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Justification of the Lattice Equation for a Nonlinear Elliptic Problem with a Periodic Potential

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Abstract: We justify the use of the lattice equation (the discrete nonlinear Schrödinger equation) for the *tight-binding approximation* of stationary localized solutions in the context of a continuous nonlinear elliptic problem with a periodic potential. We rely on properties of the Floquet band-gap spectrum and the Fourier–Bloch decomposition for a linear Schrödinger operator with a periodic potential. Solutions of the nonlinear elliptic problem are represented in terms of Wannier functions and the problem is reduced, using elliptic theory, to a set of nonlinear algebraic equations solvable with the Implicit Function Theorem. Our analysis is developed for a class of *piecewise-constant* periodic potentials with *disjoint* spectral bands, which reduce, in a singular limit, to a periodic sequence of infinite walls of a non-zero width. The discrete nonlinear Schrödinger equation is applied to classify localized solutions of the Gross–Pitaevskii equation with a periodic potential.

1. Introduction

Recent experimental and theoretical works on Bose–Einstein condensates in optical lattices [18], coherent structures in photorefractive lattices [3], and gap solitons in photonic crystals [22] have stimulated a new wave of interest in localized solutions of the nonlinear elliptic problem with a periodic potential

$$-\phi''(x) + V(x)\phi(x) + \sigma|\phi(x)|^2\phi(x) = \omega\phi(x), \quad \forall x \in \mathbb{R}, \tag{1.1}$$

where $\phi : \mathbb{R} \mapsto \mathbb{C}$ decays to zero sufficiently fast as $|x| \to \infty$, $V : \mathbb{R} \mapsto \mathbb{R}$ is a bounded 2π-periodic function, $\sigma = \pm 1$ is normalized, and ω is a free parameter. Solutions of the nonlinear elliptic problem (1.1) correspond to *stationary* (time-periodic) solutions of Hamiltonian dynamical systems such as the Gross–Pitaevskii equation.

Localized solutions $\phi(x)$ of the elliptic problem (1.1) in energy space $H^1(\mathbb{R})$ have been proved to exist for ω in *every bounded* gap in the spectrum of the linear Schrödinger operator $L = -\partial_x^2 + V(x)$, as well as in the semi-infinite gap for $\sigma = -1$ [13]. It is, however, desired to obtain more precise information on classification and properties of localized solutions. The number of branches of localized solutions, counted modulo a discrete group of translations with a 2π-multiple period, is infinite even in one dimension, and the solutions can be classified, for instance, by the number of peaks in different wells of the periodic potentials. To approximate the solution shape by analytic functions or numerically, various asymptotic reductions of the nonlinear elliptic problem (1.1) have been used [14]. The asymptotic reductions are formally derived for bifurcations of small-amplitude localized solutions from the zero solution $\phi = 0$. Recent rigorous results on these bifurcations include justification of the time-dependent nonlinear Schödinger equation for pulses near a band edge of the spectrum of L [2], analysis of the coupled nonlinear Schödinger equations for a finite-amplitude two-dimensional separable potential [6], and justification of the coupled-mode system for a small-amplitude one-dimensional potential [17].

This paper addresses the tight-binding approximation of localized solutions outside a narrow band in the spectrum of L. Although the tight-binding approximation has been used by physicists for a long time, it was only recently that this approximation was formalized by means of Wannier function decompositions [1]. The rigorous analysis of the "averaged procedure" announced in [1] as Ref. [15] appears not to have been written. Moreover, as we show in this paper, one of the claims of [1] (the coupled lattice equations (12) for inter-band interactions) cannot be verified in the context of the nonlinear elliptic problem (1.1).

Our main goal here is to prove that, when the potential $V(x)$ is represented by a periodic piecewise-constant sequence of large walls of a non-zero width, a localized solution $\phi(x)$ of the nonlinear elliptic problem (1.1) on $x \in \mathbb{R}$ is a linear transform of a localized sequence $\{\phi_n\}$ on $n \in \mathbb{Z}$ satisfying the lattice equation

$$\alpha\,(\phi_{n+1} + \phi_{n-1}) + \sigma|\phi_n|^2\phi_n = \Omega\phi_n, \quad \forall n \in \mathbb{Z}, \tag{1.2}$$

where α is constant and Ω is a new parameter related to the parameter ω. The sequence $\{\phi_n\}_{n\in\mathbb{Z}}$ represents a small-amplitude solution $\phi(x)$ of the nonlinear elliptic problem (1.1) in the sense that ϕ_n corresponds to $\phi(x)$ for the value of x in the n^{th} well of the periodic potential $V(x)$. The precise statement of our main theorem can be found in Sect. 4 of our article.

Besides the formal analysis in [1], justification of the lattice equation (1.2) for the nonlinear elliptic problem (1.1) seems not to have been carried out in the literature. Nevertheless, our work has two recent counterparts in the theory of nonlinear parabolic systems. These works are relevant as time-independent solutions of nonlinear parabolic systems satisfy nonlinear elliptic equations. In particular, the stationary solutions of a nonlinear heat equation satisfy the second-order elliptic problem (1.1).

The scalar nonlinear heat equation with a periodic diffusive term was considered in [21] and the convergence of the global solutions of the continuous partial differential equation to the global solutions of a lattice differential equation is proven with the Fourier–Bloch analysis. Although the Wannier functions are never mentioned in [21], modifications of these functions (suitable for the Shannon sampling and interpolation theory [24]) are implicitly constructed in Lemma 2.5 of [21]. The lattice differential equation describes dynamics on the invariant infinite-dimensional manifold of the nonlinear heat equation.

If the dynamics is stationary (time-independent), this center manifold corresponds directly to the nonlinear elliptic problem (1.1), which we consider here. Unfortunately, our methods can not be extended to Hamiltonian dynamical systems such as the Gross–Pitaevskii equation, since the center manifold of nonlinear dispersive wave equations does not give typically any reduction of the problem. This is the main reason why we limit our consideration to the stationary solutions of the Gross–Pitaevskii equation.

A more general system of reaction–diffusion equations was considered in [25] and the lattice differential equations were derived to describe dynamics of an infinite sequence of interacting pulses which are located far apart from each other (see also [5] for analysis of a periodic sequence of interacting pulses). The infinite sequence of equally spaced pulses introduces an effective periodic potential in the linearization of the reaction–diffusion equations, which explains the similarity between the two problems. However, the Fourier–Bloch theory cannot be used for strongly nonlinear non-equally spaced pulses. As a result, direct methods of projections in exponentially weighted spaces are applied in [25] to catch a weak tail–tail interaction of neighboring pulses. Similar analysis of the pulse tail–tail interaction was earlier developed for a finite sequence of nonlinear pulses in the reaction–diffusion systems [20].

Our paper is structured as follows. The spectral theory of operators with periodic potentials and the related Fourier–Bloch decomposition are reviewed in Sect. 2. The Wannier functions are introduced and studied in Sect. 3. The main theorem is formulated in Sect. 4 after the analysis of piecewise-constant potentials, which reduce, in a singular limit, to a periodic sequence of infinite walls of a non-zero width. The main theorem is proved in Sect. 5 using elliptic theory and the Wannier decomposition. Examples of localized solutions of the lattice equation (1.2) are given in Sect. 6. Other examples of periodic potentials with similar properties are discussed in Sect. 7. Extensions of analysis for multi-dimensional elliptic problems with a separable periodic potential are developed in Sect. 8. Appendix A reviews the Shannon decomposition which is an alternative to the Wannier decomposition. Appendices B and C give proofs of important technical lemmas about the spectrum of the Schrödinger operator with a periodic piecewise–constant potential. Appendix D describes a relationship between the lattice equation (1.2) and the Poincaré map for the second-order equation (1.1).

Notations and basic facts. In what follows, we consider scalar complex-valued functions u on $\mathbb{R}$ in the Sobolev space $H^m(\mathbb{R})$ for an integer $m \geq 0$ equipped with the squared norm

$$\|u\|^2_{H^m(\mathbb{R})} = \sum_{k=0}^{m} \int_{\mathbb{R}} |\partial_x^k u(x)|^2 dx, \tag{1.3}$$

and complex-valued vectors $\vec{\mathbf{u}}$ for sequences $\{u_n\}_{n\in\mathbb{Z}}$ in the weighted spaces $l^1_q(\mathbb{Z})$ and $l^2_s(\mathbb{Z})$ for $q, s \geq 0$ equipped with the norms

$$\|\vec{\mathbf{u}}\|_{l^1_q(\mathbb{Z})} = \sum_{n\in\mathbb{Z}} (1+n^2)^{q/2}|u_n|, \quad \|\vec{\mathbf{u}}\|^2_{l^2_s(\mathbb{Z})} = \sum_{n\in\mathbb{Z}} (1+n^2)^{s}|u_n|^2. \tag{1.4}$$

Furthermore, we use the space of bounded continuous functions $C^0_b(\mathbb{R})$ and recall Sobolev's embeddings

$$\|u\|_{C^0_b(\mathbb{R})} \leq C_1(s)\|u\|_{H^s(\mathbb{R})}, \quad \|\vec{\mathbf{u}}\|_{l^1_q(\mathbb{Z})} \leq C_2(s,q)\|\vec{\mathbf{u}}\|_{l^2_{s+q}(\mathbb{Z})}, \quad \forall s > \frac{1}{2}, \quad \forall q \geq 0, \tag{1.5}$$

for some constants $C_1(s), C_2(s,q) > 0$. We also recall that the Sobolev space $H^s(\mathbb{R})$ forms a Banach algebra for $s > \frac{1}{2}$ such that

$$\forall u, v \in H^s(\mathbb{R}): \quad \|uv\|_{H^s(\mathbb{R})} \leq C(s)\|u\|_{H^s(\mathbb{R})}\|v\|_{H^s(\mathbb{R})}, \quad \forall s > \frac{1}{2}, \tag{1.6}$$

for some constant $C(s) > 0$. We denote $\mathbb{N} = \{1, 2, 3, \ldots\} \subset \mathbb{Z}$ and $\mathbb{T} = \left[-\frac{1}{2}, \frac{1}{2}\right] \subset \mathbb{R}$.

2. Review of Spectral Theory

We consider the Schrödinger operator $L = -\partial_x^2 + V(x)$ with a real-valued, bounded and 2π-periodic function V with respect to $x \in \mathbb{R}$. The operator L is defined for functions in $C_0^\infty(\mathbb{R})$. It is extended to a self-adjoint operator which maps continuously $H^2(\mathbb{R})$ to $L^2(\mathbb{R})$.

By Theorem XIII.100 on p. 309 in [19], if $V \in L^2_{\rm per}(\mathbb{R})$, then the spectrum of $L = -\partial_x^2 + V(x)$ in $L^2(\mathbb{R})$, denoted by $\sigma(L)$, is real, purely continuous, and consists of the union of spectral bands. According to Floquet analysis (see Sects. 6.4, 6.6 and 6.7 in [7]), for each fixed $k \in \mathbb{T}$, where $\mathbb{T} = \left[-\frac{1}{2}, \frac{1}{2}\right]$, there exists a Bloch function $u_l(x; k) = e^{ikx} w_l(x; k)$ corresponding to the eigenvalue $\omega_l(k)$, such that $w_l(x+2\pi; k) = w_l(x; k)$. The band function $\omega_l(k)$ and the periodic function $w_l(x; k)$ for a fixed $k \in \mathbb{T}$ correspond to the $l^{\rm th}$ eigenvalue–eigenvector pair of the operator $L_k = -\partial_x^2 - 2ik\partial_x + k^2 + V(x)$, so that

$$L_k w_l(x; k) = \omega_l(k) w_l(x; k), \quad \text{or, equivalently,} \quad L u_l(x; k) = \omega_l(k) u_l(x; k). \tag{2.1}$$

The Bloch functions are uniquely defined up to a scalar multiplication factor. We shall assume that the amplitude factors of the Bloch functions are normalized by the orthogonality relations

$$\int_{\mathbb{R}} u_l(x, k)\bar{u}_{l'}(x, k')dx = \delta_{l,l'}\delta(k - k'), \quad \forall l, l' \in \mathbb{N}, \quad \forall k, k' \in \mathbb{T}, \tag{2.2}$$

where $\delta_{l,l'}$ is the Kronecker symbol and $\delta(k)$ is the Dirac delta function in the sense of distributions. In addition, if $u_l(x; k)$ is a Bloch function for $\omega_l(k)$, then $u_l(x; -k) = \bar{u}_l(x; k)$ can be chosen as a Bloch function for $\omega_l(-k) = \bar{\omega}_l(k) = \omega_l(k)$, to normalize uniquely the phase factors of the Bloch functions. Similar normalization was used recently for construction of Bloch functions in [12].

Proposition 1. *If $V \in L^2_{\rm per}(\mathbb{R})$, then there exists a unitary Fourier–Bloch transformation $\mathcal{T} : L^2(\mathbb{R}) \mapsto l^2(\mathbb{N}, L^2(\mathbb{T}))$ given by*

$$\forall \phi \in L^2(\mathbb{R}): \quad \hat{\phi}(k) = \mathcal{T}\phi, \quad \hat{\phi}_l(k) = \int_{\mathbb{R}} \phi(y)\bar{u}_l(y; k)dy, \quad \forall l \in \mathbb{N}, \ \forall k \in \mathbb{T}. \tag{2.3}$$

The inverse transformation is given by

$$\forall \hat{\phi} \in l^2(\mathbb{N}, L^2(\mathbb{T})): \quad \phi(x) = \mathcal{T}^{-1}\hat{\phi} = \sum_{l \in \mathbb{N}} \int_{\mathbb{T}} \hat{\phi}_l(k) u_l(x; k)dk, \quad \forall x \in \mathbb{R}. \tag{2.4}$$

Proof. The statement follows by Theorems XIII.97 and XIII.98 on pp. 303–304 in [19], which prove orthogonality and completeness of the set of Bloch functions $\{u_l(x; k)\}$ on $l \in \mathbb{N}$ and $k \in \mathbb{T}$. The orthogonality relations are given by (2.2), while the completeness relation can be written in the form

$$\sum_{l \in \mathbb{N}} \int_{\mathbb{T}} u_l(x, k)\bar{u}_l(x'; k)dk = \delta(x - x'), \quad \forall x, x' \in \mathbb{R}, \tag{2.5}$$

where $\delta(x)$ is again the Dirac delta function in the sense of distributions. □

Let E_l for a fixed $l \in \mathbb{N}$ be the invariant closed subspace of $L^2(\mathbb{R})$ associated with the l^{th} spectral band of $\sigma(L)$. Then,

$$\forall \phi \in E_l \subset L^2(\mathbb{R}) : \quad \phi(x) = \int_{\mathbb{T}} \hat{\phi}_l(k) u_l(x;k) dk, \tag{2.6}$$

where $\hat{\phi}_l(k)$ is defined by the integral in (2.3). According to the Fourier–Bloch decomposition (2.3)–(2.4), the space $L^2(\mathbb{R})$ is decomposed into a direct sum of invariant closed bounded subspaces $\oplus_{l\in\mathbb{N}} E_l$. The Fourier–Bloch decomposition can be used for representation of classical solutions of partial differential equations with periodic coefficients [2,6]. This decomposition is, however, inconvenient for a reduction of a continuous PDE problem to a lattice problem. Other decompositions, such as the Wannier and Shannon decompositions, are found to be more useful in the recent works [1] and [21], respectively. Properties of the Wannier functions are described in the next section, while the Shannon functions are reviewed in Appendix A.

3. Properties of the Wannier Functions

Since the band function $\omega_l(k)$ and the Bloch function $u_l(x;k)$ are periodic with respect to $k \in \mathbb{T}$ for any $l \in \mathbb{N}$, we represent them by the Fourier series

$$\omega_l(k) = \sum_{n\in\mathbb{Z}} \hat{\omega}_{l,n} e^{i2\pi nk}, \quad u_l(x;k) = \sum_{n\in\mathbb{Z}} \hat{u}_{l,n}(x) e^{i2\pi nk}, \quad \forall l \in \mathbb{N}, \ \forall k \in \mathbb{T}, \tag{3.1}$$

where the inverse transformation is

$$\hat{\omega}_{l,n} = \int_{\mathbb{T}} \omega_l(k) e^{-i2\pi nk} dk, \quad \hat{u}_{l,n}(x) = \int_{\mathbb{T}} u_l(x;k) e^{-i2\pi nk} dk, \quad \forall l \in \mathbb{N}, \quad \forall n \in \mathbb{Z}. \tag{3.2}$$

Since $\omega_l(k) = \bar{\omega}_l(k) = \omega_l(-k)$ and $u_l(x;k) = \bar{u}_l(x;-k)$ for any $k \in \mathbb{T}$ and any $l \in \mathbb{N}$, the coefficients of the Fourier series (3.1) satisfy the constraints

$$\hat{\omega}_{l,n} = \bar{\hat{\omega}}_{l,-n} = \hat{\omega}_{l,-n}, \quad \hat{u}_{l,n}(x) = \bar{\hat{u}}_{l,n}(x), \quad \forall n \in \mathbb{Z}, \quad \forall l \in \mathbb{N}, \quad \forall x \in \mathbb{R}. \tag{3.3}$$

In particular, the functions $\hat{u}_{l,n}(x)$ are always real-valued. Since $u_l(x + 2\pi; k) = u_l(x;k)e^{i2\pi k}$ for any $x \in \mathbb{R}$, $k \in \mathbb{T}$, and $l \in \mathbb{N}$, we obtain another constraint on the functions $\hat{u}_{l,n}(x)$:

$$\hat{u}_{l,n}(x) = \hat{u}_{l,n-1}(x - 2\pi) = \hat{u}_{l,0}(x - 2\pi n), \qquad \forall n \in \mathbb{Z}, \ \forall l \in \mathbb{N}, \ \forall x \in \mathbb{R}. \tag{3.4}$$

By substituting the Fourier series representation (3.1) into the linear problem (2.1), we obtain a system of equations for the set of functions $\{\hat{u}_{l,n}(x)\}_{n\in\mathbb{Z}}$ and coefficients $\{\hat{\omega}_{l,n}\}_{n\in\mathbb{Z}}$ for a fixed $l \in \mathbb{N}$:

$$-\hat{u}''_{l,n}(x) + V(x)\hat{u}_{l,n}(x) = \sum_{n'\in\mathbb{Z}} \hat{\omega}_{l,n-n'} \hat{u}_{l,n'}(x), \qquad \forall n \in \mathbb{Z}. \tag{3.5}$$

We shall now make rigorous the formal representations above.

Definition 1. *The functions in the set* $\{\hat{u}_{l,n}(x)\}$ *for* $n \in \mathbb{Z}$ *and* $l \in \mathbb{N}$ *are called the Wannier functions.*

Assumption 1. *Let V be a real-valued, piecewise-continuous and 2π-periodic function with respect to $x \in \mathbb{R}$. Assume that the spectrum of $L = -\partial_x^2 + V(x)$ consists of the union of disjoint spectral bands.*

Proposition 2. *Let V satisfy Assumption 1. There exists a unitary transformation $\mathcal{W} : L^2(\mathbb{R}) \mapsto l^2(\mathbb{N} \times \mathbb{Z})$ given by*

$$\forall \phi \in L^2(\mathbb{R}) : \quad \vec{\boldsymbol{\phi}} = \mathcal{W}\phi, \quad \phi_{l,n} = \int_{\mathbb{R}} \hat{u}_{l,n}(x)\phi(x)dx, \quad \forall l \in \mathbb{N}, \quad \forall n \in \mathbb{Z}. \tag{3.6}$$

The inverse transformation is given by

$$\forall \vec{\boldsymbol{\phi}} \in l^2(\mathbb{N} \times \mathbb{Z}) : \quad \phi(x) = \mathcal{W}^{-1}\vec{\boldsymbol{\phi}} = \sum_{l\in\mathbb{N}} \sum_{n\in\mathbb{Z}} \phi_{l,n}\hat{u}_{l,n}(x), \quad \forall x \in \mathbb{R}. \tag{3.7}$$

Moreover, there exists $\eta_l > 0$ and $C_l > 0$ for a fixed $l \in \mathbb{N}$, such that

$$|\hat{u}_{l,n}(x)| \leq C_l e^{-\eta_l |x-2\pi n|}, \quad \forall n \in \mathbb{Z}, \quad \forall x \in \mathbb{R}. \tag{3.8}$$

Proof. We need to prove that the set of Wannier functions of Definition 1 forms an orthonormal basis in $L^2(\mathbb{R})$ according to the orthogonality relation

$$\int_{\mathbb{R}} \hat{u}_{l,n}(x)\hat{u}_{l',n'}(x)dx = \delta_{l,l'}\delta_{n,n'}, \quad \forall l, l' \in \mathbb{N}, \quad \forall n, n' \in \mathbb{Z} \tag{3.9}$$

and the completeness relation

$$\sum_{l\in\mathbb{N}} \sum_{n\in\mathbb{Z}} \hat{u}_{l,n}(x)\hat{u}_{l,n}(x') = \delta(x - x'), \quad \forall x, x' \in \mathbb{R}. \tag{3.10}$$

The orthogonality relation (3.9) for the Wannier functions follows from the orthogonality relation (2.2) for the Bloch functions

$$\begin{aligned}
\int_{\mathbb{R}} \hat{u}_{l,n}(x)\hat{u}_{l',n'}(x)dx &= \int_{\mathbb{R}} \int_{\mathbb{T}} \int_{\mathbb{T}} u_l(x; k)\bar{u}_{l'}(x; k')e^{i2\pi(k'n'-kn)}dkdk'dx \\
&= \delta_{l',l} \int_{\mathbb{T}} \int_{\mathbb{T}} \delta(k' - k)e^{i2\pi k(n'-n)}dkdk' \\
&= \delta_{l',l} \int_{\mathbb{T}} e^{i2\pi k(n'-n)}dk = \delta_{l',l}\delta_{n',n},
\end{aligned}$$

after the integrations in $x \in \mathbb{R}$ and $k, k' \in \mathbb{T}$ are interchanged. Similarly, the completeness relation (3.10) for the Wannier functions follows from the completeness relation (2.5) for the Bloch functions

$$\begin{aligned}
\sum_{l\in\mathbb{N}} \sum_{n\in\mathbb{Z}} \hat{u}_{l,n}(x)\hat{u}_{l,n}(x') &= \sum_{l\in\mathbb{N}} \sum_{n\in\mathbb{Z}} \int_{\mathbb{T}} \int_{\mathbb{T}} u_l(x; k)\bar{u}_l(x'; k)e^{i2\pi(k'-k)n}dkdk' \\
&= \sum_{l\in\mathbb{N}} \int_{\mathbb{T}} \int_{\mathbb{T}} u_l(x; k)\bar{u}_l(x'; k) \sum_{n\in\mathbb{Z}} e^{i2\pi(k'-k)n}dkdk' \\
&= \sum_{l\in\mathbb{N}} \int_{\mathbb{T}} u_l(x; k)\bar{u}_l(x'; k)dk = \delta(x - x'),
\end{aligned}$$

where we have used the well-known orthogonality relation

$$\sum_{n\in\mathbb{Z}} e^{i2\pi n(k-k')} = \delta(k-k'), \qquad \forall k, k' \in \mathbb{T}.$$

The Wannier decomposition (3.6)–(3.7) follows by the standard theory of orthonormal bases in $L^2(\mathbb{R})$. It remains to show that the function $\hat{u}_{l,n}(x)$ for any $l \in \mathbb{N}$ and $n \in \mathbb{Z}$ is uniformly and absolutely bounded with respect to $x \in \mathbb{R}$ by an exponentially decaying function centered at $x = 2\pi n$. By Theorem XIII.95 on p.301 in [19], if the potential V satisfies Assumption 1, the band function $\omega_l(k)$ and the Bloch function $u_l(x;k) = w_l(x;k)e^{ikx}$ are analytic on $k \in \left(-\frac{1}{2}, 0\right) \cup \left(0, \frac{1}{2}\right)$ and are continued analytically along a Riemann surface near $k = 0$ and $k = \pm\frac{1}{2}$. Let us consider a rectangle D_{η_l} with vertices $\left(-\frac{1}{2}, 0\right)$, $\left(\frac{1}{2}, 0\right)$, $\left(\frac{1}{2}, i\eta_l\right)$, $\left(-\frac{1}{2}, i\eta_l\right)$ in the domain of analyticity of $u_l(x;k)$. By using the Cauchy complex integration, we obtain the identity

$$0 = \oint_{\partial D_{\eta_l}} u_l(x;k)dk = \int_{\mathbb{T}} u_l(x;k)dk - \int_{\mathbb{T}} u_l(x;k+i\eta_l)dk + \int_{\frac{1}{2}}^{\frac{1}{2}+i\eta_l} \left(u_l(x;k) - u_l(x;k-1)\right) dk.$$

The last integral is zero due to the periodicity of $u_l(x;k)$ with period 1 in k. As a result, we obtain a uniform upper bound for the Wannier function $\hat{u}_{l,0}(x)$:

$$|\hat{u}_{l,0}(x)| = \left|\int_{\mathbb{T}} u_l(x;k)dk\right| = \left|\int_{\mathbb{T}} u_l(x;k+i\eta_l)dk\right| = \left|\int_{\mathbb{T}} w_l(x;k+i\eta_l)e^{ikx-\eta_l x}dk\right| \leq C_l e^{-\eta_l x}, \quad \forall x \geq 0,$$

where $C_l = \sup_{k\in D_{\eta_l}} |w_l(x;k)|$. A similar computation extends the bound for $x \leq 0$. The decay bound (3.8) follows from the relation (3.4). □

Remark 1. The class of *piecewise-continuous* potentials with *disjoint* spectral bands provides a *sufficient* condition for existence of the unitary transformation (3.6)–(3.7) and the exponential decay (3.8). More general potentials are expected to exist for which Proposition 2 remains valid. Moreover, we do not need in our analysis the assumption that *all* spectral bands are disjoint. It is sufficient for the exponential decay of functions $\{\hat{u}_{l,n}(x)\}_{n\in\mathbb{Z}}$ for a fixed $l \in \mathbb{N}$ that the particular l^{th} band is disjoint from the rest of the spectrum of L.

Remark 2. Since the transformation $\omega \to \omega + \omega_0$, $V(x) \to V(x) + \omega_0$ leaves the elliptic problem (1.1) invariant, we will assume without loss of generality that $V(x)$ is bounded from below. For convenience, we choose $V(x) \geq 0$, $\forall x \in \mathbb{R}$. Then, $\sigma(L) \geq 0$.

Lemma 1. *Let $\vec{\boldsymbol{\phi}}$ be represented by the set of vectors $\{\vec{\boldsymbol{\phi}}_l\}_{l\in\mathbb{N}}$, where $\vec{\boldsymbol{\phi}}_l$ for a fixed $l \in \mathbb{N}$ is represented by the set of elements $\{\phi_{l,n}\}_{n\in\mathbb{Z}}$. If $\vec{\boldsymbol{\phi}} \in l_1^1(\mathbb{N}, l^1(\mathbb{Z}))$, then $\phi = \mathcal{W}^{-1}\vec{\boldsymbol{\phi}} \in H^1(\mathbb{R})$.*

Proof. We use the triangle inequality

$$\|\phi\|_{H^1(\mathbb{R})} \le \sum_{l\in\mathbb{N}}\sum_{n\in\mathbb{Z}} |\phi_{l,n}|\|\hat{u}_{l,n}\|_{H^1(\mathbb{R})} = \sum_{l\in\mathbb{N}} \|\hat{u}_{l,0}\|_{H^1(\mathbb{R})} \sum_{n\in\mathbb{Z}} |\phi_{l,n}|$$

and the fact that $\|f\|_{H^1(\mathbb{R})} \le \|(1+L)^{1/2} f\|_{L^2(\mathbb{R})}$ for any $f \in \mathrm{Dom}(L)$, since $L = -\partial_x^2 + V(x)$ and $V(x) \ge 0$. By using the integral representation (3.2) and the orthogonality relations (3.9), we obtain

$$\begin{aligned}\|(1+L)^{1/2}\hat{u}_{l,0}\|^2_{L^2(\mathbb{R})} &= \int_{\mathbb{R}} \hat{u}_{l,0}(x)(1+L)\hat{u}_{l,0}(x)dx \\ &= \int_{\mathbb{R}}\int_{\mathbb{T}}\int_{\mathbb{T}} \bar{u}_l(x;k')(1+L)u_l(x;k)dkdk'dx = \int_{\mathbb{T}} (1+\omega_l(k))\,dk.\end{aligned}$$

By Theorem 4.2.3 on p. 57 of [7], there are k-independent constants $C_\pm > 0$ such that

$$C_- l^2 \le |\omega_l(k)| \le C_+ l^2, \qquad \forall l \in \mathbb{N}, \quad \forall k \in \mathbb{T}. \tag{3.11}$$

As a result,

$$\|\phi\|_{H^1(\mathbb{R})} \le C \sum_{l\in\mathbb{N}} (1+l^2)^{1/2} \sum_{n\in\mathbb{Z}} |\phi_{l,n}| = C\|\vec{\boldsymbol{\phi}}\|_{l^1_1(\mathbb{N},l^1(\mathbb{Z}))},$$

for some $C > 0$. $\square$

Lemma 2. *If $\vec{\boldsymbol{\phi}}_l \in l^1(\mathbb{Z})$ for a fixed $l \in \mathbb{N}$ and $\phi(x) = \sum_{n\in\mathbb{Z}} \phi_{l,n}\hat{u}_{l,n}(x)$, then ϕ belongs to the invariant closed subspace $E_l \subset L^2(\mathbb{R})$. Moreover, $\phi \in H^1(\mathbb{R})$, such that the function ϕ is bounded, continuous, and decaying to zero as $|x| \to \infty$.*

Proof. By Lemma 1, we observe that if $\vec{\boldsymbol{\phi}}_l \in l^1(\mathbb{Z})$ and $\phi(x) = \sum_{n\in\mathbb{Z}} \phi_{l,n}\hat{u}_{l,n}(x)$, then $\phi \in H^1(\mathbb{R})$. By Sobolev's embedding (1.5), we obtain that $\phi \in C^0_b(\mathbb{R})$ and $\phi(x)$ decays to zero as $|x| \to \infty$. By the orthogonality property (3.9) and since $\|\vec{\boldsymbol{\phi}}_l\|_{l^2(\mathbb{Z})} \le \|\vec{\boldsymbol{\phi}}_l\|_{l^1(\mathbb{Z})}$, it follows that $\phi \in E_l \subset L^2(\mathbb{R})$. $\square$

Remark 3. If $\hat{u}_{l,n}(x)$ satisfies the exponential decay (3.8) for a fixed $l \in \mathbb{N}$, direct computations show that $\phi \in C^0_b(\mathbb{R})$, i.e.

$$|\phi(x)| \le \sum_{n\in\mathbb{Z}} |\phi_{l,n}||\hat{u}_{l,n}(x)| \le C_l \sum_{n\in\mathbb{Z}} |\phi_{l,n}|e^{-\eta_l|x-2\pi n|} \le C_l\|\vec{\boldsymbol{\phi}}_l\|_{l^1(\mathbb{Z})}, \quad \forall x \in \mathbb{R}.$$

Lemma 3. *If $\hat{u}_{l,n}(x)$ satisfies the exponential decay (3.8) for a fixed $l \in \mathbb{N}$ and $|\phi_{l,n}| \le Cr^{|n|}$ uniformly on $n \in \mathbb{Z}$ for some $C > 0$ and $0 < r < 1$, then $\phi(x) = \sum_{n\in\mathbb{Z}} \phi_{l,n}\hat{u}_{l,n}(x)$ decays to zero exponentially fast as $|x| \to \infty$.*

Proof. It is sufficient to prove that $|\phi(2\pi m)| \le Cq^m$ uniformly on $m \ge 0$ for some $C > 0$ and $0 < q < 1$. A similar analysis applies to $m \le 0$. Using the decay bound (3.8) with $C_l \equiv C$ and $\eta_l \equiv \eta$, we obtain that

$$\begin{aligned}|\phi(2\pi m)| \le C\Bigg(&\sum_{n=1}^{\infty} |\phi_{l,m+n}|e^{-2\pi\eta n} + \sum_{n=0}^{m} |\phi_{l,m-n}|e^{-2\pi\eta n} \\ &+ e^{-2\pi\eta m}\sum_{n=1}^{\infty} |\phi_{l,-n}|e^{-2\pi\eta n}\Bigg), \quad \forall m \ge 0.\end{aligned}$$

Since $r < 1$, $e^{-2\pi\eta} < 1$ and $re^{-2\pi\eta} < 1$, the first sum is bounded by $C_1 r^m$, while the third sum is bounded by $C_3 e^{-2\pi\eta m}$. The second sum is bounded by

$$r^m + r^{m-1}e^{-2\pi\eta} + \cdots + e^{-2\pi\eta m} = \begin{cases} r^m \frac{1-p^{m+1}}{1-p}, & p < 1, \\ r^m p^m \frac{1-p^{-m-1}}{1-p^{-1}}, & p > 1, \end{cases}$$

where $pr = e^{-2\pi\eta}$. If $p \leq 1$, the sum is bounded by $C_2 r^m$. If $p \geq 1$, the sum is bounded by $C_2 e^{-2\pi\eta m}$. All three terms decay to zero exponentially fast as $m \to \infty$. □

Remark 4. The Fourier series (3.1) for the Bloch function $u_l(x; k)$ is an example of the Wannier decomposition over the basis $\{\hat{u}_{l,n}(x)\}_{n\in\mathbb{Z}}$ for a fixed $l \in \mathbb{N}$ with the explicit representation

$$\phi(x) = u_l(x; k), \quad \phi_{l,n} = e^{i2\pi nk}.$$

This decomposition corresponds to the case when $\vec{\boldsymbol{\phi}}_l \notin l^1(\mathbb{Z})$ and $\phi \notin E_l \subset L^2(\mathbb{R})$.

4. Main Results

We shall now describe our main example of the potential function $V(x)$ which enables us to reduce the continuous elliptic problem (1.1) to the lattice equation (1.2). The potential function transforms, in a singular limit, to a sequence of infinite walls of a non-zero width. Since Proposition 2 is established only for bounded potentials, we need to show that the main properties of the Wannier functions such as the exponential decay (3.8) hold also in the singular limit. To do so, we develop analysis of the one-dimensional Schrödinger operator in Appendices B and C.

Assumption 2. *Let V be given by a piecewise-constant function $V(x) = b$ on $x \in (0, a)$ and $V(x) = 0$ on $x \in (a, 2\pi)$ for fixed $0 < a < 2\pi$ and $b = 1/\varepsilon^2 > 0$, periodically continued with period 2π.*

Figure 1 shows the potential function $V(x)$ defined by Assumption 2 with $a = \pi$ and $b = 4$ ($\varepsilon = \frac{1}{2}$).

Lemma 4. *Let V satisfy Assumption 2. For any fixed $l_0 \in \mathbb{N}$, there exist $\varepsilon_0, \zeta_0, \omega_0, c_1^{\pm}, c_2 > 0$, such that, for any $\varepsilon \in [0, \varepsilon_0)$, the band functions of the operator $L = -\partial_x^2 + V(x)$ satisfy the properties*

(i) *(band separation)* $$\min_{\forall l\in\mathbb{N}\backslash\{l_0\}} \inf_{\forall k\in\mathbb{T}} |\omega_l(k) - \hat{\omega}_{l_0,0}| \geq \zeta_0, \tag{4.1}$$

(ii) *(band boundness)* $$|\hat{\omega}_{l_0,0}| \leq \omega_0, \tag{4.2}$$

(iii) *(tight-binding approximation)* $$c_1^- \varepsilon e^{-\frac{a}{\varepsilon}} \leq |\hat{\omega}_{l_0,1}| \leq c_1^+ \varepsilon e^{-\frac{a}{\varepsilon}}, \quad |\hat{\omega}_{l_0,n}| \leq c_2 \varepsilon^2 e^{-\frac{2a}{\varepsilon}}, \tag{4.3}$$

where $n \geq 2$.

Proof. The proof of the lemma is given in Appendix B. □

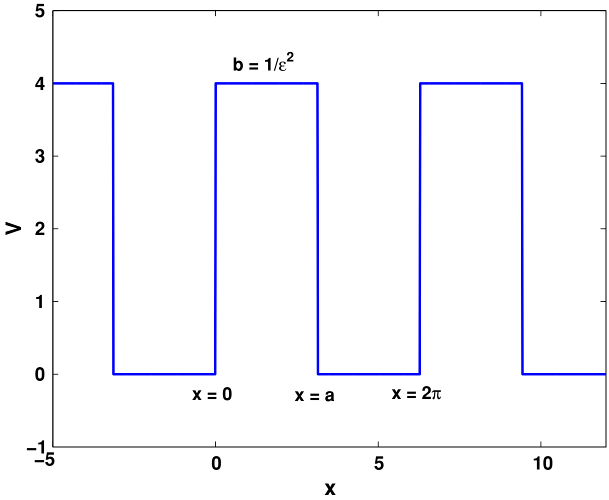

Fig. 1. The potential function $V(x)$ with $a = \pi$ and $b = 4$

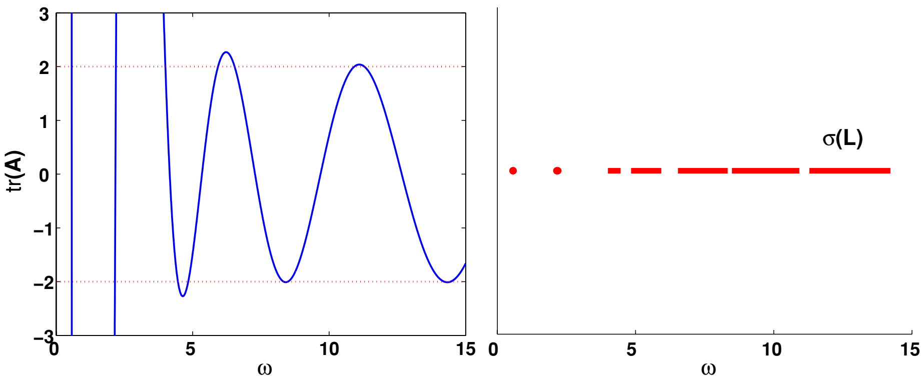

Fig. 2. Left: The trace of the monodromy matrix A versus ω for the potential function $V(x)$ with $a = \pi$ and $b = 4$. Right: The corresponding band-gap structure of the spectrum $\sigma(L)$

Figure 2 illustrates properties (4.1)–(4.3) of Lemma 4 for the potential function $V(x)$ with $a = \pi$ and $b = 4$. The left panel shows the behavior of the trace of the monodromy matrix A versus ω. The right panel shows the spectral bands defined by the intervals with $|\text{tr}(A)| \leq 2$. The first two bands are narrow for this value of $b = 1/\varepsilon^2$, according to the tight-binding approximation.

Lemma 5. *Let $V(x)$ satisfy Assumption 2. For any fixed $l_0 \in \mathbb{N}$, there exists $\varepsilon_0, C_0, C > 0$, such that, for any $\varepsilon \in [0, \varepsilon_0)$, the Wannier functions of the operator $L = -\partial_x^2 + V(x)$ satisfy the properties:*

$$\text{(i) (compact support)} \qquad |\hat{u}_{l_0,0}(x) - \hat{u}_0(x)| \leq C_0 \varepsilon, \quad \forall x \in [0, 2\pi], \tag{4.4}$$

$$\text{(ii) (exponential decay)} \qquad \left|\hat{u}_{l_0,0}(x)\right| \leq C \varepsilon^n e^{-\frac{na}{\varepsilon}}, \tag{4.5}$$

$$\forall x \in [-2\pi n, -2\pi(n-1)] \cup [2\pi n, 2\pi(n+1)], \quad n \in \mathbb{N},$$

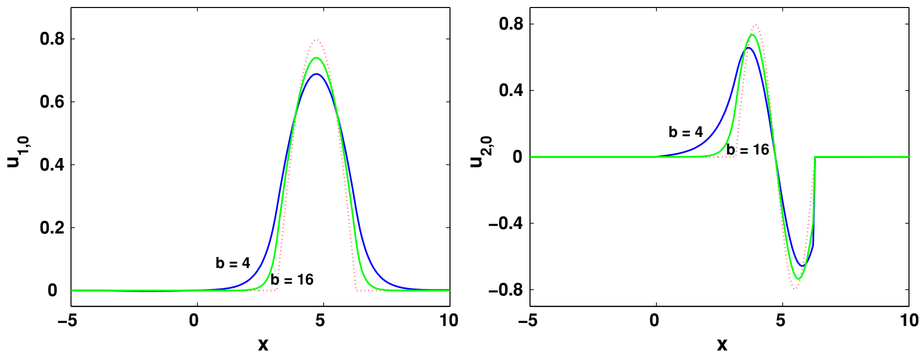

Fig. 3. The Wannier functions $\hat{u}_{l,0}(x)$ for $l = 1$ (left) and $l = 2$ (right). The solid lines show the Wannier functions for $b = 4$ and $b = 16$. The dashed lines show the limiting function (4.6)

where

$$\hat{u}_0(x) = \begin{cases} 0, & \forall x \in [0, a], \\ \frac{\sqrt{2}}{\sqrt{2\pi - a}} \sin \frac{\pi l_0 (2\pi - x)}{2\pi - a}, & \forall x \in [a, 2\pi]. \end{cases} \tag{4.6}$$

Proof. The proof of the lemma is given in Appendix C. □

Figure 3 illustrates properties (4.4)–(4.5) of Lemma 5 for the potential function $V(x)$ with $a = \pi$ and $b = 4, 16$. The left and right panels show the Wannier functions $\hat{u}_{1,0}(x)$ and $\hat{u}_{2,0}(x)$, respectively. The two functions were computed by using the integral representation (3.2) and the numerical approximations of the corresponding Bloch functions. The dashed line shows the limiting function (4.6).

Let us sketch a formal derivation of the lattice equation (1.2) from the continuous nonlinear problem (1.1) by using the Wannier function decomposition for a particular l_0^{th} band. Let V satisfy Assumption 2 and denote $\mu = \varepsilon e^{-\frac{a}{\varepsilon}}$. Fix $l_0 \in \mathbb{N}$, let $\omega = \hat{\omega}_{l_0,0} + \mu\Omega$, and consider the substitution

$$\phi(x) = \left(\frac{\mu}{\beta}\right)^{1/2} (\varphi(x) + \mu\psi(x)), \quad \varphi(x) = \sum_{n\in\mathbb{Z}} \phi_n \hat{u}_{l_0,n}(x), \tag{4.7}$$

where $\beta = \|\hat{u}_{l_0,0}\|^4_{L^4(\mathbb{R})}$ and ψ is orthogonal to $E_{l_0} \subset L^2(\mathbb{R})$. Using the ODE system (3.5), we find that $\psi(x)$ satisfies the inhomogeneous system

$$-\psi''(x) + V(x)\psi(x) - \hat{\omega}_{l_0,0}\psi(x) = -\frac{1}{\mu} \sum_{n\in\mathbb{Z}} \sum_{m\in\mathbb{N}} \hat{\omega}_{l_0,m} (\phi_{n+m} + \phi_{n-m}) \hat{u}_{l_0,n}(x)$$
$$+\Omega(\varphi(x) + \mu\psi(x)) - \frac{\sigma}{\beta} |\varphi(x) + \mu\psi(x)|^2 (\varphi(x) + \mu\psi(x)) . \tag{4.8}$$

Since $\psi \in \text{Dom}(L)$ and $\psi \perp E_{l_0}$, where $L = -\partial_x^2 + V(x)$, then $(\hat{u}_{l_0,n}, L\psi) = 0$ for all $n \in \mathbb{Z}$. As a result, the projection equations for components of the vector $\vec{\boldsymbol{\phi}} = (\ldots, \phi_{-2}, \phi_{-1}, \phi_0, \phi_1, \phi_2, \ldots)$ satisfy the system

$$\frac{1}{\mu}\sum_{m\in\mathbb{N}}\hat{\omega}_{l_0,m}\left(\phi_{n+m}+\phi_{n-m}\right)+\frac{\sigma}{\beta}\sum_{(n_1,n_2,n_3)}K_{n,n_1,n_2,n_3}\phi_{n_1}\bar{\phi}_{n_2}\phi_{n_3}$$
$$=\Omega\phi_n-\frac{\sigma}{\beta}R_n(\vec{\boldsymbol{\phi}},\psi),\quad \forall n\in\mathbb{Z}, \tag{4.9}$$

where

$$K_{n,n_1,n_2,n_3}=\int_{\mathbb{R}}\hat{u}_{l_0,n}(x)\hat{u}_{l_0,n_1}(x)\hat{u}_{l_0,n_2}(x)\hat{u}_{l_0,n_3}(x)dx,\quad \forall n,n_1,n_2,n_3\in\mathbb{Z}, \tag{4.10}$$

and

$$R_n(\vec{\boldsymbol{\phi}},\psi)=\int_{\mathbb{R}}\hat{u}_{l_0,n}(x)\Big[|\varphi(x)+\mu\psi(x)|^2\left(\varphi(x)\right.$$
$$\left.+\mu\psi(x)\right)-|\varphi(x)|^2\varphi(x)\Big]dx,\quad \forall n\in\mathbb{Z}. \tag{4.11}$$

By Lemma 4(iii), $\alpha=\frac{\hat{\omega}_{l_0,1}}{\mu}$ is uniformly bounded and nonzero for small $\mu>0$, while $\frac{\hat{\omega}_{l_0,m}}{\mu}=\mathrm{O}(\mu)$ for all $m\geq 2$. By Lemma 5(i), $K_{n,n,n,n}=\beta=\|\hat{u}_{l_0,0}\|^4_{L^4(\mathbb{R})}$ is uniformly bounded and nonzero for small $\mu>0$. By Lemma 5(ii), $K_{n,n_1,n_2,n_3}=\mathrm{O}\left(\mu^{|n_1-n|+|n_2-n|+|n_3-n|+|n_2-n_1|+|n_3-n_1|+|n_3-n_2|}\right)$ for all $n_1,n_2,n_3\neq n$. If system (4.9) is formally truncated at the leading-order terms as $\mu\to 0$, it becomes the lattice equation (1.2). We can now formulate the main result of our article.

Theorem 1. *Let V satisfy Assumption 2. Fix $l_0\in\mathbb{N}$ and denote $\mu=\varepsilon e^{-\frac{a}{\varepsilon}}$. Assume that there exists a solution $\vec{\boldsymbol{\phi}}_0\in l^1(\mathbb{Z})$ of the lattice equation (1.2) with $\alpha=\hat{\omega}_{l_0,1}/\mu$ and a fixed Ω such that the linearized equation at $\vec{\boldsymbol{\phi}}_0$ has one-dimensional kernel in $l^1(\mathbb{Z})\subset l^2(\mathbb{Z})$ spanned by $\{i\vec{\boldsymbol{\phi}}_0\}$ and the rest of the spectrum is bounded away from zero. There exist μ_0, $C>0$, such that the nonlinear elliptic problem (1.1) with $\omega=\hat{\omega}_{l_0,0}+\mu\Omega$ has a solution $\phi(x)$ in $H^1(\mathbb{R})$ with*

$$\forall 0<\mu<\mu_0:\quad\left\|\phi-\left(\frac{\mu}{\beta}\right)^{1/2}\sum_{n\in\mathbb{Z}}\phi_n\hat{u}_{l_0,n}\right\|_{H^1(\mathbb{R})}\leq C\mu^{3/2}, \tag{4.12}$$

where $\beta=\|\hat{u}_{l_0,0}\|^4_{L^4(\mathbb{R})}$. Moreover, $\phi(x)$ decays to zero exponentially fast as $|x|\to\infty$ if $\{\phi_n\}$ decays to zero exponentially fast as $|n|\to\infty$.

Remark 5. According to Theorem 1 in [13], there exists a bounded, continuous and exponentially decaying solution ϕ in $H^1(\mathbb{R})$ if ω is in a finite gap of the spectrum of L. Not only do we recover this result but also we specify the asymptotic correspondence between exponentially decaying solutions of the elliptic problem (1.1) and those of the lattice equation (1.2). The correspondence can be used to classify the localized solutions of these models by the number of pulses in different wells of the periodic potential $V(x)$ modulo a discrete group of translations with a 2π-multiple period. This classification is explained in Remark 9 of Sect. 6.

Remark 6. We show in Appendix D that the lattice equation (1.2) occurs naturally as the Poincaré map for the second-order equation (1.1) with a periodic coefficient. However, the map we used to turn a sequence $\{\phi_n\}_{n\in\mathbb{Z}}$ into a function $\phi(x)$ on $x\in\mathbb{R}$ involves the Wannier functions, whereas that to turn a sequence for Poincaré map iterations into a function $\phi(x)$ involves evolution of the differential equation on $[0,2\pi]$. There is a map between these two types of sequences but it is not a sitewise map.

5. Proof of Theorem 1

Using the same scaling as in the previous section, namely $\mu = \varepsilon e^{-\frac{a}{\varepsilon}}$, $\omega = \hat{\omega}_{l_0,0} + \mu\Omega$ and $\phi = \frac{\sqrt{\mu}}{\sqrt{\beta}}\tilde{\phi}(x)$, we rewrite the nonlinear elliptic problem (1.1) in the equivalent form

$$L_\mu \tilde{\phi} = \mu\left(\Omega\tilde{\phi} - \frac{\sigma}{\beta}|\tilde{\phi}|^2\tilde{\phi}\right), \qquad L_\mu = -\partial_x^2 + V(x) - \hat{\omega}_{l_0,0}, \tag{5.1}$$

where both V and $\hat{\omega}_{l_0,0}$ depend on ε and thus on μ. Let E_{l_0} be an invariant subspace of $L^2(\mathbb{R})$ associated with the l_0^{th} spectral band of $\sigma(L)$. Using the Lyapunov–Schmidt reduction theory, we decompose the solution in the form $\tilde{\phi}(x) = \varphi(x) + \mu\psi(x)$, where $\varphi \in E_{l_0} \subset L^2(\mathbb{R})$ and $\psi \in E_{l_0}^{\perp} = L^2(\mathbb{R})\backslash E_{l_0}$. Denote projection operators $P : L^2(\mathbb{R}) \mapsto E_{l_0}$ and $Q = I - P : L^2(\mathbb{R}) \mapsto E_{l_0}^{\perp}$. Then, the bifurcation problem (5.1) splits into a system of two equations

$$PL_\mu P\varphi = \mu\left(\Omega\varphi - \frac{\sigma}{\beta}P|\varphi + \mu\psi|^2(\varphi + \mu\psi)\right), \tag{5.2}$$

$$QL_\mu Q\psi = \mu\Omega\psi - \frac{\sigma}{\beta}Q|\varphi + \mu\psi|^2(\varphi + \mu\psi). \tag{5.3}$$

The proof of Theorem 1 is based on the following two lemmas that describe solutions of system (5.2)–(5.3).

Lemma 6. *Let $D_{\delta_0} \subset H^1(\mathbb{R})$ be a ball of finite radius δ_0 centered at $0 \in H^1(\mathbb{R})$ and let $R_{\mu_0} \subset \mathbb{R}$ be an interval of small radius μ_0 centered at $0 \in \mathbb{R}$. There exists a unique smooth map $\psi_\mu : D_{\delta_0} \times R_{\mu_0} \mapsto H^1(\mathbb{R})$, such that $\psi(x) = \psi_\mu(\varphi(x))$ solves Eq. (5.3) and*

$$\forall 0 < \mu < \mu_0, \ \forall \|\varphi\|_{H^1(\mathbb{R})} < \delta_0 : \quad \|\psi\|_{H^1(\mathbb{R})} \leq C_0\|\varphi\|^3_{H^1(\mathbb{R})}, \tag{5.4}$$

for some constant $C_0 > 0$. Moreover, $\psi(x)$ decays exponentially as $|x| \to \infty$.

Proof. Let $\omega \equiv \hat{\omega}_{l_0,0}$. Since $\omega \notin \sigma(E_{l_0}^{\perp})$ by Lemma 4(i), solutions $\phi(x)$ of the linear inhomogeneous problem $QL_\mu Q\phi = f(x)$ with $f \in L^2(\mathbb{R})$ belong to $L^2(\mathbb{R})$ uniformly in $\mu \in \mathbb{R}$ because of the Fourier–Bloch decomposition (see Proposition 1)

$$\phi(x) = \sum_{l \in \mathbb{N}\backslash\{l_0\}} \int_{\mathbb{T}} \frac{\hat{f}_l(k)}{\omega_l(k) - \omega} u_l(x;k)dk, \quad \forall x \in \mathbb{R} \tag{5.5}$$

and the Parseval identity

$$\begin{aligned}\|\phi\|^2_{L^2(\mathbb{R})} &= \sum_{l \in \mathbb{N}\backslash\{l_0\}} \int_{\mathbb{T}} \frac{|\hat{f}_l(k)|^2}{(\omega_l(k) - \omega)^2}dk \\ &\leq \frac{1}{\zeta_0^2} \sum_{l \in \mathbb{N}\backslash\{l_0\}} \int_{\mathbb{T}} |\hat{f}_l(k)|^2 dk \leq \frac{1}{\zeta_0^2}\|f\|^2_{L^2(\mathbb{R})},\end{aligned} \tag{5.6}$$

where the bound (4.1) has been used. Since $V(x) \geq 0$ and $\omega > 0$ according to Remark 2, we multiply $QL_\mu Q\phi = f(x)$ by the function ϕ and integrate it with respect to $x \in \mathbb{R}$ to obtain

$$\|\phi'(x)\|^2_{L^2(\mathbb{R})} + \|V^{1/2}\phi\|^2_{L^2(\mathbb{R})} \leq \omega\|\phi\|^2_{L^2(\mathbb{R})} + |(\phi, f)| \leq \omega\|\phi\|^2_{L^2(\mathbb{R})} + \|\phi\|_{L^2(\mathbb{R})}\|f\|_{L^2(\mathbb{R})}, \tag{5.7}$$

where the Cauchy–Schwarz inequality has been used. Using the bound (5.6), we find that

$$\|\phi\|_{H^1(\mathbb{R})} \leq C\|f\|_{L^2(\mathbb{R})}, \tag{5.8}$$

where $C > 0$ is ε-independent. Therefore, the operator $QL_\mu Q$ is continuously invertible and the inverse operator $(QL_\mu Q)^{-1}$ provides a continuous map from $L^2(\mathbb{R})$ to $H^1(\mathbb{R})$ uniformly in μ, such that

$$\forall 0 < \mu < \mu_0: \quad \|\left(QL_\mu Q - \mu\Omega\right)^{-1}\|_{L^2(\mathbb{R})\mapsto H^1(\mathbb{R})} \leq \tilde{C}, \tag{5.9}$$

where $\tilde{C} > 0$ is ε-independent. Therefore, system (5.3) can be rewritten in the form

$$\psi = -\frac{\sigma}{\beta}\left(QL_\mu Q - \mu\Omega\right)^{-1} Q|\varphi + \mu\psi|^2(\varphi + \mu\psi). \tag{5.10}$$

Since $H^1(\mathbb{R})$ is a Banach algebra, the nonlinear operator acting on ψ and given by the right-hand-side of system (5.10) maps an element of $H^1(\mathbb{R})$ to itself if $\varphi \in H^1(\mathbb{R})$. The existence of the map $\psi(x) = \psi_\mu(\varphi(x))$ with the desired bound (5.4) follows by the Implicit Function Theorem. By elliptic theory, solution $\psi(x)$ of system (5.10) in $H^1(\mathbb{R})$ decays exponentially as $|x| \to \infty$. □

Remark 7. One might have hoped that the operator $(QL_\mu Q)^{-1}$ provides a continuous map from $L^2(\mathbb{R})$ to $H^2(\mathbb{R})$ uniformly in μ, but we suspect this is false. Nevertheless, we do obtain a bound

$$\|\phi\|_{H^2(\mathbb{R})} \leq \frac{C}{\varepsilon}\|f\|_{L^2(\mathbb{R})} \leq C(\nu)\mu^{-\nu}\|f\|_{L^2(\mathbb{R})},$$

for a fixed $\nu > 0$ and some $C(\nu) > 0$, which may not be sharp. Indeed, this bound follows from the bounds

$$\|\phi''(x)\|_{L^2(\mathbb{R})} \leq \|V\phi\|_{L^2(\mathbb{R})} + \omega\|\phi\|^2_{L^2(\mathbb{R})} + \|f\|_{L^2(\mathbb{R})}$$

and $\|V\phi\|_{L^2(\mathbb{R})} \leq \frac{1}{\varepsilon}\|V^{1/2}\phi\|_{L^2(\mathbb{R})}$, where $\|V^{1/2}\phi\|_{L^2(\mathbb{R})}$ is uniformly bounded in ε by $\|f\|_{L^2(\mathbb{R})}$, thanks to the bounds (5.6) and (5.7).

Using the map in Lemma 6, we rewrite system (5.2) as a bifurcation equation for $\varphi(x)$,

$$PL_\mu P\varphi = \mu\left(\Omega\varphi - \frac{\sigma}{\beta}P|\varphi + \mu\psi_\mu(\varphi)|^2(\varphi + \mu\psi_\mu(\varphi))\right). \tag{5.11}$$

Using the decomposition in Lemma 2, we represent solutions of (5.11) in the form

$$\forall \varphi \in E_{l_0} \subset L^2(\mathbb{R}): \quad \varphi(x) = \sum_{n\in\mathbb{Z}} \phi_n \hat{u}_{l_0,n}(x). \tag{5.12}$$

We recall that $\varphi \in H^1(\mathbb{R})$ if $\vec{\boldsymbol{\phi}} \in l^1(\mathbb{Z})$. By Proposition 2, the orthogonal projections of the bifurcation equation (5.11) result in the lattice equation (4.9), where $\psi(x) = \psi_\mu(\varphi(x))$ is represented by the map with the bound (5.4) and $\varphi(x)$ is given by the Wannier function decomposition (5.12).

Lemma 7. *The lattice system (4.9) for vectors $\vec{\boldsymbol{\phi}}$ is closed in vector space $l^1(\mathbb{Z})$. Moreover,*

$$\forall 0 < \mu < \mu_0, \quad \forall \|\vec{\boldsymbol{\phi}}\|_{l^1(\mathbb{Z})} \leq \delta_0 : \quad \|\vec{\mathbf{R}}(\vec{\boldsymbol{\phi}}, \psi)\|_{l^1(\mathbb{Z})} \leq \mu D_0 \|\vec{\boldsymbol{\phi}}\|^5_{l^1(\mathbb{Z})}, \tag{5.13}$$

for some constant $D_0 > 0$.

Proof. We shall prove that every term of the lattice system (4.9) maps $l^1(\mathbb{Z})$ to itself. The first term is estimated as follows:

$$\|\vec{\boldsymbol{\omega}}(\vec{\boldsymbol{\phi}})\|_{l^1(\mathbb{Z})} \leq \frac{1}{\mu} \sum_{n\in\mathbb{Z}} \sum_{n'\in\mathbb{Z}\backslash\{0\}} |\hat{\omega}_{l_0,n'}||\phi_{n+n'}| \leq \frac{1}{\mu} \|\vec{\boldsymbol{\omega}}_{l_0}\|_{l^1(\mathbb{Z})} \|\vec{\boldsymbol{\phi}}\|_{l^1(\mathbb{Z})},$$

where $\vec{\boldsymbol{\omega}}_{l_0}$ is the vector of elements $\{\hat{\omega}_{l_0,n}\}$ on $n \in \mathbb{Z}\backslash\{0\}$. Since $\omega_{l_0}(k)$ is analytically extended along the Riemann surface on $k \in \mathbb{T}$ (by Theorem XIII.95 on p.301 in [19]), we obtain that $\omega_{l_0} \in H^s(\mathbb{T})$ for any $s \geq 0$ and, hence, $\vec{\boldsymbol{\omega}}_{l_0} \in l^1(\mathbb{Z})$. By Lemma 4(iii), we have $\|\vec{\boldsymbol{\omega}}_{l_0}\|_{l^1(\mathbb{Z})} \leq C\mu$ for some $C > 0$ and small $\mu > 0$. The second term of the lattice system (4.9) is estimated as follows:

$$\|\vec{\mathbf{K}}(\vec{\boldsymbol{\phi}})\|_{l^1(\mathbb{Z})} \leq \frac{\sigma}{\beta} \sum_{n\in\mathbb{Z}} \sum_{(n_1,n_2,n_3)} |K_{n,n_1,n_2,n_3}||\psi_{n_1}||\psi_{n_2}||\psi_{n_3}| \leq \frac{\sigma}{\beta} K_0 \|\vec{\boldsymbol{\phi}}\|^3_{l^1(\mathbb{Z})},$$

where $K_0 = \sup_{(n_1,n_2,n_3)} \|\vec{\mathbf{K}}_{n_1,n_2,n_3}\|_{l^1(\mathbb{Z})}$ and $\vec{\mathbf{K}}_{n_1,n_2,n_3}$ is the vector of elements $\{K_{n,n_1,n_2,n_3}\}$ on $n \in \mathbb{Z}$. Because of the exponential decay (3.8) justified in Lemma 5(ii), there exists a uniform bound

$$\sum_{n\in\mathbb{Z}} |\hat{u}_{l_0,n}(x)| \leq C_{l_0} \sum_{n\in\mathbb{Z}} e^{-\eta_{l_0}|x-2\pi n|} \leq A_0, \qquad \forall x \in \mathbb{R},$$

for some $A_0 > 0$. As a result, we obtain

$$\begin{aligned} \|\vec{\mathbf{K}}_{n_1,n_2,n_3}\|_{l^1(\mathbb{Z})} &\leq A_0 \int_{\mathbb{R}} |\hat{u}_{l_0,n_1}(x)||\hat{u}_{l_0,n_2}(x)||\hat{u}_{l_0,n_3}(x)|dx \\ &\leq A_0 \|\hat{u}_{l_0,0}\|_{L^\infty(\mathbb{R})} \|\hat{u}_{l_0,0}\|^2_{L^2(\mathbb{R})}, \end{aligned}$$

uniformly in (n_1, n_2, n_3). Since $\|\hat{u}_{l_0,0}\|_{H^1(\mathbb{R})} \leq \|(1+L)^{1/2}\hat{u}_{l_0,0}\|_{L^2(\mathbb{R})} \leq (1+\hat{\omega}_{l_0,0})^{1/2}$, we have $K_0 \leq C$ for some $C > 0$ and small $\mu > 0$, thanks to Lemma 4(ii) and Sobolev's embedding. Finally, the vector field $\vec{\mathbf{R}}(\vec{\boldsymbol{\phi}})$ of the lattice system (4.9) is estimated as follows:

$$\begin{aligned} \|\vec{\mathbf{R}}(\vec{\boldsymbol{\phi}})\|_{l^1(\mathbb{Z})} &\leq A_0 \int_{\mathbb{R}} \Big| |\varphi(x) + \mu\psi_\mu(\varphi(x))|^2 (\varphi(x) + \mu\psi_\mu(\varphi(x))) - |\varphi(x)|^2\varphi(x) \Big| dx \\ &\leq \mu A_0 B_0 \|\varphi\|^2_{H^1(\mathbb{R})} \|\psi_\mu(\varphi)\|_{H^1(\mathbb{R})} \\ &\leq \mu A_0 B_0 C_0 \|\varphi\|^5_{H^1(\mathbb{R})} \leq \mu A_0 B_0 C_0 \|\vec{\boldsymbol{\phi}}\|^5_{l^1(\mathbb{Z})}, \end{aligned}$$

for some $B_0 > 0$, where we have used the property (1.6), the bound (5.4), and Lemma 2. The last computation proves the desired bound (5.13) with $D_0 = A_0 B_0 C_0$. □

Proof of Theorem 1. By Lemmas 4(iii) and 7, the first term of the lattice system (4.9) can be rewritten in the form

$$\frac{1}{\mu}\sum_{m\in\mathbb{N}}\hat{\omega}_{l_0,m}\left(\phi_{n+m}+\phi_{n-m}\right)=\alpha\left(\phi_{n+1}+\phi_{n-1}\right)+\mu L_n(\boldsymbol{\phi},\mu),$$

where $\alpha=\hat{\omega}_{l_0,1}/\mu$ is uniformly bounded and nonzero for $\mu>0$ and

$$\forall 0<\mu<\mu_0,\quad \forall\|\vec{\boldsymbol{\phi}}\|_{l^1(\mathbb{Z})}\le\delta_0:\quad \|\vec{\mathbf{L}}(\vec{\boldsymbol{\phi}},\mu)\|_{l^1(\mathbb{Z})}\le D_1\|\vec{\boldsymbol{\phi}}\|_{l^1(\mathbb{Z})}, \tag{5.14}$$

for some constant $D_1>0$. By Lemmas 5(ii) and 7, the second term of the lattice system (4.9) can be rewritten in the form

$$\frac{\sigma}{\beta}\sum_{(n_1,n_2,n_3)}K_{n,n_1,n_2,n_3}\phi_{n_1}\bar{\phi}_{n_2}\phi_{n_3}=\sigma|\phi_n|^2\phi_n+\mu Q_n(\boldsymbol{\phi},\mu),$$

where

$$\forall 0<\mu<\mu_0,\quad \forall\|\vec{\boldsymbol{\phi}}\|_{l^1(\mathbb{Z})}\le\delta_0:\quad \|\vec{\mathbf{Q}}(\vec{\boldsymbol{\phi}},\mu)\|_{l^1(\mathbb{Z})}\le D_2\|\vec{\boldsymbol{\phi}}\|^3_{l^1(\mathbb{Z})}, \tag{5.15}$$

for some constant $D_2>0$. As a result, we obtain the perturbed lattice system

$$\alpha\left(\phi_{n+1}+\phi_{n-1}\right)+\sigma|\phi_n|^2\phi_n-\Omega\phi_n=\mu N_n(\vec{\boldsymbol{\phi}},\mu),\quad \forall n\in\mathbb{Z}, \tag{5.16}$$

where the perturbation term satisfies the bound

$$\forall 0<\mu<\mu_0,\quad \forall\|\vec{\boldsymbol{\phi}}\|_{l^1(\mathbb{Z})}\le\delta_0:\quad \|\vec{\mathbf{N}}(\vec{\boldsymbol{\phi}},\mu)\|_{l^1(\mathbb{Z})}\le D\|\vec{\boldsymbol{\phi}}\|_{l^1(\mathbb{Z})}, \tag{5.17}$$

for some constant $D>0$. Assume that there exists a solution $\vec{\boldsymbol{\phi}}_0\in l^1(\mathbb{Z})$ of the lattice equation (1.2) with $\alpha=\hat{\omega}_{l_0,1}/\mu$ and a fixed Ω such that the linearized equation at $\vec{\boldsymbol{\phi}}_0$ has a one-dimensional kernel in $l^1(\mathbb{Z})\subset l^2(\mathbb{Z})$ spanned by $\{i\vec{\boldsymbol{\phi}}_0\}$ and the rest of the spectrum is bounded away from zero. This eigenmode is always present owing to the invariance of the lattice equation (1.2) with respect to the gauge transformation $\vec{\boldsymbol{\phi}}\to\vec{\boldsymbol{\phi}}e^{i\theta}$, $\forall\theta\in\mathbb{R}$. The perturbed lattice equation (5.16) is also invariant with respect to this transformation, since it is inherited from the properties of the nonlinear elliptic problem (1.1). Fix θ uniquely by picking a $n_0\in\mathbb{Z}$ such that $|(\boldsymbol{\phi}_0)_{n_0}|\neq 0$ and requiring that

$$\mathrm{Im}(\boldsymbol{\phi}_0)_{n_0}=0,\quad \mathrm{Im}(\boldsymbol{\phi})_{n_0}=0.$$

The vector field of the perturbed lattice equation (5.16) preserves the constraint $\mathrm{Im}(\boldsymbol{\phi})_{n_0}=0$ by symmetry and it is closed in $l^1(\mathbb{Z})\subset l^2(\mathbb{Z})$, while the linearized operator is continuously invertible under the constraint. By the Implicit Function Theorem, there exists a smooth continuation of the solution $\vec{\boldsymbol{\phi}}_0$ due to the perturbation terms of the lattice equation (5.16) such that $\mathrm{Im}(\boldsymbol{\phi})_{n_0}=0$ and

$$\forall 0<\mu<\mu_0:\quad \|\vec{\boldsymbol{\phi}}-\vec{\boldsymbol{\phi}}_0\|_{l^1(\mathbb{Z})}\le C\mu, \tag{5.18}$$

for some $C>0$. By Lemma 2, if $\vec{\boldsymbol{\phi}}\in l^1(\mathbb{Z})$, then $\varphi(x)$ in the representation (5.12) is a continuous bounded function of $x\in\mathbb{R}$, which decays to zero as $|x|\to\infty$. By Lemma 3, it decays to zero exponentially fast as $|x|\to\infty$ if $\vec{\boldsymbol{\phi}}$ decays to zero exponentially fast as $|n|\to\infty$. The same properties hold for $\psi(x)=\psi_\mu(\varphi(x))$, by Lemma 6, and thus to the full solution $\phi(x)$. These arguments finish the proof of Theorem 1. □

Remark 8. For the proof of Theorem 1, we used a different approach compared to [6, 17]. In these papers, we first formulated the elliptic problem with a periodic potential in the Bloch (Fourier) space and then reduced a closed system of equations for the Bloch–Fourier transform by using the Lyapunov–Schmidt reductions. One can think of using the same strategy here, when a full (double-series) Wannier function decomposition is used to transform the elliptic problem to an algebraic system for coefficients of the double series. We have avoided this approach since we do not know how to show that the system of the nonlinear algebraic equations is closed in the space $l_1^1(\mathbb{N}, l^1(\mathbb{Z}))$, which would ensure that $\phi \in H^1(\mathbb{R})$.

6. Examples of Localized Solutions

We review examples of localized solutions of the lattice equation (1.2) which satisfy the assumptions of Theorem 1. Following paper [11], these solutions can be efficiently characterized in the anti-continuum limit where α is sufficiently small.

We recall that all localized solutions $\{\phi_n\}_{n\in\mathbb{Z}}$ of the lattice equation (1.2) are real-valued (see, e.g., [15]). Let $\vec{\boldsymbol{\phi}}$ be a real-valued vector on $n \in \mathbb{Z}$ and rewrite the lattice equation (1.2) in the form

$$\left(\Omega - \sigma\phi_n^2\right)\phi_n = \alpha\left(\phi_{n+1} + \phi_{n-1}\right), \quad \forall n \in \mathbb{Z}. \tag{6.1}$$

The linearized equation at the real-valued solution $\vec{\boldsymbol{\phi}}$ perturbed with the real-valued vector $\vec{\boldsymbol{\psi}}$ is written in the form

$$\left(L_\alpha\vec{\boldsymbol{\psi}}\right)_n = \left(\Omega - 3\sigma\phi_n^2\right)\psi_n - \alpha\left(\psi_{n+1} + \psi_{n-1}\right), \quad \forall n \in \mathbb{Z}. \tag{6.2}$$

The nonlinear vector field of the lattice equation (6.1) maps $l^1(\mathbb{Z})$ to itself for any $\alpha \in \mathbb{R}$. If $\alpha = 0$ and $\sigma = \operatorname{sign}(\Omega)$, there exists a limiting solution of the lattice equation (6.1) in the form

$$\phi_n = \begin{cases} 0, & \forall n \in U_0, \\ \pm\sqrt{|\Omega|}, & \forall n \in U_\pm, \end{cases} \tag{6.3}$$

where $U_+ \cup U_- \cup U_0 = \mathbb{Z}$. The spectrum of the linearized operator L_0 evaluated at the limiting solution (6.3) consists of two points $\sigma(L_0) = \{-2\Omega, \Omega\}$, where eigenvalue Ω has multiplicity $\dim(U_0)$ and eigenvalue -2Ω has multiplicity $\dim(U_+) + \dim(U_-)$. If $\dim(U_+) + \dim(U_-) < \infty$, the limiting solution (6.3) is in $l^1(\mathbb{Z})$ and the linearized operator L_α is continuously invertible in $l^1(\mathbb{Z})$ for any $\Omega \neq 0$. By the Implicit Function Theorem, there exists a unique smooth solution $\vec{\boldsymbol{\phi}}_\alpha \in l^1(\mathbb{Z})$ of the lattice equation (1.2) with $|\alpha| < \alpha_0$ and $\sigma = \operatorname{sign}(\Omega)$, where $\alpha_0 > 0$ is sufficiently small, and

$$\|\vec{\boldsymbol{\phi}}_\alpha - \vec{\boldsymbol{\phi}}_0\|_{l^1(\mathbb{Z})} \leq C|\alpha|,$$

for some α-independent constant $C > 0$. Since the kernel of the linearization operator (6.2) is empty for sufficiently small α, the assumptions of Theorem 1 are satisfied for real-valued solutions $\vec{\boldsymbol{\phi}} \in l^1(\mathbb{Z})$.

Remark 9. For sufficiently small values of α, all localized solutions of the lattice equation (6.1) can be classified by the configurations U_+ and U_- in the limiting solution (6.3). Simply speaking, the limiting configuration indicates a finite number of nodes on $\mathbb{Z}$, where "up" and "down" pulses are placed. Using the bound (4.12) of Theorem 1, we can transfer this information to the localized solution of the elliptic problem (1.1) since each $n \in \mathbb{Z}$ with $\phi_n \neq 0$ corresponds to the Wannier function $\hat{u}_{l_0,n}(x) = \hat{u}_{l_0,0}(x - 2\pi n)$, which is centered at the n^{th} potential well of $V(x)$ and is exponentially decaying as $|x| \to \infty$. Therefore, the limiting configuration (6.3) indicates the finite number of "up" and "down" pulses placed in the corresponding wells of the periodic potential V.

Remark 10. Bifurcations of localized real-valued solutions may occur for larger values of α, when the linearized operator (6.2) may admit a nontrivial kernel in $l^1(\mathbb{Z}) \subset l^2(\mathbb{Z})$. Theorem 1 does not hold at the bifurcation point but can be used to prove persistence of solutions before and after the bifurcation point, provided that the linearized operator is again invertible.

7. Examples of Potential Functions V

The main example of the potential function V in Assumption 2 can be extended to other potential functions using semi-classical techniques [4,8]. This extension will not be presented here. We shall, however, review other examples of the potential function V, for which the analysis of our paper can be applied immediately.

Example 1. Let $V(x) = c\delta(x)$ on $[-\pi, \pi]$, periodically continued with the period 2π. The band function $\omega_l(k)$ for this example can be obtained from analysis of Appendix B if $a \to 0$ and $c = ab$ is fixed. The expression (B.3) for $\text{tr}(A)$ simplifies in the limit $a \to 0$ to the form

$$\text{tr}(A) = 2\cos(2\pi\sqrt{\omega}) + \frac{c}{\sqrt{\omega}}\sin(2\pi\sqrt{\omega}), \quad 0 < \omega < \infty. \tag{7.1}$$

All bands have non-zero widths if c is finite. Therefore, the delta-function potential (with infinitesimal thickness of the walls) does not satisfy the tight-binding property (4.3) of Lemma 4. In addition, the periodic potential $V(x)$ is unbounded at $x = 2\pi n$, $\forall n \in \mathbb{Z}$ for any $c > 0$.

Example 2. Let $V(x + L) = V(x)$ be L-periodic, such that $V(x) = b$ on $x \in (0, a)$ and $V(x) = 0$ on $x \in (a, L)$. We show that this function is equivalent, in the limit $L \to \infty$, to the potential function of Assumption 2 in the limit $\varepsilon \to 0$. Let

$$\epsilon = \left(\frac{2\pi}{L}\right)^2, \quad x = \frac{\tilde{x}}{\sqrt{\epsilon}}, \quad V(x) = \epsilon\tilde{V}(\tilde{x}), \quad \phi(x) = \tilde{\phi}(\tilde{x}), \quad \omega = \epsilon\tilde{\omega}.$$

Then, $\phi(x)$ and $\tilde{\phi}(\tilde{x})$ solve

$$(-\partial_x^2 + V(x))\phi(x) = \omega\phi(x), \quad (-\partial_{\tilde{x}}^2 + \tilde{V}(\tilde{x}))\tilde{\phi}(\tilde{x}) = \tilde{\omega}\tilde{\phi}(\tilde{x}),$$

respectively, while $\tilde{V}(\tilde{x}) = \tilde{b}$ on $\tilde{x} \in (0, \tilde{a})$ and $\tilde{V}(\tilde{x}) = 0$ on $\tilde{x} \in (\tilde{a}, 2\pi)$ with $\tilde{a} = \sqrt{\epsilon}a$ and $\tilde{b} = b/\epsilon$. For fixed $\frac{a}{L}$ and b, the function $\tilde{V}(\tilde{x})$ is equivalent to the one in Assumption 2. We note that the band separation property (4.1) of Lemma 4 is not satisfied for the function $V(x)$ in the limit $L \to \infty$, since the distance between spectral bands reduces as $\text{O}(\frac{1}{L^2})$. However, this property is satisfied for the rescaled function $\tilde{V}(\tilde{x})$.

Example 3. Let $V(x) = \frac{1}{2\epsilon^2}(1 - \cos x)$ be such that $V(x) = \frac{x^2}{4\epsilon^2} + O(x^4)$ near $x = 0$. According to the asymptotic analysis in [23], the tight-binding property (4.3) of Lemma 4 is satisfied in the limit $\epsilon \to 0$, while the exponentially narrow spectral bands $\omega_l(k)$ converge to eigenvalues of the parabolic potential $\frac{x^2}{4\epsilon^2}$ at $\omega = \frac{2l-1}{2\epsilon}$ for all $l \in \mathbb{N}$. The distance between different bands satisfies the band separation property (4.1) and in fact, diverges as $\epsilon \to 0$. We note, however, that the band-boundeness property (4.2) fails for this example. However, it only affects the bound (4.12) and does not affect the lattice equation (1.2) where the coefficient of the nonlinear term is scaled to unity.

We finish this section with remarks on the related works [21,25].

- The periodic piecewise-constant function $a(x)$ in the operator $L = -\partial_x a(x)\partial_x$ considered in [21] is similar to the main example of the potential function $V(x)$ used in Assumption 2. It provides both the separation of bands and the tight-banding approximation with some modifications: (i) the lowest-order band does not satisfy the property $|\hat{\omega}_{l_0,1}| \ll \hat{\omega}_{l_0,0}$ but does satisfy the property $|\hat{\omega}_{l_0,m}| \ll \hat{\omega}_{l_0,0}$ for any $|m| \geq 2$ and (ii) the lowest-order band is separated from all other bands by a distance diverging as $\epsilon \to 0$.
- Complicated projection analysis in the problem involving nonlinear pulses located far away from each other [25] is partly explained in Example 2: the bands are not separated from each other in the limit $L \to \infty$ unless a rescaling to tilded variables is applied.

8. Lattice Equations in Two and Three Dimensions

The results of our analysis were restricted to the space of one dimension since we have used the Banach algebra property of $H^1(\mathbb{R})$ and the fact that $(QL_\mu Q)^{-1}$ provides a bounded map from $L^2(\mathbb{R})$ to $H^1(\mathbb{R})$ uniformly in $\mu > 0$. According to Remark 7, no uniform bound may exist from $L^2(\mathbb{R})$ to $H^2(\mathbb{R})$. Nevertheless, thanks to the exponential smallness of bounds (4.3) and (4.5) in Lemmas 4 and 5, we are still able to extend results of our analysis to the nonlinear elliptic problem with a multi-dimensional separable potential in the form

$$-\nabla^2\phi + W(x)\phi + \sigma|\phi|^2\phi = \omega\phi, \quad \forall x \in \mathbb{R}^d, \tag{8.1}$$

where ∇^2 is the continuous d-dimensional Laplacian and $W = \sum_{j=1}^d V(x_j)$ is a separable potential with a bounded 2π-periodic function $V : \mathbb{R} \mapsto \mathbb{R}$. The Laplacian ∇^2 can be replaced by $\nabla M \nabla$ with an arbitrary positive-definite matrix M and the results will remain the same. Equivalently, the period parallelogram of W can be arbitrary. For the sake of simplicity, we restrict our attention to the case when M is the identity matrix and W has period 2π in each coordinate. The lattice equation (1.2) is generalized in the multi-dimensional setting in the form

$$\sum_{j=1}^{d} \alpha_j \left(\phi_{n+e_j} + \phi_{n-e_j}\right) + \sigma|\phi_n|^2\phi_n = \Omega\phi_n, \quad \forall n \in \mathbb{Z}^d, \tag{8.2}$$

where $(e_1, e_2, \ldots, e_d)$ is a standard basis in $\mathbb{Z}^d$ and $(\alpha_1, \alpha_2, \ldots, \alpha_d)$ are constants. Our main result is generalized as follows.

Theorem 2. *Let $W = \sum_{j=1}^{d} V(x_j)$ be a separable potential, where V satisfies Assumption 2. Fix $l_0 \in \mathbb{N}^d$ and denote $\mu = \varepsilon e^{-\frac{a}{\varepsilon}}$. Assume that there exists a solution $\vec{\boldsymbol{\phi}}_0 \in l^1(\mathbb{Z}^d)$ of the lattice equation (8.2) for $d = 1, 2, 3$ with $\alpha_j = \hat{\omega}_{(l_0)_j,1}/\mu$, $j = 1, 2, \ldots, d$, and a fixed Ω such that the linearized equation at $\vec{\boldsymbol{\phi}}_0$ has one-dimensional kernel in $l^1(\mathbb{Z}^d)$ spanned by $\{i\vec{\boldsymbol{\phi}}_0\}$ and the rest of the spectrum is bounded away from zero. Fix $\nu \in (0, 1)$. There exist $\mu_0, C(\nu) > 0$ such that the nonlinear elliptic problem (8.1) with $\omega = \omega_0 + \mu\Omega$ has a solution $\phi(x)$ in $H^2(\mathbb{R}^d)$ for $d = 1, 2, 3$ satisfying*

$$\forall 0 < \mu < \mu_0 : \quad \left\| \phi - \left(\frac{\mu}{\beta}\right)^{1/2} \sum_{n \in \mathbb{Z}^d} \phi_n \hat{u}_{l_0,n} \right\|_{H^2(\mathbb{R}^d)} \leq C(\nu)\mu^{3/2-\nu}, \tag{8.3}$$

where $\omega_0 = \sum_{j=1}^{d} \hat{\omega}_{(l_0)_j,0}$, $\hat{u}_{l_0,n}(x) = \prod_{j=1}^{d} \hat{u}_{(l_0)_j,n_j}(x_j)$ and $\beta = \|\hat{u}_{l_0,0}\|^4_{L^4(\mathbb{R}^d)}$. Moreover, $\phi(x)$ decays to zero exponentially fast as $|x| \to \infty$ if $\{\phi_n\}$ decays to zero exponentially fast as $|n| \to \infty$.

Proof. We recall that the band and Bloch functions for the l^{th} spectral band of $L_d = -\nabla^2 + \sum_{j=1}^{d} V(x_j)$ with $l = (l_1, l_2, \ldots, l_d) \in \mathbb{N}^d$ are represented by

$$\omega = \sum_{j=1}^{d} \omega_{l_j}(k_j), \qquad u = \prod_{j=1}^{d} u_{l_j}(x_j; k_j), \tag{8.4}$$

where $\omega_l(k)$ and $u_l(x; k)$ are the band and Bloch functions of the operator $L = -\partial_x^2 + V(x)$ on $x \in \mathbb{R}$. By using the same scaling of variables, we derive system (5.1) and split it into system (5.2)–(5.3) by using the orthogonal projections. Since μ is exponentially small in ε, while the operator $(QL_\mu Q)^{-1}$ provides a map from $L^2(\mathbb{R}^d)$ to $H^2(\mathbb{R}^d)$ that diverges only algebraically in ε (see Remark 7), there exists a unique map $\psi_\mu : H^2(\mathbb{R}^d) \times (0, \mu_0) \mapsto H^2(\mathbb{R}^d)$, such that $\psi(x) = \psi_\mu(\varphi(x))$ and

$$\forall 0 < \mu < \mu_0, \ \forall \|\varphi\|_{H^2(\mathbb{R})} < \delta_0 : \quad \|\psi\|_{H^2(\mathbb{R})} \leq \mu^{-\nu/6} C_0(\nu) \|\varphi\|^3_{H^2(\mathbb{R})}, \tag{8.5}$$

for a fixed $\nu \in (0, 1)$ and some constant $C_0(\nu) > 0$. Therefore, we close the bifurcation equation (5.11) using the Wannier function decomposition

$$\forall \varphi \in E_{l_0} \subset L^2(\mathbb{R}^d) : \quad \varphi(x) = \sum_{n \in \mathbb{Z}^d} \phi_n \hat{u}_{l_0,n}(x), \quad \hat{u}_{l_0,n}(x) = \prod_{j=1}^{d} \hat{u}_{(l_0)_j,n_j}(x_j). \tag{8.6}$$

As a result, we obtain the lattice equation (4.9) in $\mathbb{Z}^d$. Since

$$\|\hat{u}_{l_0,n}\|_{H^2(\mathbb{R}^d)} \leq \frac{C(d)}{\varepsilon} \|\hat{u}_{l_0,n}\|_{H^1(\mathbb{R}^d)}$$

for some $C(d) > 0$, we have

$$\|\varphi\|_{H^2(\mathbb{R}^d)} \leq \frac{C(d)}{\varepsilon} \|\vec{\boldsymbol{\phi}}\|_{l^1(\mathbb{Z}^d)} \leq \mu^{-\nu/6} \tilde{C}(\nu) \|\vec{\boldsymbol{\phi}}\|_{l^1(\mathbb{Z}^d)}$$

for the same $\nu \in (0,1)$ and some $\tilde{C}(\nu) > 0$. The lattice system (4.9) is closed in $l^1(\mathbb{Z}^d)$ by the same analysis as in Lemma 7 and, since $H^2(\mathbb{R}^d)$ is a Banach algebra for $d = 1, 2, 3$, we obtain

$$\forall 0 < \mu < \mu_0, \quad \forall \|\vec{\boldsymbol{\phi}}\|_{l^1(\mathbb{Z}^d)} \le \delta_0 : \quad \|\vec{\mathbf{R}}(\vec{\boldsymbol{\phi}}, \psi)\|_{l^1(\mathbb{Z}^d)} \le \mu^{1-\nu} D(\nu) \|\vec{\boldsymbol{\phi}}\|^5_{l^1(\mathbb{Z}^d)}$$

for some $D(\nu) > 0$. The rest of the proof repeats the proof of Theorem 1. □

Example 4. Complex-valued localized solutions of the lattice equation (8.2) in $l^1(\mathbb{Z}^d)$ were constructed in the anti-continuum limit in [16] and [10] for $d = 2$ and $d = 3$ respectively. The method of Lyapunov–Schmidt reductions was used and all examples considered in these papers were represented by isolated families of solutions with the only free parameter due to the gauge invariance of the lattice equation (8.2). As a consequence, the linearized equation at the complex-valued solution $\vec{\boldsymbol{\phi}}$ perturbed with the complex-valued vector $\vec{\boldsymbol{\psi}}$,

$$(L_\alpha \boldsymbol{\psi})_n = \left(\Omega - 2\sigma|\phi_n|^2\right)\psi_n - \sigma\phi_n^2\bar{\psi}_n - \sum_{j=1}^{d} \alpha_j \left(\psi_{n+e_j} + \psi_{n-e_j}\right), \quad \forall n \in \mathbb{Z}^d, \tag{8.7}$$

was shown to have one-dimensional kernel spanned by $\{i\vec{\boldsymbol{\phi}}\}$ for any $0 < \sum_{j=1}^d |\alpha_j| < \alpha_0$ sufficiently small. Therefore, the assumptions of Theorem 2 are satisfied and all solutions of the lattice equation (8.2) obtained in [10,16] persist as solutions of the nonlinear elliptic problem (8.1).

A. Shannon Decomposition

We review here the Shannon decomposition, which is different from the Wannier decomposition of Proposition 2. Fix $l \in \mathbb{N}$ and assume that $u_l(0; k) \neq 0$ for all $k \in \mathbb{T}$. Let us define the set of functions $\{g_n(x)\}_{n\in\mathbb{Z}}$ according to the integrals

$$g_n(x) = \int_{\mathbb{T}} \frac{u_l(x; k)}{u_l(0; k)} e^{-i2\pi kn} dk, \quad \forall x \in \mathbb{R}. \tag{A.1}$$

Since $u_l(x; k) = w_l(x; k)e^{ikx}$, where $w_l(x; k)$ is a 2π-periodic function in x, it follows from the integrals (A.1) that

$$g_n(2\pi n') = \delta_{n,n'}, \quad \forall n, n' \in \mathbb{Z}.$$

Therefore, the set $\{g_n(x)\}_{n\in\mathbb{Z}}$ can be used for interpolation of a continuous complex-valued function $u(x)$ from its values $\{u_n\}_{n\in\mathbb{Z}}$ at the points $x = 2\pi n$. This construction reminds us of the Shannon theory of sampling and interpolation (see review in [24]).

Definition 2. *The functions of the set $\{g_n(x)\}_{n\in\mathbb{Z}}$ are called the Shannon functions.*

Proposition 3. *Let V satisfy Assumption 1. Fix $l \in \mathbb{N}$ and let E_l be an invariant closed subspace of $L^2(\mathbb{R})$ associated to the l^{th} spectral band of $\sigma(L)$. There exists an isomorphism $\mathcal{S} : E_l \subset L^2(\mathbb{R}) \mapsto l^2(\mathbb{Z})$ given by the sampling*

$$\forall \phi \in E_l \subset L^2(\mathbb{R}) : \quad \vec{\boldsymbol{\phi}} = \mathcal{S}\phi, \quad \phi_n = \phi(2\pi n) \quad \forall n \in \mathbb{Z}. \tag{A.2}$$

The inverse transformation is given by the interpolation

$$\forall \vec{\boldsymbol{\phi}} \in l^2(\mathbb{Z}) : \quad \phi(x) = \mathcal{S}^{-1}\vec{\boldsymbol{\phi}} = \sum_{n\in\mathbb{Z}} \phi_n g_n(x), \quad \forall x \in \mathbb{R}. \tag{A.3}$$

Proof. By Sobolev's embeddings (1.5), there exists an n-independent constant $C > 0$ such that

$$|\phi(2\pi n)| \leq C\|\phi\|_{H^1([2\pi n-\pi, 2\pi n+\pi])}, \qquad \forall n \in \mathbb{Z}.$$

Therefore,

$$\|\vec{\boldsymbol{\phi}}\|^2_{l^2(\mathbb{Z})} = \sum_{n\in\mathbb{Z}} |\phi(2\pi n)|^2 \leq C^2 \sum_{n\in\mathbb{Z}} \|\phi\|^2_{H^1([2\pi n-\pi, 2\pi n+\pi])} \leq C^2\|\phi\|^2_{H^1(\mathbb{R})}.$$

If $\phi \in E_l \subset L^2(\mathbb{R})$, then $\phi \in H^1(\mathbb{R})$, so that the map $\mathcal{S}$ is uniformly bounded on $E_l \subset L^2(\mathbb{R})$. On the other hand, it follows from the Fourier–Bloch decomposition (2.6) that

$$\begin{aligned} \forall \phi \in E_l: \quad \phi_n = \phi(2\pi n) &= \int_{\mathbb{T}} \hat{\phi}_l(k) u_l(2\pi n; k) dk \\ &= \int_{\mathbb{T}} \hat{\phi}_l(k) u_l(0; k) e^{i2\pi nk} dk, \quad \forall n \in \mathbb{Z}. \end{aligned}$$

Inverting this representation by the Fourier series theory, we obtain that

$$\hat{\phi}_l(k) u_l(0; k) = \sum_{n\in\mathbb{Z}} e^{-i2\pi nk} \phi_n,$$

where $u_l(0; k) \neq 0$ for all $k \in \mathbb{T}$ is assumed. As a result,

$$\forall \phi \in E_l: \quad \phi(x) = \int_{\mathbb{T}} \hat{\phi}_l(k) u_l(x; k) dk = \sum_{n\in\mathbb{Z}} \phi_n g_n(x),$$

provided that the integrals (A.1) for the Shannon functions $\{g_n(x)\}_{n\in\mathbb{Z}}$ converge absolutely and uniformly on $x \in \mathbb{R}$. This property follows from the exponential decay of the Shannon functions

$$|g_n(x)| \leq C e^{-\eta|x-2\pi n|}, \qquad \forall x \in \mathbb{R},$$

for some $C > 0$ and $\eta > 0$, which is proved similarly to the decay property (3.8) for the Wannier functions. □

By Sturm–Liouville theory, the assumption $u_l(0; k) > 0$ for all $k \in \mathbb{T}$ is satisfied for the lowest spectral band with $l = 1$. This assumption, however, may fail for some higher-order spectral bands with $l > 1$. Since our analysis is expected to work for any $l \in \mathbb{N}$, we have avoided the Shannon decomposition and have used an equivalent Wannier decomposition, which does not rely on the assumption above. Shannon functions were applied to the justification of lattice equations for the lowest spectral band in [21].

B. Proof of Lemma 4

Let $L = -\partial_x^2 + V(x)$, where V is given by Assumption 2. For any $0 < \omega < b$, the solution $\phi(x)$ of the ODE $L\phi = \omega\phi$ on $[0, 2\pi]$ is obtained explicitly in the form

$$\phi(x) = \begin{cases} \phi(0)\cosh\sqrt{b-\omega}x + \frac{\phi'(0)}{\sqrt{b-\omega}}\sinh\sqrt{b-\omega}x, & \forall x \in [0, a], \\ \phi(2\pi)\cos\sqrt{\omega}(x-2\pi) + \frac{\phi'(2\pi)}{\sqrt{\omega}}\sin\sqrt{\omega}(x-2\pi), & \forall x \in [a, 2\pi]. \end{cases} \tag{B.1}$$

The continuity of $\phi(x)$ and $\phi'(x)$ across the jump point $x = a$ leads to the 2-by-2 transfer matrix

$$\phi(2\pi) = a_{11}\phi(0) + a_{12}\phi'(0), \qquad \phi'(2\pi) = a_{21}\phi(0) + a_{22}\phi'(0), \tag{B.2}$$

where the explicit expressions for $\{a_{ij}\}_{1\le i,j\le 2}$ show that $a_{11}a_{22} - a_{12}a_{21} = \det(A) = 1$ and $a_{11} + a_{22} = \mathrm{tr}(A)$ is given explicitly by

$$\begin{aligned} \mathrm{tr}(A) &= 2\cosh(a\sqrt{b-\omega})\cos\left[(2\pi - a)\sqrt{\omega}\right] \\ &\quad + \frac{b-2\omega}{\sqrt{\omega(b-\omega)}}\sinh(a\sqrt{b-\omega})\sin\left[(2\pi-a)\sqrt{\omega}\right]. \end{aligned} \tag{B.3}$$

This equation is valid for $0 < \omega < b$ and it is analytically extended for $\omega > b$ to the equation

$$\begin{aligned} \mathrm{tr}(A) &= 2\cos(a\sqrt{\omega-b})\cos\left[(2\pi - a)\sqrt{\omega}\right] \\ &\quad + \frac{b-2\omega}{\sqrt{\omega(\omega-b)}}\sin(a\sqrt{\omega-b})\sin\left[(2\pi-a)\sqrt{\omega}\right]. \end{aligned} \tag{B.4}$$

The band functions $\omega_l(k)$ enumerated by $l \in \mathbb{N}$ and parameterized by $k \in \mathbb{T}$ correspond to the values of ω in the interval $|\mathrm{tr}(A)| \le 2$. They are defined by the equation $\mathrm{tr}(A) = 2\cos(2\pi k)$. In the limit $\varepsilon \to 0$, where $b = \frac{1}{\varepsilon^2}$, $|\mathrm{tr}(A)|$ is bounded near the particular values $\omega = \left(\frac{\pi l}{2\pi - a}\right)^2$ for any $l \in \mathbb{N}$, such that the distance between the two consequent values of ω is finite. We shall rewrite the algebraic equation $\mathrm{tr}(A) = 2\cos(2\pi k)$, where $\mathrm{tr}(A)$ is given by (B.3) with $b = \frac{1}{\varepsilon^2}$ in the equivalent form:

$$\begin{aligned} &\sin\left[(2\pi-a)\sqrt{\omega}\right] + \frac{2\varepsilon\sqrt{\omega(1-\varepsilon^2\omega)}}{1-2\varepsilon^2\omega}\cos\left[(2\pi-a)\sqrt{\omega}\right] \\ &= \frac{4\varepsilon\sqrt{\omega(1-\varepsilon^2\omega)}}{1-2\varepsilon^2\omega}e^{-\frac{a\sqrt{1-\varepsilon^2\omega}}{\varepsilon}}\cos(2\pi k) \\ &\quad - \left(\sin\left[(2\pi-a)\sqrt{\omega}\right] - \frac{2\varepsilon\sqrt{\omega(1-\varepsilon^2\omega)}}{1-2\varepsilon^2\omega}\sin\left[(2\pi-a)\sqrt{\omega}\right]\right)e^{-\frac{2a\sqrt{1-\varepsilon^2\omega}}{\varepsilon}}. \end{aligned} \tag{B.5}$$

At $\varepsilon = 0$, all roots of the algebraic equation (B.5) are simple. By the Lyapunov–Schmidt theory, the simple roots persist, and owing to the analyticity of the trigonometric functions, they persist in the form

$$\omega_l(k) = \hat{\omega}_{l,0}(\varepsilon) + \sum_{n\in\mathbb{N}} \varepsilon^n e^{-\frac{na}{\varepsilon}}\hat{\omega}_{l,n}(\varepsilon)\cos^n(2\pi k), \tag{B.6}$$

where all parameters $\hat{\omega}_{l,n}$ are continuous functions of ε, uniformly bounded in the limit $\varepsilon \to 0$. In particular,

$$\hat{\omega}_{l,0}(\varepsilon) = \frac{(\pi l)^2}{(2\pi - a)^2} + \mathrm{O}(\varepsilon), \quad \hat{\omega}_{l,1}(\varepsilon) = \frac{8(-1)^l(\pi l)^2}{(2\pi - a)^3} + \mathrm{O}(\varepsilon), \quad \text{etc.}$$

Properties (4.1)–(4.3) follow from the representation (B.6) for sufficiently small $\varepsilon > 0$.

C. Proof of Lemma 5

Let us first rewrite the system of Eq. (3.5) in the form

$$-\hat{u}''_{l,0}(x) + V(x)\hat{u}_{l,0}(x) = \sum_{n\in\mathbb{Z}} \hat{\omega}_{l,n}\hat{u}_{l,n}(x), \qquad \forall n \in \mathbb{Z}. \tag{C.1}$$

Consider the ODE $(L - \omega)\phi = f(x)$ for $L = -\partial_x^2 + V(x)$ on $[0, 2\pi]$. The explicit solution is

$$\phi(x) = \begin{cases} Ae^{\frac{\sqrt{1-\varepsilon^2\omega}}{\varepsilon}(x-a)} + Be^{-\frac{\sqrt{1-\varepsilon^2\omega}}{\varepsilon}(x-a)} - \frac{\varepsilon}{2\sqrt{1-\varepsilon^2\omega}}\int_0^a e^{-\frac{\sqrt{1-\varepsilon^2\omega}}{\varepsilon}|x-\xi|} f(\xi)d\xi, & \forall x \in [0,a], \\ C\cos\sqrt{\omega}(x-a) + D\sin\sqrt{\omega}(x-a) - \int_a^{2\pi} \frac{\sin\sqrt{\omega}|x-\xi|}{2\sqrt{\omega}} f(\xi)d\xi, & \forall x \in [a, 2\pi], \end{cases} \tag{C.2}$$

where (A, B, C, D) are arbitrary constants. Because of the property (3.4), the ODE above corresponds to system (C.1) for $\omega = \hat{\omega}_{l,0}$, $\phi = \hat{u}_{l,0}$ and $f = \sum_{n\in\mathbb{Z}\backslash\{0\}} \hat{\omega}_{l,n}\hat{u}_{l,0}(x - 2\pi n)$. Because $\hat{\omega}_{l,n} = \mathcal{O}(\varepsilon^n e^{-\frac{na}{\varepsilon}})$ by the expansion (B.6), whereas $\hat{u}_{l,0}(x)$ are uniformly bounded in ε, we have

$$\begin{aligned} \sup_{x\in[0,2\pi]} |f(x)| \le \varepsilon e^{-\frac{a}{\varepsilon}}(F_+ + F_-), \quad F_+ = \sup_{x\in[0,2\pi]} |\hat{u}_{l,0}(x+2\pi)|, \\ F_- = \sup_{x\in[0,2\pi]} |\hat{u}_{l,0}(x-2\pi)|. \end{aligned} \tag{C.3}$$

Matching the two solutions at $x = a$ for $\phi(x)$ and $\phi'(x)$, we find that

$$A = \frac{1}{2}\left(C + \frac{\varepsilon\sqrt{\omega}}{\sqrt{1-\varepsilon^2\omega}}D\right) + \varepsilon e^{-\frac{a}{\varepsilon}}\tilde{A}, \quad B = \frac{1}{2}\left(C - \frac{\varepsilon\sqrt{\omega}}{\sqrt{1-\varepsilon^2\omega}}D\right) + \varepsilon e^{-\frac{a}{\varepsilon}}\tilde{B},$$

where $\tilde{A}$ and $\tilde{B}$ are uniformly bounded in $|\varepsilon| < \varepsilon_0$. As $\varepsilon \to 0$, the homogeneous solution is bounded only if $B = \varepsilon e^{-\frac{a}{\varepsilon}} B'$, where B' is a new parameter. This constraint results in the relation

$$C = \frac{\varepsilon\sqrt{\omega}}{\sqrt{1-\varepsilon^2\omega}}D + \varepsilon e^{-\frac{a}{\varepsilon}}\tilde{C},$$

where $\tilde{C}$ is uniformly bounded in $|\varepsilon| < \varepsilon_0$. As a result, we rewrite the solution (C.2) in the form

$$\hat{u}_{l,0} = \begin{cases} D\frac{\varepsilon\sqrt{\hat{\omega}_{l,0}}}{\sqrt{1-\varepsilon^2\hat{\omega}_{l,0}}} e^{\frac{\sqrt{1-\varepsilon^2\hat{\omega}_{l,0}}}{\varepsilon}(x-a)} + B'\varepsilon e^{-\frac{\sqrt{1-\varepsilon^2\hat{\omega}_{l,0}}}{\varepsilon}x}, & \forall x \in [0,a] \\ D\sin\sqrt{\hat{\omega}_{l,0}}(x-a) + D\frac{\varepsilon\sqrt{\hat{\omega}_{l,0}}}{\sqrt{1-\varepsilon^2\hat{\omega}_{l,0}}}\cos\sqrt{\hat{\omega}_{l,0}}(x-a), & \forall x \in [a, 2\pi] \end{cases} + \mathrm{O}(\varepsilon e^{-\frac{a}{\varepsilon}}). \tag{C.4}$$

The parameter D is fixed by the normalization condition $\|\hat{u}_{l,0}\|_{L^2(\mathbb{R})} = 1$, from which the property (4.4) on $[0, 2\pi]$ is proved.

Consider now the same ODE $(L - \omega)\phi = f(x)$ on $[2\pi, 4\pi]$. The explicit solution $\phi \equiv \phi_1$ is now written in the form

$$\phi_1(x) = \begin{cases} A_1 e^{\frac{\sqrt{1-\varepsilon^2\omega}}{\varepsilon}(x-2\pi-a)} + B_1 e^{-\frac{\sqrt{1-\varepsilon^2\omega}}{\varepsilon}(x-2\pi-a)} \\ \qquad - \frac{\varepsilon}{2\sqrt{1-\varepsilon^2\omega}} \int_{2\pi}^{a+2\pi} e^{-\frac{\sqrt{1-\varepsilon^2\omega}}{\varepsilon}|x-\xi|} f(\xi) d\xi, \quad \forall x \in [2\pi, 2\pi + a], \\ C_1 \cos\sqrt{\omega}(x - 2\pi - a) + D_1 \sin\sqrt{\omega}(x - 2\pi - a) - \int_{a+2\pi}^{4\pi} \frac{\sin\sqrt{\omega}|x-\xi|}{2\sqrt{\omega}} f(\xi) d\xi, \quad \forall x \in [2\pi + a, 4\pi]. \end{cases}$$

We have

$$\sup_{x\in[2\pi,4\pi]} |f(x)| \le \varepsilon e^{-\frac{a}{\varepsilon}} \left(1 + \sup_{x\in[0,2\pi]} |\hat{u}_{l,0}(x + 4\pi)| \right),$$

where we have used the bound (4.4). By matching the solution at $x = 2\pi + a$, we obtain the constraints on parameters of the solution:

$$A_1 = \frac{1}{2}\left(C_1 + \frac{\varepsilon\sqrt{\omega}}{\sqrt{1-\varepsilon^2\omega}} D_1 \right) + \varepsilon e^{-\frac{a}{\varepsilon}} \tilde{A}_1, \quad B_1 = \frac{1}{2}\left(C_1 - \frac{\varepsilon\sqrt{\omega}}{\sqrt{1-\varepsilon^2\omega}} D_1 \right) + \varepsilon e^{-\frac{a}{\varepsilon}} \tilde{B}_1,$$

where $\tilde{A}_1$ and $\tilde{B}_1$ are uniformly bounded in $|\varepsilon| < \varepsilon_0$. Now we apply the continuity conditions $\phi(2\pi) = \phi_1(2\pi)$ and $\phi'(2\pi) = \phi_1'(2\pi)$, which relate coefficients A_1 and B_1 to D:

$$\begin{aligned} A_1 e^{-\frac{a\sqrt{1-\varepsilon^2\omega}}{\varepsilon}} &= \frac{1 - 2\varepsilon^2\omega}{2(1-\varepsilon^2\omega)} D \Bigg[\sin\left[(2\pi - a)\sqrt{\omega}\right] + \frac{2\varepsilon\sqrt{\omega(1-\varepsilon^2\omega)}}{1 - 2\varepsilon^2\omega} \\ &\quad \times \cos\left[(2\pi - a)\sqrt{\omega}\right] \Bigg] + \varepsilon e^{-\frac{a}{\varepsilon}} F_1, \\ B_1 e^{\frac{a\sqrt{1-\varepsilon^2\omega}}{\varepsilon}} &= \frac{1}{2(1-\varepsilon^2\omega)} D \sin\left[(2\pi - a)\sqrt{\omega}\right] + \varepsilon e^{-\frac{a}{\varepsilon}} G_1, \end{aligned}$$

where F_1 and G_1 are uniformly bounded in $|\varepsilon| < \varepsilon_0$. If $\omega = \hat{\omega}_{l,0}$, the second equation implies that $B_1 = \varepsilon e^{-\frac{a}{\varepsilon}} B_1'$, such that

$$C_1 = \frac{\varepsilon\sqrt{\omega}}{\sqrt{1-\varepsilon^2\omega}} D_1 + \varepsilon e^{-\frac{a}{\varepsilon}} \tilde{C}_1,$$

where B_1' and $\tilde{C}_1$ are uniformly bounded in $|\varepsilon| < \varepsilon_0$. Substituting the expansion (B.6) into the algebraic equation (B.5), we find that, if $\omega = \hat{\omega}_{l,0}$, then $A_1 = \varepsilon F_1 + \mathrm{O}(\varepsilon^2 e^{-\frac{a}{\varepsilon}})$. Since F_1 is linear with respect to $\tilde{C}$ and $\tilde{C}$ is linear with respect to B', one can choose B' so that $F_1 = \mathrm{O}\left(\varepsilon e^{-\frac{a}{\varepsilon}}\right)$, after which

$$A_1 = \mathrm{O}\left(\varepsilon^2 e^{-\frac{a}{\varepsilon}}\right), \quad C_1 = \mathrm{O}\left(\varepsilon^2 e^{-\frac{a}{\varepsilon}}\right), \quad D_1 = \mathrm{O}\left(\varepsilon e^{-\frac{a}{\varepsilon}}\right).$$

Moreover, since

$$F_+ = \sup_{x\in[0,2\pi]} |\hat{u}_{l,0}(x+2\pi)| = \mathrm{O}\left(\varepsilon e^{-\frac{a}{\varepsilon}}\right),$$

it is also clear that $B' = \mathrm{O}\left(\varepsilon e^{-\frac{a}{\varepsilon}}\right)$. This construction proves the bound (4.5) on $[2\pi, 4\pi]$. Continuing the ODE analysis on the intervals $[2\pi n, 2\pi(n+1)]$ with $n \geq 2$, the bound (4.5) is extended for any $x \in [2\pi, 2\pi(n+1)]$. It is left for a reader's exercise to use the same method to prove the bound (4.5) for $x < 0$.

D. Poincaré Mappings

We review here the Poincaré map for the second-order equation (1.1) with a 2π-periodic coefficient V, in comparison with the second-order difference equation (1.2). Denote $\phi(2\pi n) = \phi_n$ and $\phi'(2\pi n) = \psi_n$, $\forall n \in \mathbb{Z}$ and consider the initial value problem for the second-order equation (1.1) on the interval $[2\pi n, 2\pi(n+1)]$ for a fixed $n \in \mathbb{Z}$. By the theorem on local existence and smoothness of solutions of the initial-value problem, there exists a continuously differentiable solution $\phi(x)$ on $[2\pi n, 2\pi(n+1)]$ if the function V is piecewise continuous and $\delta_0 := |\phi_n| + |\psi_n|$ is sufficiently small. The Poincaré map is then defined in the form

$$\mathbf{u}_{n+1} = \mathbf{P}(\mathbf{u}_n), \quad \mathbf{u}_n = \begin{pmatrix} \phi_n \\ \psi_n \end{pmatrix}, \quad \forall n \in \mathbb{Z}, \tag{D.1}$$

where $\mathbf{P} : \mathbb{C}^2 \mapsto \mathbb{C}^2$ is a continuously differentiable function. On one hand, the difference map (D.1) is *exactly* equivalent to the second-order equation (1.1) with the periodic function V. On the other hand, the Poincaré map $\mathbf{P}(\mathbf{u}_n)$ is *generally different* from the second-order difference equation (1.2). We will show that the Poincaré map (D.1) reduces to the scalar equation (1.2) in the *near-linear* limit, when the cubic term $|\phi_n|^2\phi_n$ is small compared to the second-order difference term $\phi_{n+1} + \phi_{n-1}$. This limit differs from the domain of applicability of the lattice equation (1.2) justified in Theorem 1, where all terms are considered to be of the same order.

In the linear theory, $\mathbf{P}(\mathbf{u}_n) = A\mathbf{u}_n$, where A is a monodromy matrix with the elements a_{ij} for $1 \leq i, j \leq 2$. Since the Wronskian determinant of the second-order ODE (1.1) is constant in x, the coefficients satisfy the constraint $\det(A) = a_{11}a_{22} - a_{12}a_{21} = 1$. Eliminating ψ_n from the system (D.1) with $\mathbf{P}(\mathbf{u}_n) = A\mathbf{u}_n$, we obtain that

$$\phi_{n+1} + \phi_{n-1} = \Delta(\omega)\phi_n, \qquad \forall n \in \mathbb{Z}, \tag{D.2}$$

where $\Delta(\omega) = \mathrm{tr}(A) = a_{11} + a_{22}$. The Floquet theory follows immediately from the linear second-order map (D.2) since the spectral bands are found from solutions of the equation $\Delta(\omega) = 2\cos(2\pi k)$ for all $k \in \mathbb{T}$. It is proved in [7] that this equation admits infinitely many solutions, which can be enumerated by the index $l \in \mathbb{N}$ and ordered as follows: $\omega_1(k) \leq \omega_2(k) \leq \cdots \leq \omega_l(k) \leq \cdots$ for any $k \in \mathbb{T}$.

Consider the nonlinear Poincaré map (D.1) in the limit where the cubic terms are small, i.e. when $\sup_{x\in[2\pi n, 2\pi(n+1)]}\left(|\phi(x)| + |\phi'(x)|\right) := \delta$ is sufficiently small. Expanding $\mathbf{P}(\mathbf{u}_n)$ into the Taylor series in $\mathbf{u}_n$ and eliminating ψ_n from the second equation by using the near-identity transformations, we obtain the perturbed second-order difference map,

$$\begin{aligned}\phi_{n+1} + \phi_{n-1} - \Delta(\omega)\phi_n = \sigma \Big[& \alpha_1 |\phi_n|^2 \phi_n + \alpha_2 |\phi_n|^2 (\phi_{n+1} + \phi_{n-1}) + \alpha_3 \phi_n^2 (\bar{\phi}_{n+1} + \bar{\phi}_{n-1}) \\ & + \alpha_4 (|\phi_{n+1}|^2 + |\phi_{n-1}|^2)\phi_n + \alpha_5 (\bar{\phi}_{n+1}\phi_{n-1} + \phi_{n+1}\bar{\phi}_{n-1})\phi_n \\ & + \alpha_6 (\phi_{n+1}^2 + \phi_{n-1}^2)\bar{\phi}_n + \alpha_7 \phi_{n+1}\phi_{n-1}\bar{\phi}_n \\ & + \alpha_8 (|\phi_{n+1}|^2 \phi_{n+1} + |\phi_{n-1}|^2 \phi_{n-1}) + \alpha_9 (\phi_{n+1}^2 \bar{\phi}_{n-1} + \phi_{n-1}^2 \bar{\phi}_{n+1}) \\ & + \alpha_{10} (|\phi_{n+1}|^2 \phi_{n-1} + |\phi_{n-1}|^2 \phi_{n+1}) \Big], \qquad \forall n \in \mathbb{Z}, \end{aligned} \tag{D.3}$$

where $(\alpha_1, \alpha_2, \dots, \alpha_{10})$ are some coefficients. The perturbed equation (D.3) contains all cubic terms, which preserve the gauge invariance and reversibility of the original ODE (1.1), such that if $\{\phi_n\}_{n\in\mathbb{Z}}$ is a solution, then $\{\phi_n e^{i\theta}\}_{n\in\mathbb{Z}}$ and $\{\phi_{-n}\}_{n\in\mathbb{Z}}$ are also solutions for any $\theta \in \mathbb{R}$. The actual values of the coefficients of the cubic terms depend on the potential function V. See [15] for analysis of localized solutions of the second-order difference equation (D.3).

Proposition 4. *Let $\{\phi_n\}_{n\in\mathbb{Z}}$ be a real-valued solution of the lattice equation (D.3) such that $\|\vec{\phi}\|_{l^2(\mathbb{Z})}$ is small. There exists a near-identity transformation*

$$\phi_n = \varphi_n + \sigma B(\omega)\varphi_n^3 + \mathrm{O}\left(\|\vec{\varphi}\|_{l^2(\mathbb{Z})}^5\right), \tag{D.4}$$

which transforms the lattice equation (D.3) to the canonical form

$$\varphi_{n+1} + \varphi_{n-1} - \Delta(\omega)\varphi_n = \sigma A(\omega)\varphi_n^3 + \mathrm{O}\left(\|\vec{\varphi}\|_{l^2(\mathbb{Z})}^5\right), \tag{D.5}$$

for some constants $A(\omega)$ and $B(\omega)$.

Proof. Let $\{\phi_n\}_{n\in\mathbb{Z}}$ be a real-valued solution of the lattice equation (D.3), such that the right-hand-side can be rewritten in the form

$$\begin{aligned}\beta_1 \phi_n^3 + \beta_2 \phi_n^2 (\phi_{n+1} + \phi_{n-1}) + \beta_3 (\phi_{n+1}^2 + \phi_{n-1}^2)\phi_n + \beta_4 \phi_{n+1}\phi_{n-1}\phi_n \\ + \beta_5 (\phi_{n+1}^3 + \phi_{n-1}^3) + \beta_6 \phi_{n+1}\phi_{n-1}(\phi_{n+1} + \phi_{n-1}),\end{aligned}$$

where $\beta_1 = \alpha_1$, $\beta_2 = \alpha_2 + \alpha_3$, $\beta_3 = \alpha_4 + \alpha_6$, $\beta_4 = 2\alpha_5 + \alpha_7$, $\beta_5 = \alpha_8$ and $\beta_6 = \alpha_9 + \alpha_{10}$. Substituting the leading-order equation (D.2) to the terms above, we obtain

$$\begin{aligned}&\left(\beta_1 + \Delta\beta_2 + \frac{1}{3}\Delta^2(\beta_3 + \beta_4) + \frac{1}{3}\Delta^3 \beta_6\right)\phi_n^3 \\ &\quad + \left(\beta_5 - \frac{1}{3}\beta_6 - \frac{1}{3\Delta}(\beta_4 - 2\beta_3)\right)(\phi_{n+1}^3 + \phi_{n-1}^3).\end{aligned}$$

Using the near-identity transformation (D.4) with $B(\omega) = \beta_5 - \frac{1}{3}\beta_6 - \frac{1}{3\Delta}(\beta_4 - 2\beta_3)$, we arrive to the canonical form (D.5) with $A(\omega) = \beta_1 + \Delta\beta_2 + \frac{1}{3}\Delta^2(\beta_3 + \beta_4) + \frac{1}{3}\Delta^3\beta_6 + \Delta B(\omega)$. □

The canonical form (D.5) does not hold when the potential function V is defined by Assumption 2 for sufficiently small ε. In the lattice equation (1.2) justified by Theorem 1, the cubic term $|\phi_n|^2\phi_n$ can not be considered to be small compared to the second-order difference term $\phi_{n+1}+\phi_{n-1}$, which implies that $\Delta(\omega)$ in the canonical form (D.5) is large. Compared to the Poincaré map (D.1), the Wannier decomposition replaces the second-order equation by the lattice system with infinite coupling between lattice sites, which is reduced *asymptotically* to the second-order difference map. Notice that the analysis above implies that the lattice system for coefficients of the Wannier functions must be satisfied *exactly* by the second-order Poincaré map (D.1) after a nonlocal transformation.

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