\right\|_F^2 \mathrm{d}k + \frac{a}{2\pi}\int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} \|A(k)\|_F^2\,\mathrm{d}k\,, \tag{128}$$

where we have used (110) and $\Omega = \frac{2\pi}{a}$. We observe that only the second term in (128) depends on the gauge choice. Hence, using (126) and (128) turns the total spread in Lemma 4.5 into the following exact decomposition:

$$\begin{aligned}\mathcal{S} = {} & \frac{a^2}{2\pi}\int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} \left\|\frac{\mathrm{d}}{\mathrm{d}k}\boldsymbol{P}(k)\widetilde{\boldsymbol{\mathcal{V}}}(k)\right\|_F^2 \mathrm{d}k + \sum_{\substack{i,j=1\\(i\neq j)}}^{n_b} \frac{a}{2\pi}\int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} |A_{ij}(k)|^2\,\mathrm{d}k \\ & + \sum_{i=1}^{n_b}\frac{a}{2\pi}\int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} \left(A_{ii}(k) - \langle x\rangle_i\right)^2\,\mathrm{d}k\,,\end{aligned} \tag{129}$$

where the $\|A(k)\|_F^2$ in (128) is split into the off-diagonal and diagonal part (which is real as A is Hermitian). The decomposition in (129) reveals the optimality conditions:

1. $A(k)$ is diagonal for all $k \in I_{\rm bz}$;

2. $A_{ii}(k) = \langle x \rangle_i = \text{constant for all } k \in I_{\text{bz}}\,, \quad i = 1, 2, \ldots, n_b\,.$

leaving only the gauge-invariant part in (129); thus any gauge achieving these two conditions is globally optimal.

The optimality conditions are satisfied by the constant matrix W_0 from (119), which diagonalizes A_{zak}. To see it, we set

$$W(k) = W_0\,, \quad k \in I_{\text{bz}}\,, \tag{130}$$

which turns $A(k)$ in (125) into D_{zak}, the diagonal form of A_{zak}. We next show that this choice is unique, up to the freedom of selecting the diagonalizer W_0 of A_{zak}. Suppose there exists other $W(k)$ turning $A(k)$ in (125) into a constant real diagonal matrix, denoted by B. Then (125) becomes a differential equation for $W(k)$:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}k}W(k) = W(k)B - A_{\text{zak}}W(k)\,, \tag{131}$$

whose solution is given by

$$W(k) = e^{\mathrm{i}A_{\text{zak}}\left(k+\frac{\Omega}{2}\right)}C_0 e^{-\mathrm{i}B\left(k+\frac{\Omega}{2}\right)}\,, \tag{132}$$

where C_0 is a constant matrix to be fixed by the boundary condition (123). Imposing this boundary condition (123) and right multiplying by $e^{-\mathrm{i}\Omega B}$ gives

$$U_{\text{zak}}C_0 = C_0 e^{\mathrm{i}\Omega B}\,, \tag{133}$$

which is the eigenvalue equation for U_{zak} as in (118). Thus C_0 diagonalizes U_{zak} with $B = -D_{\text{zak}}$ in (119) (up to permutation). It then follows that $C_0 e^{-\mathrm{i}B\left(k+\frac{\Omega}{2}\right)}C_0^* = e^{\mathrm{i}A_{\text{zak}}\left(k+\frac{\Omega}{2}\right)}$, which turns (132) into

$$W(k) = C_0\,. \tag{134}$$

Comparing (130) with (134) shows that the global optimal choice in (130) is unique up to the degrees of freedom in choosing the diagonalizer for A_{zak}.

Theorem 4.9. Let $\boldsymbol{\mathcal{V}}$ and $U_\star$ be same as in Theorem 4.8 and let $A_{\text{zak}} = W_0 D_{\text{zak}} W_0^*$, with $D_{\text{zak}} = \frac{1}{\Omega}\,\text{diag}\,(\varphi_1, \ldots, \varphi_{n_b})$. Then the globally optimal gauge choice minimizing the total spread $\mathcal{S}$ is given by the formula

$$\widetilde{\boldsymbol{\mathcal{V}}}(k) = \boldsymbol{\mathcal{V}}(k)U_\star(k)W_0\,, \quad k \in I_{\text{bz}}\,, \tag{135}$$

that satisfies the differential equation

$$\frac{\mathrm{d}\widetilde{\boldsymbol{\mathcal{V}}}(k)}{\mathrm{d}k} = \frac{\mathrm{d}\boldsymbol{P}(k)}{\mathrm{d}k}\widetilde{\boldsymbol{\mathcal{V}}}(k) - \mathrm{i}\widetilde{\boldsymbol{\mathcal{V}}}(k)D_{\text{zak}}\,. \tag{136}$$

Furthermore, the global optimum (135) is unique up to the choice of the diagonalizer W_0 for A_{zak}. At this optimum, the sum of Wannier centers and the total spread $\mathcal{S}$ of the corresponding Wannier functions are given by the formulas

$$\sum_{i=1}^{n_b}\langle x \rangle_i = \text{Tr}(A_{\text{zak}}) = \frac{a}{2\pi}\sum_{i=1}^{n_b}\varphi_i\,, \qquad \mathcal{S} = \frac{a^2}{2\pi}\int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}}\left\|\frac{\mathrm{d}\boldsymbol{P}(k)}{\mathrm{d}k}\widetilde{\boldsymbol{\mathcal{V}}}(k)\right\|_F^2 \mathrm{d}k\,, \tag{137}$$

which both only contain gauge-invariant quantities.

Remark 4.6. As explained in Remark 4.5, different branch choices lead to different A_{zak}, but this will only cause the individual Wannier centers in (126) and their sum (137) to be shifted by integer lattice points. This only results in identical Wannier functions centered at different lattice points due to (33).

Remark 4.7. Gauge invariance of the total center sum follows directly by substituting (125) into (127) to obtain

$$\sum_{i=1}^{n_b} \langle x \rangle_i = \frac{a}{2\pi} \int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} \operatorname{Tr}(W^*(k) A_{\text{zak}} W(k))\, \mathrm{d}k + \frac{a}{2\pi} \mathrm{i} \int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} \operatorname{Tr}\big(W^*(k) W'(k)\big)\, \mathrm{d}k\,, \quad (138)$$

where the first term is the gauge-invariant part and the second term vanishes since $\operatorname{Tr}(W^*(k)W'(k)) = \frac{\mathrm{d}}{\mathrm{d}k} \log\det W(k)$ vanishes after integration due to periodicity (123). For the total spread $\mathcal{S}$, we observe that the projector $\boldsymbol{P} = \frac{1}{a}\widetilde{\boldsymbol{\mathcal{V}}}\widetilde{\boldsymbol{\mathcal{V}}}^*$, where the $1/a$ factor is due to normalization in (104), gives the following equivalent expressions

$$\mathcal{S} = \frac{a}{2\pi} \int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} \operatorname{Tr}\left(\boldsymbol{P}'^*(k) \boldsymbol{P}'(k) \boldsymbol{P}(k)\right)\, \mathrm{d}k = \frac{a}{2\pi} \int_{-\frac{\Omega}{2}}^{\frac{\Omega}{2}} \left\| \boldsymbol{P}'(k)\boldsymbol{P}(k) \right\|_F^2 \mathrm{d}k\,, \quad (139)$$

which is obviously gauge-invariant.

4.7 Reality of Wannier functions

In this section, we show that the time-reversal symmetry condition (142) implies the analytic Bloch frames constructed in Theorems 4.8 and 4.9 can be chosen to yield real Wannier functions after a simple modification, as alluded to in Remark 4.2. The initial condition $\boldsymbol{\mathcal{U}}(-\Omega/2)$ in Lemma 4.6 is arbitrary up to multiplication by a constant unitary matrix U_0. Such a modification does not change Theorem 4.8 and 4.9, but different initial conditions lead to different Wannier functions. In what follows, we show that this remaining ambiguity can be removed by selecting a particular initial frame $\boldsymbol{\mathcal{U}}(-\Omega/2)$ for which all composite-band Wannier functions are real.

To introduce the modification, we first define the time-reversal operator $T : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ by complex conjugation composed with index reversal,

$$T(\boldsymbol{u})_m = \overline{\boldsymbol{u}}_{-m}\,, m \in \mathbb{Z}\,. \quad (140)$$

We observe that T is an antiunitary operator and it is easy to verify that

$$T^{-1} = T^* = T\,. \quad (141)$$

The time-reversal symmetry in (5) implies that the ℓ^2-version $\boldsymbol{H}$ in (79) satisfies

$$T\boldsymbol{H}(k)T^* = \boldsymbol{H}(-k)\,. \quad (142)$$

Combining (142) with (80) and (81) shows that

$$T\boldsymbol{P}(k)T^* = \boldsymbol{P}(-k)\,, \quad T\boldsymbol{P}'(k)T^* = -\boldsymbol{P}'(-k)\,. \quad (143)$$

Next, we compose the right-shift operator R with T and denote the composition by $S = TR$. More explicitly, it is given by the formula

$$(S\boldsymbol{u})_m = (TR\boldsymbol{u})_m = \overline{\boldsymbol{u}}_{-m-1}\,, \quad m \in \mathbb{Z}\,. \quad (144)$$

We combine (142)–(143) with (89) and (91) to conclude that

$$\boldsymbol{H}(-\Omega/2) = S\boldsymbol{H}(-\Omega/2)S^* \quad (145)$$

and

$$\boldsymbol{P}(-\Omega/2) = S\boldsymbol{P}(-\Omega/2)S^*\,. \quad (146)$$

4.7.1 Construction of the initial frame for reality

Starting from the initial frame $\boldsymbol{\mathcal{U}}(-\Omega/2)$ in (86), whose columns are eigenvectors of $\boldsymbol{H}(k)$ at $k = -\Omega/2$, we apply the symmetry relations (145)–(146) to construct a new initial frame invariant under S defined in (144).

First, we investigate the action of S on $\boldsymbol{\mathcal{U}}(-\Omega/2)$. The relation in (145) implies that vectors in $S\boldsymbol{\mathcal{U}}(-\Omega/2)$ (with S applied column-wise) are also eigenvectors of $\boldsymbol{H}(-\Omega)$ while (146) ensures that columns in $S\boldsymbol{\mathcal{U}}(-\Omega/2)$ span the same subspace as those in $\boldsymbol{\mathcal{U}}(-\Omega/2)$. Since the subspace is S-invariant, the frames differ only by a constant unitary matrix:

$$S\boldsymbol{\mathcal{U}}(-\Omega/2) = \boldsymbol{\mathcal{U}}(-\Omega/2)U_0\,, \tag{147}$$

which can be combined with orthogonality (75) to compute $U_0 \in \mathrm{U}_{n_b}$ via

$$U_0 = a\boldsymbol{\mathcal{U}}^*(-\Omega/2)S\boldsymbol{\mathcal{U}}(-\Omega/2)\,. \tag{148}$$

Because T is antiunitary, U_0 is complex symmetric (i.e. $U_0 = U_0^T$). Indeed, a direct calculation using (144) shows that, for any indices $k, l = 1, 2, \ldots, n_b$, we have

$$U_{0,kl} = \sum_{m=-\infty}^{\infty} \overline{\boldsymbol{u}}_m^{(j_k)} S(\boldsymbol{u}^{(j_l)})_m = \sum_{m=-\infty}^{\infty} \overline{\boldsymbol{u}}_m^{(j_k)} \overline{\boldsymbol{u}}_{-m-1}^{(j_l)} = \sum_{n=-\infty}^{\infty} \overline{\boldsymbol{u}}_{-n-1}^{(j_k)} \overline{\boldsymbol{u}}_n^{(j_l)} = U_{0,lk}\,, \tag{149}$$

where we use (144) to obtain the second equality and the third one by setting $n = -m-1$.

We now construct an S-invariant initial frame. Since U_0 is unitary, we apply the spectral theorem to define its matrix square root (assuming the principal branch):

$$U_S = U_0^{\frac{1}{2}}\,, \tag{150}$$

and it is also a complex-symmetric unitary matrix as U_0. This then implies $U_S^* = U_S^{-1} = \overline{U_S}$. We transform the initial frame by U_S via the formula

$$\widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2) = \boldsymbol{\mathcal{U}}(-\Omega/2)U_S\,, \tag{151}$$

and its S-invariance is easily verified:

$$S\widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2) = \boldsymbol{\mathcal{U}}(-\Omega/2)U_0\overline{U_S} = \boldsymbol{\mathcal{U}}(-\Omega/2)U_S = \widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2)\,. \tag{152}$$

This leads to the following lemma.

Lemma 4.10. Suppose that $\boldsymbol{H}$ satisfies the time-reversal symmetry as in (142). Let $\boldsymbol{\mathcal{U}}(-\Omega/2)$ be the initial frame in (86) and define

$$\widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2) = \boldsymbol{\mathcal{U}}(-\Omega/2)U_S\,, \tag{153}$$

where $U_S = U_0^{\frac{1}{2}}$ is a complex symmetric unitary matrix defined in (150). Then the new $\widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2)$ satisfies

$$S\widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2) = \widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2)\,. \tag{154}$$

In other words, it is invariant under the combined time-reversal-shift operator S.

This lemma establishes a canonical S-invariant initial condition, which will be used in Section 4.7.3 to achieve the reality of Wannier functions.

Remark 4.8. If an eigenvalue of $\boldsymbol{H}(-\Omega/2)$ is non-degenerate, the symmetries in (145)–(146) implies that the corresponding eigenvector $\boldsymbol{u}^{(j_i)}(-\Omega/2)$ satisfies

$$S\left(\boldsymbol{u}^{(j_i)}(-\Omega/2)\right) = e^{\mathrm{i}\theta_i}\boldsymbol{u}^{(j_i)}(-\Omega/2)\,, \quad \text{for some } \theta_i \in (-\pi, \pi]\,. \tag{155}$$

Hence U_0 is a diagonal matrix given by

$$U_0 = \mathrm{diag}(e^{\mathrm{i}\theta_1}, e^{\mathrm{i}\theta_2}, \ldots, e^{\mathrm{i}\theta_{n_b}})\,. \tag{156}$$

When a degeneracy occurs (with multiplicity 2 the only possibility in one dimension by Lemma 3.1), the corresponding block of U_0 is a 2×2 unitary matrix acting within that degenerate subspace. Consequently, U_S in (150) inherits the same block-unitary structure as U_0 within each degenerate subspace.

4.7.2 Reality of Berry connections

Before we construct real Wannier functions, we show that the Berry connection A_{zak} in (116) is a real symmetric matrix, if we replace the initial frame $\boldsymbol{\mathcal{U}}(-\Omega/2)$ in Lemma 4.6 with its S-invariant $\widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2)$ in Lemma 4.10. More explicitly, the new initial condition is given by

$$\boldsymbol{\mathcal{V}}(-\Omega/2) = \widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2)\,. \tag{157}$$

We now show that the Berry connection associated with the S-invariant initial condition is real symmetric.

Lemma 4.11. Suppose that the initial condition in Lemma 4.6 is replaced by (157). Then the Berry connection A_{zak} in Theorem 4.8 is a real symmetric matrix.

Proof. By the definition of A_{zak} in (111), it suffices to show that U_{zak} in (95) is complex symmetric, $U_{\mathrm{zak}} = U_{\mathrm{zak}}^T$; combined with unitarity, it is always possible to choose its diagonalizer W_0 to be real, implying that A_{zak} is real symmetric by (119).

To show the complex symmetry of U_{zak}, we first observe that under this assumption $\boldsymbol{\mathcal{V}}$ satisfies the same equation as in (86) with the modified initial condition (157):

$$\boldsymbol{\mathcal{V}}'(k) = \boldsymbol{P}'(k)\boldsymbol{\mathcal{V}}(k)\,, \quad \boldsymbol{\mathcal{V}}(-\Omega/2) = \widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2)\,. \tag{158}$$

Then the time-reversed pair defined by $\boldsymbol{\mathcal{V}}_{\mathrm{TR}}(k) = \boldsymbol{\mathcal{V}}(-k)$ satisfies

$$\boldsymbol{\mathcal{V}}_{\mathrm{TR}}'(k) = -\boldsymbol{\mathcal{V}}'(-k) = -\boldsymbol{P}'(-k)\boldsymbol{\mathcal{V}}(-k) = -\boldsymbol{P}'(-k)\boldsymbol{\mathcal{V}}_{\mathrm{TR}}(k)\,. \tag{159}$$

We apply T in (140) to the above equation and use (143) to conclude that

$$(T\boldsymbol{\mathcal{V}}_{\mathrm{TR}})'(k) = \boldsymbol{P}'(k)T\boldsymbol{\mathcal{V}}_{\mathrm{TR}}(k) \tag{160}$$

with the initial condition

$$T\boldsymbol{\mathcal{V}}_{\mathrm{TR}}(-\Omega/2) = T\boldsymbol{\mathcal{V}}(\Omega/2) = T\left(R\boldsymbol{\mathcal{V}}(-\Omega/2)U_{\mathrm{zak}}\right) = S\left(\boldsymbol{\mathcal{V}}(-\Omega/2)\right)\overline{U_{\mathrm{zak}}}\,, \tag{161}$$

where we used (101) for the second equality. Apply the S-invariance in Lemma 4.10 and we obtain

$$T\boldsymbol{\mathcal{V}}_{\mathrm{TR}}(-\Omega/2) = \boldsymbol{\mathcal{V}}(-\Omega/2)\overline{U_{\mathrm{zak}}}\,. \tag{162}$$

Comparing (158) with (160) and (162), we conclude that $\boldsymbol{\mathcal{V}}$ and $T\boldsymbol{\mathcal{V}}_{\mathrm{TR}}U_{\mathrm{zak}}^T$ satisfy the same differential equation and initial condition. By the uniqueness theorem of initial value problems on Banach spaces [16], it follows that

$$\boldsymbol{\mathcal{V}}(k) = T\boldsymbol{\mathcal{V}}_{\mathrm{TR}}(k)U_{\mathrm{zak}}^T = T\boldsymbol{\mathcal{V}}(-k)U_{\mathrm{zak}}^T\,, \quad k \in I_{\mathrm{bz}}\,. \tag{163}$$

Due to (141), we have $T^2 = \boldsymbol{I}$. Hence, we reverse $k \mapsto -k$ in (163), followed by applying T, to obtain

$$T\boldsymbol{\mathcal{V}}(-k) = \boldsymbol{\mathcal{V}}(k)U_{\text{zak}}^*, \quad k \in I_{\text{bz}}. \tag{164}$$

Substituting (164) into the (163) produces

$$\boldsymbol{\mathcal{V}}(k) = \boldsymbol{\mathcal{V}}(k)U_{\text{zak}}^* U_{\text{zak}}^T. \tag{165}$$

Left multiplying $\boldsymbol{\mathcal{V}}^*(k)$ and using the orthogonality in (75) gives $U_{\text{zak}}^* U_{\text{zak}}^T = I_{n_b}$. Since U_{zak} is unitary, we prove the complex symmetry $U_{\text{zak}} = U_{\text{zak}}^T$. □

4.7.3 Time-reversal invariance and real Wannier functions

We state conditions for real exponentially localized Wannier functions, and then for real globally optimal ones.

We recall that the construction leading to Theorem 4.8 started with solving the parallel transport equation in Lemma 4.6, followed by the gauge transformation $U_\star$ in Theorem 4.8 for obtaining exponential localization. To obtain real and exponentially localized Wannier functions, it suffices to repeat the construction of Theorem 4.8 with the initial condition in Lemma 4.6 replaced by the S-invariant $\widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2)$ in (157).

Theorem 4.12. Suppose that the initial condition in Lemma 4.6 is replaced by (157). Then the resulting Wannier functions corresponding to the analytic family of frames $\widetilde{\boldsymbol{\mathcal{V}}}(k) = \boldsymbol{\mathcal{V}}(k)U_\star(k)$ for $k \in I_{\text{bz}}$ in Theorem 4.8 are real and exponentially localized.

Proof. We first observe that $\widetilde{\boldsymbol{\mathcal{V}}}(k)$ satisfies (136) with the modified initial condition (157):

$$\widetilde{\boldsymbol{\mathcal{V}}}'(k) = \boldsymbol{P}'(k)\widetilde{\boldsymbol{\mathcal{V}}}(k) - \mathrm{i}\widetilde{\boldsymbol{\mathcal{V}}}(k)A_{\text{zak}}, \quad \text{with} \quad \widetilde{\boldsymbol{\mathcal{V}}}(-\Omega/2) = \widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2). \tag{166}$$

Next, we define that the time-reversed pair $\widetilde{\boldsymbol{\mathcal{V}}}_{\text{TR}}(k) = \widetilde{\boldsymbol{\mathcal{V}}}(-k)$. By applying the chain rule, we have

$$\widetilde{\boldsymbol{\mathcal{V}}}_{\text{TR}}'(k) = -\widetilde{\boldsymbol{\mathcal{V}}}'(-k) = -\boldsymbol{P}'(-k)\widetilde{\boldsymbol{\mathcal{V}}}(-k) + \mathrm{i}\widetilde{\boldsymbol{\mathcal{V}}}(-k)A_{\text{zak}}. \tag{167}$$

Next, we apply T in (140) to the above equation. Using (143) and the fact that A_{zak} is a real matrix by Lemma 4.11, it follows that

$$(T\widetilde{\boldsymbol{\mathcal{V}}}_{\text{TR}})'(k) = \boldsymbol{P}'(k)T\widetilde{\boldsymbol{\mathcal{V}}}_{\text{TR}}(k) - \mathrm{i}T\widetilde{\boldsymbol{\mathcal{V}}}_{\text{TR}}(k)A_{\text{zak}}, \tag{168}$$

which has the same form as (166). The initial condition is given by

$$T\widetilde{\boldsymbol{\mathcal{V}}}_{\text{TR}}(-\Omega/2) = T\widetilde{\boldsymbol{\mathcal{V}}}(\Omega/2), \tag{169}$$

where we have used that $U_\star(\Omega/2) = U_{\text{zak}}$. Moreover, by the construction in Theorem 4.8, we have $R(\widetilde{\boldsymbol{\mathcal{V}}}(\Omega/2)) = \widetilde{\boldsymbol{\mathcal{V}}}(-\Omega/2)$. Combining this with the S-invariance of $\widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2)$ in (154), we conclude that the initial condition is given by

$$T\widetilde{\boldsymbol{\mathcal{V}}}_{\text{TR}}(-\Omega/2) = TR\widetilde{\boldsymbol{\mathcal{V}}}(-\Omega/2) = TR\widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2) = \widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2), \tag{170}$$

which is identical to that in (166). It follows that $\widetilde{\boldsymbol{\mathcal{V}}}$ and $T\widetilde{\boldsymbol{\mathcal{V}}}_{\text{TR}}$ satisfy the same differential equation and initial condition. By the uniqueness theorem of initial value problems on Banach spaces [16], it follows that

$$\widetilde{\boldsymbol{\mathcal{V}}}(k) = T\widetilde{\boldsymbol{\mathcal{V}}}_{\text{TR}}(k), \quad k \in I_{\text{bz}}. \tag{171}$$

We observe that this is equivalent to $\widetilde{\alpha}^{(i)}$ in Theorem 4.8 satisfying

$$\widetilde{\alpha}^{(i)}(k) = \overline{\widetilde{\alpha}^{(i)}}(-k), \quad k \in \mathbb{R}, \quad i = 1, 2, \ldots, n_b, \tag{172}$$

which implies that the corresponding Wannier functions in (117) are real. □

To achieve global optimality after obtaining real and exponential localized Wannier functions, we apply a constant gauge transformation by W_0, the diagonalizer of A_{zak} as in Theorem 4.9. As shown in Lemma 4.11, A_{zak} is a real symmetric matrix once the new initial condition (157) is in place. Hence, W_0 can be chosen as an orthogonal matrix (thus a real matrix). Combining the reality of W_0 with same reasoning in Theorem 4.12 shows that the globally optimal Wannier functions are also real.

Theorem 4.13. Suppose that the initial condition in Lemma 4.6 is replaced by (157). We choose W_0 in $A_{\text{zak}} = W_0 D_{\text{zak}} W_0^T$ to be a real (orthogonal) matrix. Then the resulting Wannier functions corresponding to the analytic family of frames $\widetilde{\boldsymbol{\mathcal{V}}}(k) = \boldsymbol{\mathcal{V}}(k)U_\star(k)W_0$ for $k \in I_{\text{bz}}$ in Theorem 4.9 are both real and globally optimal.

This completes the construction of real and globally optimal Wannier functions in one dimension.

5 Construction of optimal Wannier functions

We now summarize the full constructive procedure in Section 4 for obtaining real, exponentially localized, and globally optimal Wannier functions.

Let a and $\Omega = 2\pi/a$ be the lattice and reciprocal lattice constants, respectively, that determine the first Brillouin zone $I_{\text{bz}} = [-\Omega/2, \Omega/2)$. Let $V : \mathbb{R} \to \mathbb{R}$ be a piecewise smooth potential with period a that determines the eigenvalue equation (8) for $k \in I_{\text{bz}}$. Choose an isolated group of n_b bands with band index $j_1, j_2, \ldots, j_{n_b}$ (which can be done by computing the eigenvalues at $k = 0, \pm\Omega/2$ to detect degeneracy by Lemma 3.1). The information about the chosen set of bands is encoded in the Bloch functions (46):

$$\Psi_k = \left(\psi_k^{(j_1)}, \psi_k^{(j_2)}, \ldots, \psi_k^{(j_{n_b})}\right), \quad k \in I_{\text{bz}}, \tag{173}$$

from which we fix the subspace $\mathcal{S}_k = \text{Range}\,(\Psi_k)$ of interest at every $k \in I_{\text{bz}}$. This in turn determines the projector $\boldsymbol{P}(k)$ in (80) for $k \in I_{\text{bz}}$ after transforming to the Fourier $\ell^2(\mathbb{Z})$ domain.

In order to form an analytic family of Bloch frames Φ_k with $\text{Range}\,(\Phi_k) = \text{Range}\,(\Psi_k)$, we compute the Bloch functions in Ψ_k at $k = -\Omega/2$, followed by obtaining their Fourier series by (52). Then we use the Fourier coefficients and the definition (72) to form the initial frame $\boldsymbol{\mathcal{U}}(-\Omega/2)$. To obtain real Wannier functions, we compute U_S in (150) by the formula

$$U_S = U_0^{1/2}, \quad \text{with} \quad U_0 = a\,\boldsymbol{\mathcal{U}}^*(-\Omega/2) S\left(\boldsymbol{\mathcal{U}}(-\Omega/2)\right), \tag{174}$$

where $S = TR$ is the composition of time-reversal operator T and the right-shift operator R in (144). Then we use

$$\widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2) = \boldsymbol{\mathcal{U}}(-\Omega/2)U_S \tag{175}$$

as the initial condition for the parallel-transport equation (86), given by the formula

$$\frac{\mathrm{d}\boldsymbol{\mathcal{V}}(k)}{\mathrm{d}k} = \frac{\mathrm{d}\boldsymbol{P}(k)}{\mathrm{d}k}\boldsymbol{\mathcal{V}}(k), \quad \boldsymbol{\mathcal{V}}(-\Omega/2) = \widetilde{\boldsymbol{\mathcal{U}}}(-\Omega/2). \tag{176}$$

We solve the parallel-transport equation on I_{bz} and the solution $\boldsymbol{\mathcal{V}}$ determines an analytic family of Bloch frames via (73)–(74) by Lemma 4.6. (We observe that (174)–(175) are unnecessary if reality is not required; any choice of $\boldsymbol{\mathcal{U}}(-\Omega/2)$ is a valid initial condition.)

Next, to fix the discontinuities across the zone boundaries, we compute U_{zak} and A_{zak} in (95) and (111) via

$$U_{\text{zak}} = a\,\boldsymbol{\mathcal{V}}^*(-\Omega/2) R\left(\boldsymbol{\mathcal{V}}(\Omega/2)\right) \quad \text{and} \quad A_{\text{zak}} = \frac{\mathrm{i}}{\Omega}\log\left(U_{\text{zak}}\right), \tag{177}$$

and carry out the gauge transformation:

$$\widetilde{\boldsymbol{\mathcal{V}}}(k) = \boldsymbol{\mathcal{V}}(k)U_\star(k)\,, \quad \text{with} \quad U_\star(k) = \exp\left(-\mathrm{i}A_{\mathrm{zak}}\left(k + \frac{\Omega}{2}\right)\right), k \in I_{\mathrm{bz}}\,. \tag{178}$$

By Theorem 4.8, the Wannier functions associated with $\widetilde{\boldsymbol{\mathcal{V}}}$ are exponentially localized; and they are also real by Theorem 4.12. To achieve global optimality for minimizing the total spread $\mathcal{S}$, we diagonalize

$$A_{\mathrm{zak}} = W_0 D_{\mathrm{zak}} W_0^*\,, \tag{179}$$

where W_0 is chosen to be a real matrix (see Lemma 4.11). Finally, we apply the constant W_0 gauge transformation so that

$$\widetilde{\boldsymbol{\mathcal{V}}}(k) \mapsto \widetilde{\boldsymbol{\mathcal{V}}}(k)W_0 = \boldsymbol{\mathcal{V}}(k)U_\star(k)W_0\,, \quad k \in I_{\mathrm{bz}}\,. \tag{180}$$

By Theorem 4.9, the Wannier functions corresponding to the transformed $\widetilde{\boldsymbol{\mathcal{V}}}$ are globally optimal with the Wannier functions given by

$$W_0^{(i)}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{2\pi}{\Omega}\widetilde{\alpha}^{(i)}(\xi)\, e^{\mathrm{i}\xi x}\,\mathrm{d}\xi\,, \quad i = 1, 2, \ldots, n_b\,, \tag{181}$$

where

$$\widetilde{\alpha}^{(i)}(k + m\Omega) = \widetilde{\boldsymbol{\mathcal{V}}}_{mi}(k)\,, \quad k \in I_{\mathrm{bz}}\,, \quad m \in \mathbb{Z}\,. \tag{182}$$

By Theorem 4.13, the Wannier functions in (181) are real.

At this point, all gauge degrees of freedom are fixed, up to (1) the branch choice for computing A_{zak} in (177), which only shifts the Wannier centers by integer lattice translations (Remark 4.5), and (2) the square-root choice in (174) which merely introduces overall $\pm$ signs in the resulting Wannier functions due to the block-unitary structure described in Remark 4.8. Hence the constructive procedure for real and globally optimal Wannier functions in one dimension is complete.

6 Conclusion and generalization

We have developed a constructive analytic framework for obtaining real and globally optimal Wannier functions in one dimension for an isolated group of bands. Although the results in [3] and in this paper concern one-dimensional Schrödinger operators, the approach readily generalizes to other systems (see Remark 4.4), including Maxwell and Dirac operators. Moreover, the seemingly innocent one-dimensional setting already captures nearly all analytic difficulties of the Wannier problem. In higher dimensions, the remaining challenges are no longer analytic but geometric and topological. For example, in the context of matrix models, [17] shows that one must modify Kato's equations along different directions to address the non-integrability induced by the Berry curvature; when topological obstructions are present, continuous assignments of eigenvectors become impossible. Together with [17] and its forthcoming multiband sequel, the present results provide a unified constructive framework for Wannier functions of Schrödinger operators in higher dimensions, shedding light on how to efficiently compute optimal Wannier functions. These extensions have been completed and papers are in preparation for publication.

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