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Localized Modes of the Linear Periodic Schrödinger Operator with a Nonlocal Perturbation

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Abstract

We consider the existence of localized modes corresponding to eigenvalues of the periodic Schrödinger operator $-\partial_x^2 + V(x)$ with an interface. The interface is modeled by a jump either in the value or the derivative of $V(x)$ and, in general, does not correspond to a localized perturbation of the perfectly periodic operator. The periodic potentials on each side of the interface can, moreover, be different. As we show, eigenvalues can only occur in spectral gaps. We pose the eigenvalue problem as a C^1 gluing problem for the fundamental solutions (Bloch functions) of the second order ODEs on each side of the interface. The problem is thus reduced to finding intersections of the ratio functions $R_\pm = \frac{\psi'_\pm(0)}{\psi_\pm(0)}$, where $\psi_\pm$ are those Bloch functions that decay on the respective half-lines. These ratio functions are analyzed with the help of the Prüfer transformation. The limit values of $R_\pm$ at band edges depend on the ordering of Dirichlet and Neumann eigenvalues at gap edges. We show that the ordering can be determined in the first two gaps via variational analysis for potentials satisfying certain monotonicity conditions. Numerical computations of interface eigenvalues are presented to corroborate the analysis.

1 Introduction

Localization for perturbed periodic Schrödinger operators $L = -\Delta + V_0(x) + W(x)$, where $V_0(x)$ is periodic in $x \in \mathbb{R}^n, n \in \mathbb{N}$ is a classical problem traditionally treated by spectral theory. Most commonly it is studied for perturbations $W(x)$ that are either compactly supported [6, 1, 3] or fast decaying, e.g. $W \in L^{n/2}(\mathbb{R}^n)$, see [19, 1]. Both of these scenarios can lead to eigenvalues of L and thus to localization. Potentials W describing random perturbation also yield eigenvalues due to Anderson localization [12, 17]. We investigate localization in the one-dimensional case $n = 1$ due to the presence of deterministic interfaces which cannot be represented as localized perturbations of $-\partial_x^2 + V_0(x)$. Such an interface typically arises, for instance, when $W(x)$ is periodic on one side of the interface and vanishes on the other side (we assume commensurability of the periods of W and V_0 to preserve periodicity on each side of the interface). This topic has been previously studied mainly by E. Korotyaev via spectral theory [13, 14]. We, on the other hand, use the properties of the fundamental solutions of the 1D spectral problems of the periodic operators corresponding to each side of the interface and pose the eigenvalue problem as a C^1-gluing problem for the decaying Floquet-Bloch solutions from either interface side. This approach allows us to provide some concrete conditions on V_0 and the perturbation W directly (without conditions on the spectrum of $-\partial_x^2 + V_0(x)$) that ensure eigenvalue existence in semi-infinite and the first finite gap of the continuous spectrum of L. Our approach is also arguably conceptually simpler than that of [13, 14].

In detail, within the framework of the eigenvalue problem

$$L\psi = \lambda\psi, \qquad L = -\partial_x^2 + V(x),\ x \in \mathbb{R} \tag{1.1}$$

we study the following two interface problems. Firstly, an *interface made of two even periodic potentials*

$$V(x) = \chi_{\{x<0\}}V_-(x) + \chi_{\{x\geq 0\}}V_+(x), \tag{1.2}$$

with periods $d_\pm > 0$, i.e., $V_\pm(x + d_\pm) = V_\pm(x)$, $V_\pm(-x) = V_\pm(x)$. Secondly, an *interface made of dislocated even periodic potentials*

$$V(x) = \chi_{\{x<0\}}V_0(x + s) + \chi_{\{x\geq 0\}}V_0(x + t), \tag{1.3}$$

with period $d > 0$, i.e., $V_0(x + d) = V_0(x)$ and $V_0(-x) = V_0(x)$, and dislocation parameters $t, s \in \mathbb{R}$. Here χ is the characteristic function. Unless otherwise stated, the potentials $V_\pm$ and V_0 are continuous and hence bounded.

One of the simplest examples of the interface (1.2) is the *additive interface*

$$V_-(x) = V_0(x),\ V_+(x) = V_0(x) + \alpha, \quad V_0(x + d) = V_0(x),\ V_0(-x) = V_0(x), \quad \alpha \in \mathbb{R},\ d > 0, \tag{1.4}$$

generated by merely changing the average value of the potential on one half of the real axis. This example is studied in more detail in Section 3.1.1 since the conditions on eigenvalue existence become rather specific in this particular case.

Schematic pictures of the two potentials (1.2) and (1.3) are displayed in Figure 1.

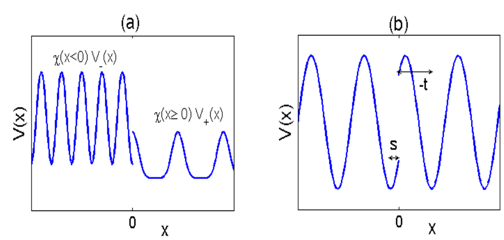

Figure 1: A cartoon of example potentials V for the case (1.2) in (a) and (1.3) in (b).

Equation (1.1) finds applications in many fields of natural science. Perhaps most notably it describes the wave function of an electron in a one dimensional crystal. It also directly applies to the description of light propagating transversally to the direction of periodicity of a non-dispersive, lossless, linear one-dimensional photonic crystal. Suppose the refractive index n^2 varies periodically in the $x-$direction and its mean has a jump at $x = 0$, such that $n = \sqrt{1 + W(x)}$, $W(x) = -\frac{c^2}{\omega^2}V(x)$. We assume the following form of the electric field,

$$\vec{E} = (0, \psi(x), 0)^T e^{i(kz-\omega t)},$$

such that the field is polarized in the $y-$direction, the waves propagate in the $z-$ direction and the $x-$profile is stationary. Then Maxwell's equations exactly reduce to

$$(\partial_x^2 - k^2)\psi + \frac{\omega^2}{c^2}(1 + W(x))\psi = 0.$$

With $V(x) = -\frac{\omega^2}{c^2}W(x)$ and setting $\lambda = \frac{\omega^2}{c^2} - k^2$, we recover (1.1).

Another example of an application of (1.1) is the description of matter waves in one dimensional Bose-Einstein condensates loaded onto an optical lattice [4]. The density of a condensate is described by the wavefunction u governed by the Gross-Pitaevskii equation [4, 9, 15]

$$i\hbar\partial_t u + \frac{\hbar^2}{2m}\partial_x^2 u - W(x)u - g|u|^2 u = 0,$$

where, in our setting, $W(x)$ is periodic but has a jump in its mean at $x = 0$. Here $\hbar$ is Planck's constant, m is the boson mass, W is the potential induced by the optical lattice and g is the scattering length. In the linear regime, $g = 0$, stationary waves $e^{-i\lambda t}\psi(x)$ obey (after rescaling) equation (1.1).

The rest of the paper is organized as follows. In Section 2 we review the needed facts on the spectral properties of the interface-free periodic Schrödinger operators with an even potential including the problem of ordering of spectral band edges according to even/odd symmetry of the Bloch functions. Section 3.1 discusses the interface (1.2) and introduces the main tools of our analysis, namely the C^1-matching condition and the Prüfer transformation. The theory is then applied to the additive interface example (1.4) and numerical computations of point spectrum are performed. In Section 3.2 we analyze the dislocation problem (1.3) for the cases $s = -t$ and $s = 0$ using the same tools as in Section 3.1 plus differential inequalities and variational methods. Numerical examples are, once again, provided.

2 Spectrum of the Interface-Free Problem

We review, first, some well known results on the spectrum and the eigenfunctions of the interface-free operator $L_0 = -\partial_x^2 + V_0(x)$, where $V_0(x + d) = V_0(x)$ is continuous and $V_0(-x) = V_0(x)$. Good sources on the theory of the periodic Schrödinger operator are [7, 16].

L_0 has a purely continuous spectrum (see Theorem XIII.90 in [16]) consisting of bands $[s_{2n-1}, s_{2n}]$ so that

$$\sigma(L_0) = \bigcup_{n\in\mathbb{N}} [s_{2n-1}, s_{2n}],$$

where $s_n \in \mathbb{R}$ and $s_{2n-1} < s_{2n} \leq s_{2n+1}$ [7]. When $s_{2n+1} > s_{2n}$, we say that $\sigma(L_0)$ has the finite gap $G_n := (s_{2n}, s_{2n+1})$. Clearly, $\sigma(L_0)$ has also the semi-infinite gap $G_0 := (-\infty, s_1)$. According to Floquet theory [7] the spectrum $\sigma(L_0)$ can be easily found via the use of the monodromy matrix of the second order ODE $L_0\psi = \lambda\psi$. Figure 2 presents the numerically computed spectrum of the operator L_0 with $V_0(x) = \sin^2(\pi x/10)$.

The ODE $L_0\psi = \lambda\psi$ has two linearly independent solutions, so called, Bloch functions. For $\lambda \notin \partial\sigma(L_0)$ they are of the form

$$\psi_1(x;\lambda) = p_1(x;\lambda)e^{-ik(\lambda)x}, \quad \psi_2(x;\lambda) = p_2(x;\lambda)e^{ik(\lambda)x}, \tag{2.1}$$

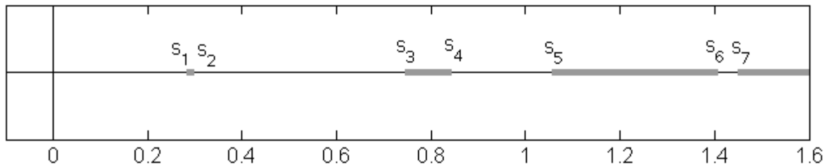

Figure 2: Spectrum of L_0 for $V_0(x) = \sin^2(\pi x/10)$.

where $k \in \mathbb{R}$ if $\lambda \in \text{int}(\sigma(L_0))$ and $k \in i\mathbb{R} \setminus \{0\}$ if $\lambda \in \mathbb{R} \setminus \sigma(L_0)$, and $p_{1,2}(x; \lambda)$ are real-values and $2d-$periodic in x. In fact, $p_{1,2}$ are either $d-$periodic of $d-$anti-periodic. If $\lambda \in \partial(\sigma(L_0))$, the Bloch functions are of the form

$$\psi_1(x; \lambda) = p_1(x; \lambda), \quad \psi_2(x; \lambda) = p_2(x; \lambda) + x p_1(x; \lambda), \tag{2.2}$$

where again $p_{1,2}(x; \lambda)$ are $2d-$periodic in x. In all cases we assume $\|p_j\|_{L^\infty(0,2d)} = 1$ for $j = 1, 2$.

The evenness of the potential $V_0(x)$ and the fact that only one linearly independent bounded Bloch function (namely $\psi_1(x; \lambda) = p_1(x; \lambda)$) exists at any $\lambda \in \partial(\sigma(L_0))$ imply that this solution must be even or odd and hence it satisfies at the boundary-points $x = 0$ and $x = d$ either Dirichlet- or Neumann-boundary conditions. For $k \in \mathbb{N}$ let (μ_k, ζ_k) denote the k-th Dirichlet eigenpair of L_0 on $[0, d]$ satisfying $\zeta_k(0) = \zeta_k(d) = 0$ and let (ν_k, η_k) be the k-th Neumann eigenpair of L_0 on $[0, d]$ such that $\eta_k'(0) = \eta_k'(d) = 0$. The following lemma may be well known, cf. [7], Theorem 1.3.4.

Lemma 2.1. *For the first gap edge we have $s_1 = \nu_1$. If $k \geq 1$ and if $s_{2k} \neq s_{2k+1}$ then $s_{2k} = \min\{\mu_k, \nu_{k+1}\}$, $s_{2k+1} = \max\{\mu_k, \nu_{k+1}\}$. Moreover, the following properties of the eigenfunctions are known (note that the even/odd-property applies with respect to reflection around $\frac{d}{2}$):*

	eigenvalue	eigenfunction properties		
Dirichlet	μ_{2k-1}	even	$d-$anti-periodic	$\zeta_{2k-1}'(\frac{d}{2}) = 0$
Dirichlet	μ_{2k}	odd	$d-$periodic	$\zeta_{2k}(\frac{d}{2}) = 0$
Neumann	ν_{2k-1}	even	$d-$periodic	$\eta_{2k-1}'(\frac{d}{2}) = 0$
Neumann	ν_{2k}	odd	$d-$anti-periodic	$\eta_{2k}(\frac{d}{2}) = 0$

Remark. Note that $\lambda \in G_n$ can never be a Dirichlet or Neumann eigenvalue since any corresponding eigenfunction could be extended to a bounded solution of $L_0\psi = \lambda\psi$ on $\mathbb{R}$ by reflection and periodic extension. Such nontrivial solutions cannot exist for $\lambda \in G_n$ by (2.1) and (2.2).

As we show in Sections 3.1 and 3.2, ordering between the Dirichlet and Neumann eigenvalues μ_k and ν_{k+1} plays an important role for existence of interface eigenvalues. It is, however, known that all orderings are in general possible, i.e., for any given ordering of the Dirichlet and Neumann eigenvalues a corresponding even potential V_0 exists, see Theorem 3 in [8]. Nevertheless, the following lemma provides an ordering of low eigenvalues under some monotonicity assumptions on the potential V_0.

Lemma 2.2. *(a) If V_0 is strictly increasing on $[0, \frac{d}{2}]$, then $\nu_2 < \mu_1$. Every Neumann eigenfunction corresponding to ν_2 is strictly monotone on $[0, d]$ and odd with respect to $\frac{d}{2}$.*

(b) *If V_0 is strictly decreasing on $[0, \frac{d}{2}]$, then $\mu_1 < \nu_2$. Every Dirichlet eigenfunction corresponding to μ_1 is strictly monotone on $[0, \frac{d}{2}]$ and even with respect to $\frac{d}{2}$.*

The proof is based on the following result.

Lemma 2.3. *Consider a potential $V_0 \in L^\infty(a,b)$ (not necessarily periodic, even or continuous) and let κ_{ND} be the first eigenvalue of $L_0 = -\partial_x^2 + V_0$ on $[a,b]$ with the boundary condition $u'(a) = 0 = u(b)$, whereas κ_{DN} denotes the first eigenvalue of the same differential operator but with boundary conditions $u(a) = 0 = u'(b)$. Then*

$$\min\{\kappa_{ND}, \kappa_{DN}\} = \min\left\{\int_a^b v'^2 + V_0(x)v^2\,dx : v \in H^1(a,b) \text{ has a zero and } \int_a^b v^2\,dx = 1\right\}. \quad (2.3)$$

Moreover, if V_0 is strictly increasing on $[a,b]$ then $\kappa_{ND} < \kappa_{DN}$ and any eigenfunction for κ_{ND} with $u(a) = 1$ is strictly decreasing on $[a,b]$. If V_0 is strictly decreasing on $[a,b]$ then $\kappa_{DN} < \kappa_{ND}$ and any eigenfunction for κ_{DN} with $u'(a) = 1$ is strictly increasing on $[a,b]$.

Proof. The proof is inspired by a similar result in [2]. Note first that the set on which the minimization is performed, is weakly closed in $H^1(a,b)$ due to the compact embedding $H^1(a,b) \to C[a,b]$. Hence a minimizer, denoted u, of the right-hand side of (2.3) exists. Let us also denote the value of the minimum by κ. The proof is now divided into five steps:

Step 1: u has exactly one zero on $[a,b]$. Since u possesses at least one zero in $[a,b]$ let it be denoted by x_0 and let $H_{x_0} = \{v \in H^1(a,b) : v(x_0) = 0\}$. Clearly u is then the minimizer of

$$\min\left\{\int_a^b v'^2 + V_0(x)v^2\,dx : v \in H_{x_0}, \int_a^b v^2\,dx = 1\right\}.$$

and therefore u satisfies the Euler-Lagrange equation

$$-u'' + V_0(x)u = \kappa u \text{ in } (a, x_0) \cup (x_0, b) \quad (2.4)$$

with boundary condition

$$u'(a) = u(x_0) = u'(b) = 0 \quad (2.5)$$

where in case $x_0 \in \{a,b\}$ one of the two Neumann conditions is dropped. Note that

$$\int_a^b u'v' + V_0(x)uv\,dx = \kappa \int_a^b uv\,dx \text{ for all } v \in H_{x_0}. \quad (2.6)$$

Now assume for contradiction that u has a second zero $x_1 \neq x_0$. Then (2.6) holds also for all $v \in H_{x_1}$ and since $H^1(a,b) = H_{x_1} \oplus H_{x_2}$ we find that (2.6) holds for all $v \in H^1(a,b)$, i.e., u is a Neumann-eigenfunction. The same applies for $|u|$, which is also a minimizer of (2.3). But then u must be the first Neumann-eigenfunction of L_0 on (a,b) and it therefore has no zero on $[a,b]$. This contradiction shows that u has exactly one zero in $[a,b]$.

Step 2: κ is strictly less than the second Neumann-eigenvalue ν_2 on $[a,b]$. Since the second Neumann eigenfunction η_2 has one zero in $[a,b]$ we find $\kappa \leq \nu_2$. Suppose for contradiction that $\kappa = \nu_2$. Testing the equation for η_2 with $\eta_2^+ = \max\{\eta_2, 0\}$ we obtain

$$\int_a^b ({\eta_2^+}')^2 + V_0(x)(\eta_2^+)^2\,dx = \nu_2 \int_a^b (\eta_2^+)^2\,dx$$

and thus η_2^+ is a minimizer for (2.3) and must have a unique zero by Step 1. However, clearly η_2^+ has a continuum of zeros. Therefore we can conclude that $\kappa < \nu_2$.

Step 3: u has its unique zero either at $x = a$ or at $x = b$. If we suppose for contradiction that the unique zero x_0 lies in the open interval (a, b) then we obtain the Euler-Lagrange equation (2.4) with boundary condition (2.5). By rescaling the minimizer u suitably on $[a, x_0]$ we can achieve that the rescaled function u is a C^1-function on $[a, b]$ solving the equation (2.4) pointwise a.e. on (a, b). Hence, the rescaled function u is a Neumann-eigenfunction with one interior zero, i.e. $\kappa = \nu_2$ in contradiction to Step 2.

Now the claim of the lemma about the value of the minimization is immediate.

Step 4: ordering of κ_{ND}, κ_{DN}. We are using the following rearrangement result of Hardy, Littlewood, Pólya [10]. Let v, w be non-negative and measurable on $[a, b]$. If $v^\sharp, w^\sharp$ are the increasing rearrangements of v, w then $\int_a^b vw\,dx \le \int_a^b v^\sharp w^\sharp\,dx$. Moreover, if v is strictly increasing then equality holds if and only if $w = w^\sharp$. A similar statement holds for the decreasing rearrangements v^*, w^*. Note, that the non-negativity of v, w can be replaced by boundedness.

A simple corollary of the Hardy, Littlewood, Pólya inequality is the following: suppose $V = V^\sharp$ is strictly increasing and both V and w are bounded. Then

$$\int_a^b V w^*\,dx \le \int_a^b V w\,dx \tag{2.7}$$

with equality if and only if $w = w^*$. The proof follows immediately from the observation that $(-w)^\sharp = -w^*$.

Let V_0 be strictly increasing on $[a, b]$. Suppose for contradiction that $\kappa_{DN} \le \kappa_{ND}$ and let u be an eigenfunction corresponding to κ_{DN}. We may assume u to be non-negative, since $|u|$ is also a minimizer of the corresponding variational problem and κ_{DN} is a simple eigenvalue. Let now u^* be the decreasing rearrangement of u on $[a, b]$ and note that $(u^2)^* = (u^*)^2$. Since the decreasing rearrangement lowers the Dirichlet energy, cf. Kawohl [11], we obtain by (2.7) applied to V_0 and u^2 the relations

$$\int_a^b (u^*)^2\,dx = \int_a^b u^2\,dx = 1, \qquad \int_a^b (u^{*\prime})^2 + V_0(x)(u^*)^2\,dx \le \int_a^b (u')^2 + V_0(x)u^2\,dx. \tag{2.8}$$

Therefore u^*, which satisfies $u^*(b) = 0$, is also a minimizer of (2.3) and hence equality has to hold in (2.8). But since V_0 is strictly increasing the sharp form of (2.7) implies that $u = u^*$ which by $u(a) = 0$ implies the contradiction that u must be identically zero. Hence $\kappa_{ND} < \kappa_{DN}$. Moreover, (2.8) shows that any non-negative minimizer u for κ_{ND} satisfies $u = u^*$, i.e., u is decreasing, and by using the differential equation for u and the strict monotonicity of V_0 it is easy to see that in fact u is strictly decreasing.

If V_0 is strictly decreasing on $[a, b]$ then a similar argument based on replacing u by its increasing rearrangement shows that $\kappa_{DN} < \kappa_{ND}$. □

Proof of Lemma 2.2. Consider the Dirichlet-eigenfunction ζ_1. By Lemma 2.1 its restriction to $[0, \frac{d}{2}]$ is the eigenfunction for κ_{DN} of Lemma 2.3. Likewise, the restriction of η_2 to$[0, \frac{d}{2}]$ is the eigenfunction for κ_{ND}. Hence $\mu_1 = \kappa_{DN}$ and $\nu_2 = \kappa_{ND}$. The statements (a) and (b) then follow from Lemma 2.3. □

3 Interface Problems

We investigate next the existence of eigenvalues of L in (1.1) for the interface potentials (1.2) and (1.3). These examples fall into a larger class of potentials, namely $V(x) = \chi_{\{x<0\}}V_1(x) + \chi_{\{x\geq 0\}}V_2(x)$, where $V_{1,2}(x+d_{1,2}) = V_{1,2}(x)$ for some $d_{1,2} \geq 0$ but where $V_{1,2}$ may not necessarily be even in x. Clearly, all solutions of $(-\partial_x^2 + V(x))\psi = \lambda\psi$ are

$$\psi(x) = \chi_{\{x<0\}}\psi_-(x) + \chi_{\{x\geq 0\}}\psi_+(x),$$

where $\psi_\pm$ are Bloch functions of $(-\partial_x^2 + V_{1,2}(x))\psi = \lambda\psi$ respectively. As decaying Bloch functions $\psi_\pm$ exist only in spectral gaps of $-\partial_x^2 + V_{1,2}(x)$ respectively, eigenvalues of L can exist only within intersections of the gaps of $\sigma(-\partial_x^2 + V_1(x))$ and $\sigma(-\partial_x^2 + V_2(x))$. *No embedded eigenvalues of L thus exist.*

3.1 Point Spectrum for Interfaces Made of Even Potentials

The eigenvalue problem (1.1) with (1.2) can be viewed as the system

$$\begin{aligned} L_-\psi &:= -\partial_x^2\psi + V_-(x)\psi = \lambda\psi \quad \text{for } x<0,\\ L_+\psi &:= -\partial_x^2\psi + V_+(x)\psi = \lambda\psi \quad \text{for } x\geq 0 \end{aligned} \tag{3.1}$$

coupled by the the C^1-matching conditions

$$\psi(0-) = \psi(0+) \qquad \text{and} \qquad \psi'(0-) = \psi'(0+). \tag{3.2}$$

As stated in Section 1, the functions $V_\pm(x)$ are continuous, even and $d_\pm$-periodic.

Based on the knowledge of the fundamental solutions in (2.1), (2.2) we conclude that an L^2-integrable solution of (1.1) with (1.2) can only exist if λ lies in the intersection of the resolvent sets, i.e. in the intersection of the spectral gaps of L_- and L_+, i.e. if $\lambda \in G_n^+ \cap G_m^-$ for some $n, m \in \mathbb{N}\cup\{0\}$, where $G_n^\pm$ is the n-th spectral gap of $L_\pm$ respectively.

For $\lambda \in G_n^+ \cap G_m^-$ with some $n, m \geq 0$, any localized eigenfunction ψ of L, therefore, has to be of the form

$$\psi(x;\lambda) = \psi_-(x;\lambda)\chi_{\{x<0\}} + \psi_+(x;\lambda)\chi_{\{x\geq 0\}},$$

where we set

$$\psi_\pm(x;\lambda) = p_\pm(x;\lambda)e^{\mp\kappa(\lambda)x} \tag{3.3}$$

with $\kappa(\lambda) > 0$ and $p_\pm(x;\lambda)$ being $2d_\pm$−periodic in x. The functions $p_\pm$ are restrictions of either p_1 or p_2 in (2.1) with $V_0 = V_\pm$ to the half-line $\mathbb{R}_\pm$ respectively.

An important remark is that, due to the linearity of the problem, the matching conditions (3.2) together with an appropriate scaling are equivalent to

$$R_+(\lambda) = R_-(\lambda), \qquad \text{where} \qquad R_\pm(\lambda) = \frac{\psi_\pm'(0;\lambda)}{\psi_\pm(0;\lambda)} \tag{3.4}$$

and the prime denotes differentiation in x.

We determine existence of solutions to (3.4) via the intermediate value theorem and by monotonicity of the functions $R_\pm(\lambda)$. The monotonicity then also implies uniqueness.

Lemma 3.1. *Within each gap G_n^+ and $G_n^-, n \geq 0$, the functions R_+ and R_- are continuous functions of $\lambda \in G_n^{\pm}$, which are strictly increasing and decreasing respectively.*

Proof. Let us start with the proof for $R_+(\lambda)$. Under the Prüfer transformation, cf. Coddington, Levinson [5]

$$\psi_+(x;\lambda) = \rho(x;\lambda)\sin(\theta(x;\lambda)), \qquad \psi_+'(x;\lambda) = \rho(x;\lambda)\cos(\theta(x;\lambda)),$$

the equation $L_+\psi_+ = \lambda\psi_+$ becomes

$$\begin{aligned}\theta' &= 1 + (\lambda - V_+(x) - 1)\sin^2(\theta),\\ \rho' &= -\rho(\lambda - V_+(x) - 1)\sin(\theta)\cos(\theta),\end{aligned}$$

where the prime denotes differentiation in x. Clearly, θ and ρ are continuous functions of both variables $x \in \mathbb{R}$ and $\lambda \in G_n^+$ and since $R_+(\lambda) = \cot(\theta(0;\lambda))$, the function $R_+(\lambda)$ is continuous in λ provided $\psi_+(0;\lambda)$ has no zero in the interior of G_n. Note that if $\psi_+(0;\lambda) = 0$ then by evenness of V_0 and the reflection symmetry of the problem $L_+\psi_+ = \lambda\psi_+$, the solution $\psi_+(x;\lambda)$ defined in (3.3) on $x \geq 0$ could be extended to a solution on $x \in \mathbb{R}$ via $\psi_+(-x;\lambda) = -\psi_+(x;\lambda)$. This solution would decay exponentially at both infinities and λ would, thus, be an eigenvalue of L_+, which is impossible. Hence continuity of $R_+(\lambda)$ is proven.

Now let us prove the monotonicity. Due to the form of ψ_+, see (3.3), we have

$$\rho(2d) = \sqrt{(\psi_+(2d))^2 + (\psi_+'(2d))^2} = e^{-2d\kappa}\rho(0). \tag{3.5}$$

Define now $z(x) := \frac{\partial\theta}{\partial\lambda}(x;\lambda)$. The function z satisfies $z' = z(\lambda - V_+(x) - 1)2\sin(\theta)\cos(\theta) + \sin^2(\theta) = -2\frac{\rho'}{\rho}z + \sin^2(\theta)$. Therefore,

$$z(x) = \left(\frac{\rho(0;\lambda)}{\rho(x;\lambda)}\right)^2 z(0) + \int_0^x \left(\frac{\rho(t;\lambda)}{\rho(x;\lambda)}\right)^2 \sin^2(\theta(t;\lambda))\,dt. \tag{3.6}$$

Because $\cot(\theta) = \frac{\psi_+'}{\psi_+}$, and due to the periodicity $\frac{\psi_+'(x+2d;\lambda)}{\psi_+(x+2d;\lambda)} = \frac{\psi_+'(x;\lambda)}{\psi_+(x;\lambda)}$, we have $\theta(2d;\lambda) = \theta(0;\lambda) + m\pi$, where due to continuity the value $m \in \mathbb{Z}$ is independent of λ.[1] Hence, $z(2d;\lambda) = z(0;\lambda)$. Using (3.5) and (3.6), we thus obtain

$$z(0) = z(2d) = e^{4d\kappa}z(0) + \int_0^{2d} \left(\frac{\rho(t;\lambda)}{\rho(2d;\lambda)}\right)^2 \sin^2(\theta(t;\lambda))\,dt. \tag{3.7}$$

Because $\kappa > 0$, we get $z(0) < 0$ and conclude that $\theta(0;\lambda)$ is strictly decreasing throughout G_n^+. Therefore, $R_+(\lambda) = \cot(\theta(0;\lambda))$ is strictly increasing with respect to λ throughout G_n^+.

In order to prove strict monotonicity of $R_-(\lambda)$, note that (3.5) is replaced by $\rho(-2d) = e^{-2d\kappa}\rho(0)$ and in (3.7) the value $2d$ is replaced by $-2d$ both in the arguments of the functions and in the upper limit of the integral. This leads to the conclusion $z(0) > 0$ which means that $R_-(\lambda)$ is strictly decreasing with respect to λ. □

In order to apply the intermediate value theorem and prove crossing of the graphs of $R_+(\lambda)$ and $R_-(\lambda)$, we use their continuity within each gap and their limits as λ approaches a gap edge.

[1] In fact, it can be easily seen that $m = 2n$, where n is the index of the gap G_n^+.

Lemma 3.2. *Let $s \in \{s_1, s_2, \ldots\}$ be one of the boundary-points of the spectral gaps $G_n^{\pm}$ of $L_{\pm}$ respectively. If s corresponds to a Dirichlet-eigenvalue of $L_{\pm}$ on $[0,d]$ then $\lim_{\lambda\to s,\lambda\in G_n} |R_{\pm}(\lambda)| = |R_{\pm}(s)| = \infty$ respectively, and if s corresponds to a Neumann-eigenvalue of $L_{\pm}$ on $[0,d]$ then $\lim_{\lambda\to s,\lambda\in G_n} R_{\pm}(\lambda) = R_{\pm}(s) = 0$ respectively.*

Proof. Let λ be inside the gap. On compact subintervals of $[0,\infty)$, $(-\infty,0]$ the H^2-norm of $\psi_{\pm}(\cdot,\lambda)$ in (3.3) is bounded in λ and hence along a sequence $\lambda_k \to s, \lambda_k \in G_n$ the functions $\psi_{\pm}(\cdot,\lambda_k)$ are convergent in H^1 to a bounded solution v of $L_{\pm}v = sv$. Therefore v coincides with the bounded, periodic Bloch function $p_1(x;s)$. The rest of the statement is obvious, cf. Lemma 2.1. □

To make the picture of the behavior of $R_{\pm}$ complete, it remains to determine their behavior at the lower end of the semi-infinite gap $G_0^{\pm}$, i.e. as $\lambda \to -\infty$.

Lemma 3.3. *Let $V_{\pm}$ be bounded potentials (not necessarily even, periodic or continuous). Then $R_{\pm}(\lambda) \to \mp\infty$ as $\lambda \to -\infty$.*

Proof. The proof is, as for Lemma 3.1, shown only for R_+ with the one for R_- being completely analogous. Consider $\lambda \in G_0^+$. We rescale the Bloch function $\psi_+(x;\lambda)$ so that $\psi_+(0;\lambda) = 1$. Note that this is possible if and only if $\psi_+(0;\lambda) \neq 0$. We show that $\psi_+(0;\lambda) \neq 0$ for all $\lambda \leq \inf V_+$. Suppose that $\psi_+(0;\lambda) = 0$. Testing $(L_+ - \lambda)\psi_+ = 0$ with ψ_+ over $x \in [0,\infty)$, we get

$$\int_0^\infty (\psi_+')^2 dx + \int_0^\infty (V_+ - \lambda)\psi_+^2 dx = 0$$

and, therefore, $\lambda > \inf V_+$.

Let now $\lambda = -\nu^2$ for some $\nu > 0$, s.t. $-\nu^2 \in G_0^+$ and $-\nu^2 \leq \inf V_+$, and define

$$\phi_\nu(x) := \psi_+(x;-\nu^2) - e^{-\nu x}. \tag{3.8}$$

We have

$$\phi_\nu'' = \nu^2\phi_\nu + V_+\psi_+, \qquad \phi_\nu(0) = 0. \tag{3.9}$$

Since $R_+(\lambda) = R_+(-\nu^2) = \psi_+'(0;-\nu^2) = -\nu + \phi_\nu'(0)$, we need to determine the behavior of $\phi_\nu'(0)$ as $\nu \to \infty$. Using the Green's function, we solve (3.9) to obtain

$$\phi_\nu(x) = -\frac{1}{\nu}\left(e^{-\nu x}\int_0^x \sinh(\nu t)V_+(t)\psi_+(t;-\nu^2)dt + \sinh(\nu x)\int_x^\infty e^{-\nu t}V_+(t)\psi_+(t;-\nu^2)dt\right).$$

Therefore, $\phi_\nu'(0) = -\int_0^\infty e^{-\nu t}V_+(t)\psi_+(t;-\nu^2)\,dt$ and

$$|\phi_\nu'(0)| \leq \|V_+\|_{L^\infty}\|e^{-\nu\cdot}\|_{L^2(0,\infty)}\|\psi_+(\cdot;-\nu^2)\|_{L^2(0,\infty)} = \frac{\|V_+\|_{L^\infty}}{\sqrt{2\nu}}\|\psi_+(\cdot;-\nu^2)\|_{L^2(0,\infty)}. \tag{3.10}$$

In order to estimate $\|\psi_+(\cdot;-\nu^2)\|_{L^2(0,\infty)}$, (3.9) yields

$$\nu^2\|\phi_\nu\|^2_{L^2(0,\infty)} = -\|\phi_\nu'\|^2_{L^2(0,\infty)} - \int_0^\infty V_+(x)\psi_+(x;-\nu^2)\phi_\nu(x)dx,$$

implying $\nu^2\|\phi_\nu\|^2_{L^2(0,\infty)} \leq \|V_+\|_{L^\infty}\|\psi_+(\cdot;-\nu^2)\|_{L^2(0,\infty)}\|\phi_\nu\|_{L^2(0,\infty)}$ and

$$\|\phi_\nu\|_{L^2(0,\infty)} \leq \frac{1}{\nu^2}\|V_+\|_{L^\infty}\|\psi_+(\cdot;-\nu^2)\|_{L^2(0,\infty)}. \tag{3.11}$$

Therefore (3.8) and (3.11) together give $\|\psi_+(\cdot;-\nu^2)\|_{L^2(0,\infty)} \leq \frac{1}{\sqrt{2\nu}} + \frac{1}{\nu^2}\|V_+\|_{L^\infty}\|\psi_+(\cdot;-\nu^2)\|_{L^2(0,\infty)}$. If $\nu^2 > \|V_+\|_{L^\infty}$, we have the estimate

$$\|\psi_+(\cdot;-\nu^2)\|_{L^2(0,\infty)} \leq \frac{(2\nu)^{-1/2}}{1-\nu^{-2}\|V_+\|_{L^\infty}}. \tag{3.12}$$

Finally, combining (3.12) and (3.10), we arrive at the bound

$$|\phi_\nu'(0)| \leq \frac{(2\nu)^{-1}\|V_+\|_{L^\infty}}{1-\nu^{-2}\|V_+\|_{L^\infty}},$$

which implies $R_+(-\nu^2) = -\nu + \phi_\nu'(0) \to -\infty$ as $\nu \to \infty$. $\square$

The behavior of the ratio functions $R_\pm(\lambda)$ for the two examples $V_+ = V_- = \sin^2(\pi x/10)$ and $V_+ = V_- = \cos^2(\pi x/10)$ is summarized in Figure 3. Note that Lemmas 2.2, 3.1, 3.2 and 3.3 imply the behavior only for $\lambda \leq s_3$. The rest in Figure 3 is obtained without a rigorous proof from numerical computations of the gap edge eigenfunctions.

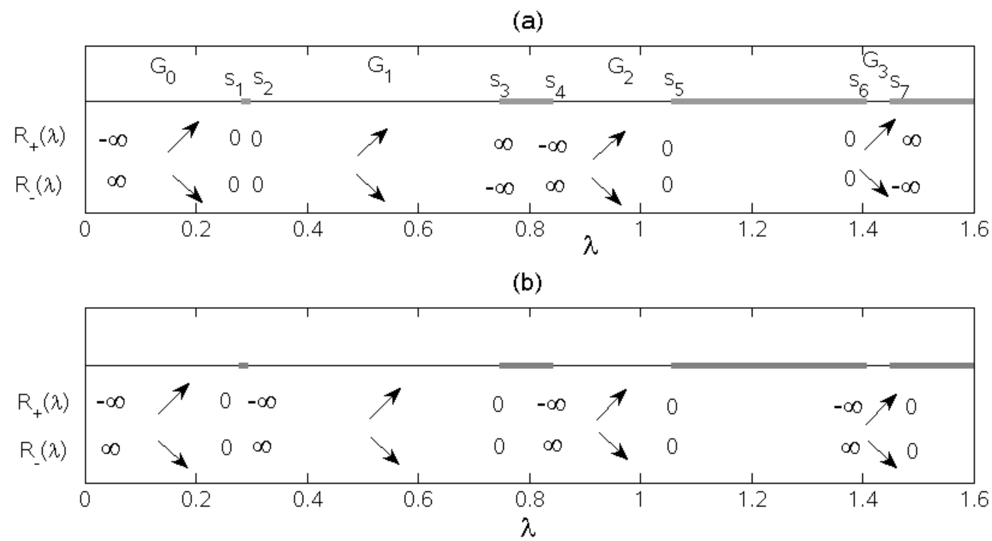

Figure 3: Behavior of the ratio functions $R_\pm(\lambda)$ within gaps of $\sigma(L_\pm)$ for $V_+ = V_- = \sin^2(\pi x/10)$ in (a) and for $V_+ = V_- = \cos^2(\pi x/10)$ in (b). The arrows denote the monotonicity type.

By the intermediate value theorem and based on the behavior of $R_\pm$, we now obtain the following theorem, which has been observed by Korotyaev [14].

Theorem 3.4. *Let G_n^-, G_m^+ be two gaps in the spectrum of L_- and L_+ respectively, such that $G_n^- \cap G_m^+ \neq \emptyset$. Then the following two statements are equivalent:*

(a) $\exists\ \lambda \in G_n^- \cap G_m^+$ such that λ is an eigenvalue of L.

(b) Either $G_n^- = (\mu_n, \nu_{n+1}), G_m^+ = (\nu_{m+1}, \mu_m)$ or $G_n^- = (\nu_{n+1}, \mu_n), G_m^+ = (\mu_m, \nu_{m+1})$.

In case (a) the eigenvalue is also unique.

Remark. Note that besides continuity and the limit values of $R_\pm(\lambda)$ their monotonicity is also needed to fulfill the conditions of the intermediate value theorem. Without monotonicity the ranges of the functions $R_+(\lambda)$ and $R_-(\lambda)$ on the intersection $G_n^- \cap G_m^+$ could be completely distinct, see Figure 4. With monotonicity of $R_\pm(\lambda)$ we, of course, obtain also uniqueness of solutions to (3.4).

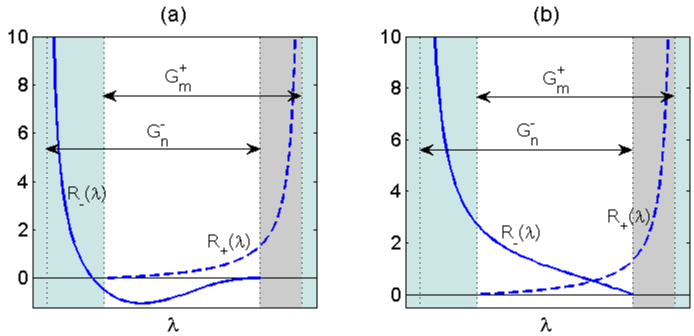

Figure 4: A cartoon of the graphs of $R_-(\lambda)$ and $R_+(\lambda)$ when the former one of the two conditions in Theorem 3.4 holds. (a) No solution to (3.4) without monotonicity of R_- (hypothetical case). (b) Existence and uniqueness of the solution to (3.4) on any $G_n^- \cap G_m^+$ with monotonicity of $R_\pm$.

Let us call the gap (μ_n, ν_{n+1}) a DN-gap and the gap (ν_{n+1}, μ_n) a ND-gap. The semi-infinite gap belongs to DN-gaps. The existence part of Theorem 3.4 can then be formulated as follows:

> *Whenever a DN/ND-gap of L_- intersects a ND/DN-gap of L_+, respectively, a unique eigenvalue of L exists in this intersection.*

3.1.1 Example: additive interface

The additive interface problem (1.1) with (1.4) is equivalent to (3.1) with $L_- = L_0 := -\partial_x^2 + V_0(x)$ and $L_+ = L_0 + \alpha$.

Because $\sigma(L_0+\alpha) = \sigma(L_0)+\alpha$, we have $G_n^+ = G_n^- + \alpha$ and because the Bloch functions of L_0 at the spectral parameter λ are the same as the Bloch functions of $L_0+\alpha$ at $\lambda+\alpha$, to check conditions of Theorem 3.4, one only needs to know $\sigma(L_0)$ and symmetries (even/odd) of the Bloch functions of L_0 at the gap edges s_n.

The existence part of Theorem 3.4 can now be formulated as follows:

> *Whenever α shifts the spectrum of L_0 so that a shifted DN/ND-gap intersects an (unshifted) ND/DN-gap, respectively, a unique eigenvalue of L exists in this intersection.*

Theorem 3.4 has several interesting and rather specific corollaries for the additive interface case. Firstly, clearly, if $|\alpha| < \alpha_*$, where $\alpha_* := \min_{n\in\mathbb{N}}(s_{2n} - s_{2n-1})$ is the width of the narrowest spectral band of L_0, the shift α is too small to make even the two gaps lying closest to each other overlap.

Corollary 3.5. *If $|\alpha| < \alpha_* := \min_{n\in\mathbb{N}}(s_{2n} - s_{2n-1})$, L has no eigenvalues.*

In the rest of this section G_n denotes the n-th spectral gap of L_0. As Lemma 2.2 dictates, when V_0 is increasing on $[0, d/2]$, the first finite gap $G_1 = (s_2, s_3)$ is a ND-gap and thus if α shifts the semi-infinite (DN) gap G_0 so that $G_0+\alpha$ intersects G_1, an eigenvalue exists. Obviously, the infimal value of $\alpha > 0$ achieving such an intersection is the width of the first spectral band s_2-s_1. Since G_0 is semi-infinite, there is no upper bound on α and if $\alpha > s_2-s_1$, the intersection is always nonempty. On the other hand, when V_0 is decreasing on $[0, d/2]$, G_1 is a DN-gap and the intersection of $G_0+\alpha$ and G_1 contains no eigenvalues. As the next Corollary clarifies, for $\alpha < -(s_2 - s_1)$ the situation is similar.

Corollary 3.6. *Let V_0 be strictly increasing/strictly decreasing on $[0, \frac{d}{2}]$. If $|\alpha| > s_2 - s_1$ then a unique eigenvalue/no eigenvalue of L exists in $G_1 \cap (G_0 + \alpha)$ for $\alpha > 0$ and in $G_0 \cap (G_1 + \alpha)$ for $\alpha < 0$.*

Numerical results The point spectrum of the additive interface problem with the potential $V_0(x) = \sin^2(\pi x/10)$ has been computed using a 4th order centered finite difference discretization. The eigenvalues are plotted in Figure 5 for a range of values of α. The shaded regions are the union of spectral bands of L_0 and $L_0 + \alpha$. The results agree with Theorem 3.4.

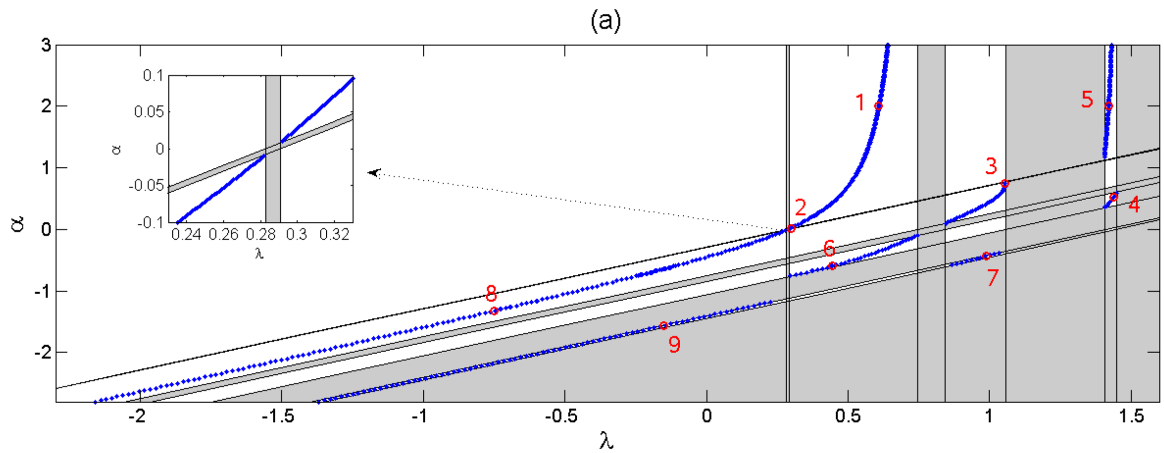

Figure 5: Numerically computed point spectrum of L with $V_0(x) = \sin^2(\pi x/10)$ for a range of values of α. The union of spectral bands of L_0 and $L_0+\alpha$ is shaded. The inset blows up the region near $\lambda = s_1$, $\alpha = 0$. Eigenfunctions for the labeled points are plotted in Figure 6.

In Figure 6 we plot eigenfunctions corresponding to nine selected eigenvalues in Figure 5. Note that the decay rate of the eigenfunctions is often very different on either side of the origin.

For the potential $V_0(x) = \cos^2(\pi x/10)$ it is clear from the numerically obtained Figure 3 (b) that the intersections $G_j \cap (G_k + \alpha)$, $j, k \in \{0, \ldots, 3\}$ contain no eigenvalues because the gaps $G_0, \ldots, G_3$ are all DN-gaps. In other words, based on the numerics, the additive interface problem (1.1), (1.4) with $V_0(x) = \cos^2(\pi x/10)$ has *no eigenvalues on* $(-\infty, s_8]$. Note that our analysis guarantees non-existence of eigenvalues only in $(-\infty, s_4]$.

3.2 Point Spectrum for Interface Problems Made of Dislocated Even Potentials

For the dislocation interface (1.3) we restrict our attention to the two representative cases $t = -s$ and $s = 0$.

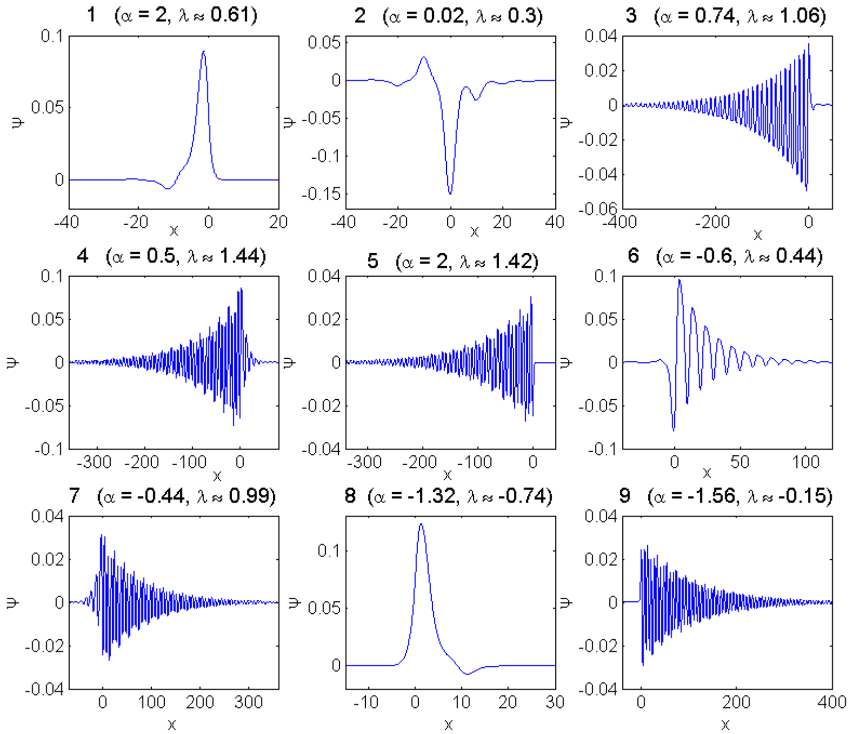

Figure 6: Eigenfunctions corresponding to the 9 labeled eigenvalues in Figure 5.

3.2.1 Symmetric Dislocations

Here we study the eigenvalue problem (1.1) with (1.3) in the case where $t = -s,\ t \in (0, d)$. This can be done via the system

$$\begin{array}{ll} L_-^t \psi^t := -\partial_x^2 \psi^t + V_0(x-t)\psi^t = \lambda \psi^t & \text{for } x < 0, \\ L_+^t \psi^t := -\partial_x^2 \psi^t + V_0(x+t)\psi^t = \lambda \psi^t & \text{for } x \geq 0 \end{array} \tag{3.13}$$

coupled by the the C^1-matching conditions

$$\psi^t(0-) = \psi^t(0+) \qquad \text{and} \qquad \frac{d}{dx}\psi^t(0-) = \frac{d}{dx}\psi^t(0+). \tag{3.14}$$

First note that the spectrum $\sigma(L_t)$ of the operator $L_t := -\partial_x^2 + V_0(x+t)$ on $\mathbb{R}$ is identical to the spectrum $\sigma(L_0)$ of $L_0 = -\partial_x^2 + V_0$ on $\mathbb{R}$ and we have $G_n^+ = G_n^-$. Moreover, the Bloch functions $\psi_{1,2}^t$ of L_t for $\lambda \in \mathbb{R} \setminus \sigma(L_t) = \mathbb{R} \setminus \sigma(L_0)$ are just shifts of the Bloch functions of L_0, i.e., $\psi_i^t(x;\lambda) = \psi_i^0(x+t;\lambda), i = 1,2$. Therefore, an L^2-solution of (1.1) with (1.3) can only exist if $\lambda \notin \sigma(L_0)$. For such λ any localized eigenfunction ψ^t of (1.1) with (1.3) must take the form

$$\psi^t(x;\lambda) = \psi_-^t(x;\lambda)\chi_{\{x<0\}} + \psi_+^t(x;\lambda)\chi_{\{x\geq 0\}},$$

where $\psi_\pm^t(x;\lambda)$ are those Bloch functions of $L_{\pm t}$, which decay on $\mathbb{R}^\pm$, respectively.

As in Section 3.1 we introduce the ratio functions

$$R^t_\pm(x;\lambda) = \frac{\frac{\partial}{\partial x}\psi^t_\pm(x;\lambda)}{\psi^t_\pm(x;\lambda)},$$

so that the matching conditions (3.14) are equivalent to $R^t_+(0;\lambda) = R^t_-(0;\lambda)$. Due to the fact, that the Bloch functions $\psi^t_\pm$ are just shifts of the Bloch functions $\psi^0_\pm$ we see that $R^t_+(x;\lambda) = R^0_+(x+t;\lambda)$ and $R^t_-(x;\lambda) = R^0_-(x-t;\lambda)$. Thus, the matching condition (3.14) amounts to

$$R^0_+(t;\lambda) = R^0_-(-t;\lambda).$$

Finally, the evenness of the potential V_0 and the fact that only one linearly independent Bloch function decaying at $+\infty$ exists, implies that $\psi^0_+(x;\lambda) = \pm\psi^0_-(-x;\lambda)$ for $\lambda \notin \sigma(L_0)$, and hence $R^0_+(t;\lambda) = -R^0_-(-t;\lambda)$ so that finding an eigenvalue of (1.1) with (1.3) amounts to finding a zero or a pole of $R^0_+(t;\lambda)$ for some $t \in (0,d)$. This is done below via the intermediate value theorem and monotonicity properties of the function $R^0_+(t;\lambda)$.

For simplicity, we write in the following $R(t;\lambda)$ instead of $R^0_+(t;\lambda)$. First, we need to generalize Lemma 3.1 on the monotonicity and continuity of $R(t;\lambda)$ as a function of t and λ. Suppose $u \in L^2(0,\infty)$ solves $L_0\psi = \lambda\psi$. We apply again the Prüfer transformation, cf. Coddington, Levinson [5], given by

$$\psi(x;\lambda) = \rho(x;\lambda)\sin(\theta(x;\lambda)), \qquad \psi'(x;\lambda) = \rho(x;\lambda)\cos(\theta(x;\lambda)),$$

which transforms the equation $L_0\psi = \lambda\psi$ into the system

$$\theta' = 1 + (\lambda - V_0(x) - 1)\sin^2(\theta), \tag{3.15}$$

$$\rho' = -\rho(\lambda - V_0(x) - 1)\sin(\theta)\cos(\theta), \tag{3.16}$$

where the prime denotes differentiation in x. Note that $R(t;\lambda)$ is a $2d$-periodic function of the variable t. Hence $\theta(t+2d;\lambda) = \theta(t;\lambda) + m\pi$, where m is an integer which is constant in λ within each spectral gap. In fact, it can be shown that $m = 2n$ when $\lambda \in G_n$.

In the subsequent arguments we use the following result on differential inequalities, cf. Walter [18], which we quote in a slightly simplified way. Functions v, w satisfying (3.17) below are called sub-, supersolutions, respectively.

Lemma 3.7. *Let $f : [a,b] \times \mathbb{R} \to \mathbb{R}$ be continuous and continuously differentiable with respect to the second variable. If $v, w \in C^1[a,b]$ satisfy*

$$v' \le f(t,v), \quad w' \ge f(t,w) \text{ on } [a,b] \text{ with } v(a) \le w(a), \tag{3.17}$$

then $v \le w$ in $[a,b]$. More precisely, either $v < w$ in $[a,b]$ or there exists $c \in (a,b]$ such that $v = w$ on $[a,c]$ and $v < w$ on $(c,b]$. Moreover, if one of the differential inequalities holds strictly almost everywhere in $[a,b]$, then $v(t) < w(t)$ holds for all $t \in (a,b]$.

Lemma 3.8 (Monotonicity in λ). *Let $G_n = (s_{2n}, s_{2n+1}), n \ge 0$ be a fixed gap. For $\lambda \in \overline{G_n}$ and $t \in [0,d]$ the function R is continuous except in the set $S = \bigcup_{t\in[0,d]} S_t$, where either $S_t = \emptyset$ or $S_t = \{(t,\lambda_t)\}$ and*

$$\lim_{\lambda\to\lambda_t-} R(t;\lambda) = +\infty, \qquad \lim_{\lambda\to\lambda_t+} R(t;\lambda) = -\infty. \tag{3.18}$$

For a fixed t the function $R(t;\lambda)$ is strictly increasing for $\lambda \in [s_{2n}, \lambda_t)$ and for $\lambda \in (\lambda_t, s_{2n}]$. Moreover, if $\lambda, \mu \in \overline{G_n}$ then $\lambda < \lambda_t < \mu$ implies $R(t;\lambda) > R(t;\mu)$ and $\lambda \ne \mu$ implies $R(t;\lambda) \ne R(t;\mu)$.

Proof. As we have seen in Lemma 3.1 the Prüfer-variables θ and ρ are continuous functions of both variables $t \in \mathbb{R}$ and $\lambda \in G_n$. Since $R(t;\lambda) = \cot(\theta(t;\lambda))$ the function $R(t;\lambda)$ is continuous except for those values, where $\theta(t;\lambda)$ passes through $k\pi, k \in \mathbb{Z}$. Since $R(t;\lambda)$ is increasing in λ at points of continuity by Lemma 3.1, the relation (3.18) follows. The fact that there is at most one blow-up point λ_{t_0} with respect to λ will follow from the next statement. Let $\lambda < \lambda_{t_0} < \mu$ and suppose for contradiction that $R(t_0;\lambda) \le R(t_0;\mu)$. By lowering μ if necessary and keeping the order $\lambda < \lambda_{t_0} < \mu$, we may achieve $R(t_0;\lambda) = R(t_0;\mu)$, i.e., there exists $k \in \mathbb{Z}$ such that $\theta(t_0;\lambda) = \theta(t_0;\mu) + k\pi$. Note that

$$\begin{aligned}
\theta'(t;\lambda) &= 1 + (\lambda - V_0(t) - 1)\sin^2(\theta(t;\lambda)),\\
\theta'(t;\mu) &= 1 + (\mu - V_0(t) - 1)\sin^2(\theta(t;\mu)) > 1 + (\lambda - V_0(t) - 1)\sin^2(\theta(t;\mu))
\end{aligned}$$

for almost all $t \ge t_0$. By the comparison principle of Lemma 3.7 we obtain $\theta(t;\lambda) < \theta(t;\mu) + k\pi$ for all $t > t_0$. Here we have used that θ and $\theta + k\pi$ solve the same differential equation. It follows in particular, that

$$\theta(t_0;\lambda) + m\pi = \theta(t_0 + 2d;\lambda) < \theta(t_0 + 2d;\mu) + k\pi = \theta(t_0;\mu) + (m+k)\pi$$

contradictory to our assumption $\theta(t_0;\lambda) = \theta(t_0;\mu) + k\pi$. This proves the lemma. □

Corollary 3.9. *For $t = -s$ the number of dislocation eigenvalues in any gap $G_n, n \ge 0$, is* 0, 1 *or* 2.

Proof. It follows from Lemma 3.8 that for fixed t the function $R(t;\lambda)$ as a function of λ can have at most one zero and at most one pole. □

Lemma 3.10 (Monotonicity in t). *Suppose V_0 is an even, $d-$periodic C^1-function. Let $G_n = (s_{2n}, s_{2n+1}), n \ge 0$, be a fixed gap and let $\lambda \in \partial G_n$.*

(a) If V_0 is increasing on $[0, \frac{d}{2}]$ then either $\frac{\partial R}{\partial t}(t;\lambda) \le 0$ on $[0,d]$ or there exists $t_0 \in (0, \frac{d}{2})$ such that $\frac{\partial R}{\partial t}(t;\lambda) \le 0$ on $[0,t_0] \cup [d - t_0, d]$ and $\frac{\partial R}{\partial t}(t;\lambda) \ge 0$ for all $t \in [t_0, d - t_0]$.

(b) If V_0 is decreasing on $[0, \frac{d}{2}]$ then either $\frac{\partial R}{\partial t}(t;\lambda) \le 0$ on $[0,d]$ or there exists $t_0 \in (0, \frac{d}{2})$ such that $\frac{\partial R}{\partial t}(t;\lambda) \ge 0$ on $[0,t_0] \cup [d - t_0, d]$ and $\frac{\partial R}{\partial t}(t;\lambda) \le 0$ for all $t \in [t_0, d - t_0]$.

Note that in both cases, $R(t;\lambda)$ can change monotonicity with respect to t only once. Furthermore, the monotonicity of $\theta(t;\lambda)$ is the reverse of the monotonicity of $R(t;\lambda)$ with respect to t.

Proof. We give the proof in case (a). The proof for case (b) needs only minor modifications. Since $\cot(\theta) = R$, we need to prove the reverse monotonicity for the function θ. Recall from Lemma 2.1 that for $\lambda \in \partial G_n$ the evenness of V_0 implies $\theta(\frac{d}{2};\lambda) \in \{k\pi, k\pi + \frac{\pi}{2}; k \in \mathbb{Z}\}$. Hence, for some $l \in \mathbb{Z}$ we have

$$\theta\left(\frac{d}{2} + s;\lambda\right) = l\pi - \theta\left(\frac{d}{2} - s;\lambda\right) \quad \forall s \in \left[0, \frac{d}{2}\right] \tag{3.19}$$

due to the evenness of $V_0(x)$ about $x = d/2$ (implied by $d-$periodicity and evenness about $x = 0$). In any of the two cases, the monotonicity of θ in $[0, \frac{d}{2}]$ has its counterpart in $[\frac{d}{2}, d]$. Differentiation of (3.15) with respect to t yields

$$\begin{aligned}
(\theta')' =& 2(\lambda - V_0(t) - 1)\sin(\theta)\cos(\theta)\theta' - V_0'(t)\sin^2(\theta)\\
&\begin{cases} \le 2(\lambda - V_0(t) - 1)\sin(\theta)\cos(\theta)\theta' & \text{on } [0, \frac{d}{2}],\\ \ge 2(\lambda - V_0(t) - 1)\sin(\theta)\cos(\theta)\theta' & \text{on } [\frac{d}{2}, d]. \end{cases}
\end{aligned} \tag{3.20}$$

Note that there is always a point $\tau \in (0, \frac{d}{2})$ where $\theta'(\tau; \lambda) \geq 0$. Since 0 is a subsolution to (3.20) on $[\frac{d}{2}, d]$, we conclude by Lemma 3.7 and by (3.19) that there are two intervals $[0, t_0] \cup [d - t_0, d]$ with $t_0 \in [0, d/2]$, where $\theta' \geq 0$. Let us choose t_0 to be the maximal value. Either $t_0 = d/2$ and $\theta' \geq 0$ on $[0, d]$ or $t_0 < d/2$, $\theta'(t_0) = 0$ and $\theta' < 0$ in a right-sided neighborhood of t_0. In the latter case, since 0 is a supersolution to (3.20) on $[0, \frac{d}{2}]$, we conclude that $\theta' \leq 0$ on $[t_0, d - t_0]$. This concludes the proof of the lemma. □

Theorem 3.11. *Suppose V_0 satisfies the basic assumptions, i.e., even, d-periodic and continuous. Let $s = -t$ in* (1.3) *and consider the semi-infinite gap $G_0 = (-\infty, s_1)$.*

(a) If V_0 is strictly increasing on $[0, d/2]$, then there is exactly zero/one dislocation eigenvalue in G_0 for $t \in (0, d/2]$ / $(d/2, d)$ respectively.

(b) If V_0 is strictly decreasing on $[0, d/2]$, then there is exactly one/zero dislocation eigenvalue in G_0 for $t \in (0, d/2)$ / $[d/2, d)$ respectively.

Proof. It suffices to prove part (a), since (b) follows from (a) via shifting the potential by the half-period $\frac{d}{2}$ due to the evenness of $V_0(x)$ about $x = d/2$. Recall that the first band edge s_1 is a Neumann eigenvalue. Due to the $d-$periodicity and evenness of V_0, the first Neumann eigenfunction u has an extremum at $x = d/2$. It can be thus viewed as the first Neumann eigenfunction on the interval $x \in [0, d/2]$, i.e. the minimizer of the energy

$$\int_0^{d/2} v'^2 + V_0(x)v^2 \, dx : v \in H^1(0, d/2) \quad \text{with} \quad \int_0^{d/2} v^2 dx = 1.$$

Without loss of generality assume that u is positive. As the decreasing rearrangement u^* of u decreases the energy, u has to be strictly decreasing on $[0, d/2]$ and hence on $[0, d]$. We claim that $u' < 0$ on $(0, d)$. To see this, consider the corresponding Prüfer angle θ and note that $\theta'(\frac{d}{2}) = 1$. Hence, the comparison principle of Lemma 3.7 and the fact that 0 is a subsolution to (3.20) on $[\frac{d}{2}, d]$ imply that $\theta' > 0$ on $[\frac{d}{2}, d]$ and by the symmetry relation (3.19) $\theta' > 0$ on the whole interval $[0, d]$. Therefore, θ is strictly increasing on $[0, d]$ with range $[\frac{\pi}{2}, \frac{3\pi}{2}]$ so that $u' < 0$ on $(0, d)$. Therefore, $R(t; s_1) < 0$ for $t \in (0, d/2)$ and $R(t; s_1) > 0$ for $t \in (d/2, d)$.

Recall now from Lemma 3.3 that that $R(t; \lambda) \to -\infty$ as $\lambda \to -\infty$ for any $t \in [0, d]$. Moreover, $R(t; \lambda)$ is continuous in $\lambda \in G_1$ because continuity can be broken only by a pole. But because $R(t; \lambda) \to -\infty$ as $\lambda \to -\infty$ and $R(t; \lambda)$ is increasing in λ within each continuity segment, a pole would mean that $R(t; \lambda)$ takes the same value for some $\lambda_1 \neq \lambda_2 \in G_1$, which is impossible by Lemma 3.8.

As a result $R(t; \lambda)$ stays negative for $t \in (0, d/2)$ throughout $\lambda \in G_0$, goes through 0 once for $t \in (d/2, d)$, and takes the zero value at $\lambda = s_1 \notin G_0$ for $t = d/2$. □

Theorem 3.12. *Suppose V_0 is an even, d-periodic C^1-function, let $s = -t$ in* (1.3) *and consider the first finite gap $G_1 = (s_2, s_3)$.*

(a) Suppose V_0 is strictly increasing on $[0, \frac{d}{2}]$ so that $G_1 = (\nu_2, \mu_1)$. The second Neumann-eigenfunction is strictly monotone on $[0, d]$. For the first Dirichlet-eigenfunction u we have the alternative:

(a1) u is strictly monotone on $[0, \frac{d}{2}]$. Then there is exactly one dislocation-eigenvalue in G_1 for $t \in (0, d) \setminus \{\frac{d}{2}\}$ and none for $t = \frac{d}{2}$.

(a2) u changes monotonicity on $[0, \frac{d}{2}]$ exactly once at the extremal point $d_0 \in (0, \frac{d}{2})$. Then the number of dislocation-eigenvalues in G_1 is as follows:

dislocation parameter	$t \in (0, d_0)$	$t \in [d_0, \frac{d}{2}]$,	$t \in (\frac{d}{2}, d - d_0)$	$t \in [d - d_0, d)$	$t = d$
number of eigenvalues	1	0	2	1	0

(b) Suppose V_0 is strictly decreasing on $[0, \frac{d}{2}]$ so that $G_1 = (\mu_1, \nu_2)$. The first Dirichlet-eigenfunction is strictly monotone on $[0, \frac{d}{2}]$. For the second Neumann-eigenfunction u we have the alternative:

(b1) u is strictly monotone on $[0, \frac{d}{2}]$. Then there is exactly one dislocation-eigenvalue in G_1 for $t \in (0, d) \setminus \{\frac{d}{2}\}$ and none for $t = \frac{d}{2}$.

(b2) u changes monotonicity on $[0, \frac{d}{2}]$ exactly once at the extremal point $d_0 \in (0, \frac{d}{2})$. Then the number of dislocation-eigenvalues in G_1 is as follows:

dislocation parameter	$t \in (0, d_0)$	$t \in [d_0, \frac{d}{2})$,	$t = \frac{d}{2}$	$t \in (\frac{d}{2}, d - d_0)$	$t \in [d - d_0, d)$
number of eigenvalues	2	1	0	1	0

Proof. As in Theorem 3.11 it suffices to prove part (a) when, in addition, the roles of ν_2 and μ_1 are switched in the proof of (b). The strict monotonicity of the second Neumann eigenfunction was already stated in Lemma 2.2. For the monotonicity alternative of the first Dirichlet eigenfunction u, recall that

$$u(x) = \rho(x; \mu_1) \sin \theta(x; \mu_1), \quad u'(x) = \rho(x; \mu_1) \cos \theta(x; \mu_1).$$

We can assume that $\theta(0; \mu_1) = 0$, $\theta(\frac{d}{2}; \mu_1) = \frac{\pi}{2}$ and that $\theta(x; \mu_1)$ ranges in $[0, \pi)$ for $x \in [0, \frac{d}{2}]$. According to the monotonicity alternative for θ in Lemma 3.10 there are two possibilities: either $\theta(x; \mu_1)$ is increasing and hence $\cos(\theta(x; \mu_1)) > 0$ for $x \in (0, \frac{d}{2})$, or $\theta(x; \mu_1)$ is increasing for $t \in [0, t_0]$ and decreasing for $t \in [t_0, \frac{d}{2}]$. In this case $\theta(x; \mu_1)$ crosses the value $\frac{\pi}{2}$ at $d_0 \in (0, t_0)$ and hence $u' > 0$ on $[0, d_0)$ and $u' < 0$ on $(d_0, \frac{d}{2}]$. This proves the monotonicity alternative (a1), (a2), and it remains to discuss the number of dislocation eigenvalues.

We may suppose that the Neumann eigenfunction is strictly decreasing on $[0, d]$ with its unique zero at $\frac{d}{2}$. Thus $\theta(t; \nu_2)$ ranges within $[\frac{\pi}{2}, \frac{3\pi}{2}]$ with $\theta(\frac{d}{2}; \nu_2) = \pi$, $\theta'(\frac{d}{2}; \nu_2) = 1$. Therefore, taking into account Lemma 3.10(a), we find that θ must be increasing on $[0, d]$ and hence $R(t; \nu_2)$ is decreasing in t with

$$R(0+; \nu_2) = 0-, \quad R\left(\frac{d}{2}-; \nu_2\right) = -\infty, \quad R\left(\frac{d}{2}+; \nu_2\right) = +\infty, \quad R(d-; \nu_2) = 0+. \tag{3.21}$$

Case (a1): We may suppose that the Dirichlet eigenfunction is strictly increasing and positive on $[0, \frac{d}{2}]$ and even around $\frac{d}{2}$. In this case $\theta(t; \mu_1)$ ranges through $[0, \frac{\pi}{2}]$ for $t \in [0, \frac{d}{2}]$ and through $[\frac{\pi}{2}, \pi]$ for $t \in [\frac{d}{2}, d]$. As before, Lemma 3.10(a) implies that θ is increasing on $[0, d]$ and hence $R(t; \mu_1)$ is decreasing in t with

$$R(0+; \mu_1) = +\infty, \quad R\left(\frac{d}{2}-; \mu_1\right) = 0+, \quad R\left(\frac{d}{2}+; \mu_1\right) = 0-, \quad R(d-; \mu_1) = -\infty.$$

For $t \in (0, \frac{d}{2})$ we have $R(t;\nu_2) < 0 < R(t;\mu_1)$ and hence there exists a value $\lambda \in (\nu_2, \mu_1)$ with $R(t;\lambda) = 0$. Lemma 3.8 shows that this is the only zero. Moreover, $R(t;\lambda)$ cannot have a pole, since this would imply the existence of a second zero. Thus we have the uniqueness of the dislocation eigenvalue. For $t = \frac{d}{2}$, the zero appears at $\lambda = \mu_1$ which is not inside the gap, i.e., there is no dislocation eigenvalue. Finally, for $t \in (\frac{d}{2}, d)$ we have $R(t;\nu_2) > 0 > R(t;\mu_1)$ and hence there exists a value $\lambda \in (\nu_2, \mu_1)$, where $R(t;\lambda)$ has a pole. No further poles or zeros can exists, which shows again uniqueness of the dislocation eigenvalue.

Case (a2): We may suppose that the positive Dirichlet eigenfunction is strictly increasing on $[0, d_0]$, strictly decreasing on $[d_0, \frac{d}{2}]$ and even around $\frac{d}{2}$. In this case $\theta(t;\mu_1)$ has the following properties:

$$\begin{array}{llll}
\text{increasing from } 0 \text{ to } \frac{\pi}{2} & \text{for } t \in [0, d_0], & \text{increasing from } \frac{\pi}{2} \text{ to } \theta^* & \text{for } t \in [d_0, t_0], \\
\text{decreasing from } \theta^* \text{ to } \frac{\pi}{2} & \text{for } t \in [t_0, \frac{d}{2}], & \text{decreasing from } \frac{\pi}{2} \text{ to } \theta_* & \text{for } t \in [\frac{d}{2}, d - t_0], \\
\text{increasing from } \theta_* \text{ to } \frac{\pi}{2} & \text{for } t \in [d - t_0, d - d_0], & \text{increasing from } \frac{\pi}{2} \text{ to } \pi & \text{for } t \in [d - d_0, d],
\end{array}$$

which translates as follows into the following behavior of $R(t;\mu_1)$:

$$\begin{array}{llll}
\text{decreasing from } +\infty \text{ to } 0 & \text{for } t \in [0, d_0], & \text{decreasing from } 0 \text{ to } R_* & \text{for } t \in [d_0, t_0], \\
\text{increasing from } R_* \text{ to } 0 & \text{for } t \in [t_0, \frac{d}{2}], & \text{increasing from } 0 \text{ to } R^* & \text{for } t \in [\frac{d}{2}, d - t_0], \\
\text{decreasing from } R^* \text{ to } 0 & \text{for } t \in [d - t_0, d - d_0], & \text{decreasing from } 0 \text{ to } -\infty & \text{for } t \in [d - d_0, d].
\end{array}$$

If we combine this information with (3.21) we conclude as follows:

(i) For $t \in (0, d_0)$ we have $R(t;\nu_2) < 0 < R(t;\mu_1)$ and hence there exists a value $\lambda \in (\nu_2, \mu_1)$ with $R(t;\lambda) = 0$. No other zero/pole can occur, which shows the uniqueness of the dislocation eigenvalue.

(ii) For $t = d_0$ the zero has moved toward the right-end of the gap.

(iii) Next, we claim that

$$R(t;\nu_2) < R(t;\mu_1) < 0 \text{ for all } t \in [d_0, d/2) \tag{3.22}$$

This is obvious for t near d_0 and has to hold by continuity for all $t \in [d_0, \frac{d}{2})$ since equality is excluded by Lemma 3.8. Moreover, (3.22) also implies that there cannot be a pole of $R(t;\lambda)$ for $\lambda \in (\nu_2, \mu_1)$ since such a pole would yield that $R(t;\lambda)$ attains all values between $R(t;\nu_2)$ and $R(t;\mu_1)$ twice, in contradiction to Lemma 3.8. Thus, $R(t;\lambda)$ increases continuously from $R(t;\nu_2)$ to $R(t;\mu_1)$ as λ runs through (ν_2, μ_1) with no zero or pole, i.e., there is no dislocation eigenvalue for $t \in [d_0, \frac{d}{2})$.

(iv) For $t = \frac{d}{2}$ dislocation eigenvalues are excluded as before.

(v) Next we consider $t \in (\frac{d}{2}, d - d_0)$. For such t we claim that $R(t;\nu_2) > R(t;\mu_1) > 0$. Whereas positivity is obvious, the ordering is clear for t near $\frac{d}{2}$, cf. (3.21), and has to hold by continuity for all $t \in (\frac{d}{2}, d - d_0)$. Hence, there exists a pole $\lambda_1 \in (\nu_2, \mu_1)$ of $R(t;\lambda)$ and also a zero $\lambda_2 \in (\lambda_1, \mu_1)$, which yields exactly two dislocation eigenvalues for $t \in (\frac{d}{2}, d - d_0)$.

(vi) For $t = d - d_0$, the previous argument shows the existence of a pole, but the zero has moved to the right end of the interval (ν_2, μ_1) leaving us with only one dislocation eigenvalue.

(vii) Finally, consider $t \in (d - d_0, d_0)$. For such t we have $R(t;\nu_2) > 0 > R(t;\mu_1)$ which forces the existence of a pole at some value $\lambda \in (\nu_2, \mu_1)$ with no further zeros, i.e., there is exactly one dislocation eigenvalue. This completes the verification of the number of dislocation eigenvalues. $\square$

Finally, we give a partial answer to the question which of the cases (a1), (a2) or (b1), (b2) for a given potential V_0 actually occur. The condition given in the next theorem is a sufficient condition on the potential V_0 such that (a2), (b2) occur.

Theorem 3.13. *Suppose V_0 satisfies the basic assumptions, i.e., even, d-periodic, and continuous.*

(i) Assume that V_0 is strictly increasing on $[0, d/2]$ and

$$V_0(x) \leq \overline{V}(x) := \beta + (\alpha - \beta)\left(\frac{2x}{d} - 1\right)^2 \text{ with } \beta > \alpha \text{ for all } x \in [0, d/2],$$

where $\beta := V_0(\frac{d}{2})$. If

$$(\beta - \alpha)d^2 > 80(13 - 2\sqrt{37}) \approx 66.75, \tag{3.23}$$

then only the case (a2) of Theorem 3.12 occurs, i.e., the first Dirichlet-eigenfunction on $[0, d]$ is even around $\frac{d}{2}$ but changes its monotonicity at $d_0 \in (0, \frac{d}{2})$.

(ii) Assume that V_0 is strictly decreasing on $[0, d/2]$ and

$$V_0(x) \leq \overline{V}(x) := \alpha + (\beta - \alpha)\frac{4}{d^2}x^2 \text{ with } \alpha > \beta \text{ for all } x \in [0, d/2],$$

where $\alpha := V_0(0)$. If

$$(\alpha - \beta)d^2 > 80(13 - 2\sqrt{37}) \approx 66.75, \tag{3.24}$$

then only the case (b2) of Theorem 3.12 occurs, i.e., the second Neumann-eigenfunction on $[0, d]$ is odd around $\frac{d}{2}$ but changes its monotonicity at $d_0 \in (0, \frac{d}{2})$.

Remark. It will become clear from the proof that (3.23) is not the only condition that leads to the conclusion of the theorem. In fact, by choosing different upper bounds $\overline{V}$ and by choosing a different candidate function $w(x)$ in the proof below, one may obtain a sufficient condition which is different from (3.23). Since there are manifold ways to derive such conditions, we decided to give only the simplest one. Nevertheless, (3.23) is already sufficient to cover the example potentials such as $V_0(x) = \sin^2(\pi x/10)$ and $V_0(x) = \cos^2(\pi x/10)$.

Proof. Suppose V_0 is increasing on $[0, \frac{d}{2}]$. Let μ_1 be the first Dirichlet eigenvalue on $[0, d]$ with corresponding positive eigenfunction u. Then $\mu_1 = \kappa_{DN}$, where κ_{DN} denotes the first eigenvalue on $[0, \frac{d}{2}]$ with Dirichlet boundary condition at 0 and Neumann boundary condition at $\frac{d}{2}$. Let θ be the Prüfer-angle for u normalized by $\theta(0) = 0$, which implies $\theta(\frac{d}{2}) = \frac{\pi}{2}$. The non-monotonicity of u can be shown by proving that $\theta'(\frac{d}{2}) < 0$, i.e., $\theta > \frac{\pi}{2}$ in a left-neighborhood of $\frac{d}{2}$ since θ can change monotonicity only once on $[0, \frac{d}{2}]$. By the differential equation for θ we obtain

$$\theta'\left(\frac{d}{2}\right) = 1 + \left(\mu_1 - V\left(\frac{d}{2}\right) - 1\right)\sin^2\theta\left(\frac{d}{2}\right) = \mu_1 - V\left(\frac{d}{2}\right).$$

Using the variational characterization of $\mu_1 = \kappa_{DN}$, it suffices to find one function $w \in H^1(0, \frac{d}{2})$ with $w(0) = 0$ such that

$$\frac{\int_0^{\frac{d}{2}} w'^2 + V_0(x)w^2\,dx}{\int_0^{\frac{d}{2}} w^2\,dx} < V_0\left(\frac{d}{2}\right) = \beta. \tag{3.25}$$

Using the upper bound $V_0(x) \le \overline{V}(x)$ and the quadratic candidate function $w(x) = x(2c - x)$ with $c \in \mathbb{R}$ to be determined, the condition (3.25) amounts to

$$\int_0^{\frac{d}{2}} w'^2 + \overline{V}(x) w^2 \, dx - \beta \int_0^{\frac{d}{2}} w^2 \, dx$$
$$= \frac{d}{3360}\big(56(120-\gamma)c^2 - 14(240-\gamma)c + (560-\gamma)d^2\big) < 0, \qquad \text{where } \gamma := (\beta - \alpha)d^2. \quad (3.26)$$

If $\gamma \ge 120$ then (3.26) can be achieved by an appropriate choice of c. If $\gamma < 120$ then the optimal choice for c is $c = \frac{d(\gamma-240)}{8(\gamma-120)}$ and hence (3.26) amounts to

$$\frac{d^3(\gamma^2 - 2080\gamma + 134400)}{8 \cdot 3360(120-\gamma)} < 0,$$

which is fulfilled for $\gamma \in \big(80(13 - 2\sqrt{37}), 80(13 + 2\sqrt{37})\big) \approx (66.75, 2013.24)$. Altogether, the statement (i) of the theorem holds true for $\gamma = (\beta - \alpha)d^2 > 80(13 - 2\sqrt{37})$. This concludes the proof of statement (i). Part (ii) can be obtained from part (i) by reflecting the interval $[0, \frac{d}{2}]$. $\square$

Numerical Results We present results of numerical computations of the point spectrum of L with the dislocation interface (1.3) with $s = -t$ and $V_0 = \sin^2(\pi x/10)$ as well as $V_0 = \cos^2(\pi x/10)$. The number of eigenvalues in the semi-infinite gap agrees with Theorem 3.11.

As $V_0 = \sin^2(\pi x/10)$ satisfies the conditions of Theorem 3.13 (with $\beta = 1$ and, for instance, $\alpha = 0.3$), we know that the first Dirichlet eigenfunction changes monotonicity at some $d_0 \in (0, d/2) = (0, 5)$. The case $(a2)$ of Theorem 3.12, therefore, applies. We obtain numerically $d_0 \approx 2.16$, see Fig. 7 top. The number of eigenvalues in the gap $G_1 = (s_2, s_3)$ agrees with the theory at each $t \in (0, d)$, see Figure 7 bottom. Eigenvalues in the gaps G_2 and G_3 are also plotted although for these our analysis provides no explanation other than the statement of Corollary 3.9.

Figure 8 shows the eigenfunctions corresponding to the 9 labeled eigenvalues in Figure 7.

The results for $V_0(x) = \cos^2(\pi x/10)$, as an example of a potential that falls in the case (b) of Theorem 3.12, are, in fact, contained in the lower part of Figure 7 because $\cos^2(\pi(x - t)/10) = \sin^2(\pi(x - (t + 5))/10)$. As $\cos^2(\pi x/10)$ satisfies the conditions of Theorem 3.23 (with $\alpha = 1$ and, for instance, $\beta = 0.3$), we know that the alternative (b2) has to apply.

3.2.2 One-sided Dislocations

As the second representative example of the dislocation problem (1.1) with (1.3) we choose $s = 0, t \in (0, d)$, which is equivalent to the system

$$\begin{array}{ll} L_-^0 \psi^t := -\partial_x^2 \psi^t + V_0(x)\psi^t = \lambda \psi^t & \text{for } x < 0, \\ L_+^t \psi^t := -\partial_x^2 \psi^t + V_0(x+t)\psi^t = \lambda \psi^t & \text{for } x \ge 0 \end{array} \qquad (3.27)$$

coupled by the the C^1-matching conditions (3.14). Localized eigenfunctions ψ^t, once again, exist only for $\lambda \notin \sigma(L_0)$ and have the form

$$\psi^t(x;\lambda) = \psi_-^0(x;\lambda)\chi_{\{x<0\}} + \psi_+^t(x;\lambda)\chi_{\{x\ge 0\}},$$

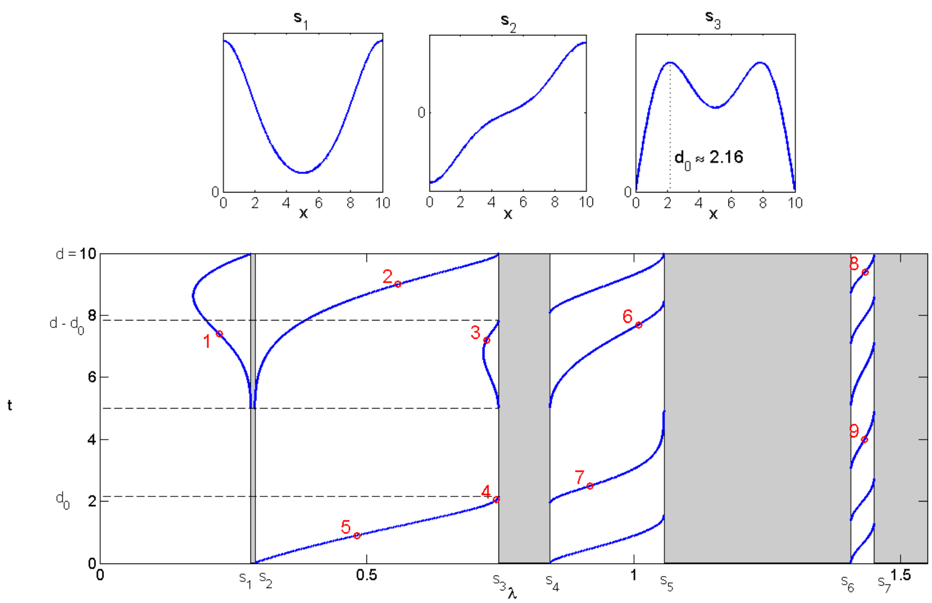

Figure 7: top: the first three band edge Bloch functions of L_0 with $V_0(x) = \sin^2(\pi x/10)$; bottom: point spectrum of L for (1.3) with $s = -t$ and $V_0 = \sin^2(\pi x/10)$ for $t \in [0, d)$. The spectral bands of L are shaded. Eigenfunctions for the labeled points are plotted in Figure 8.

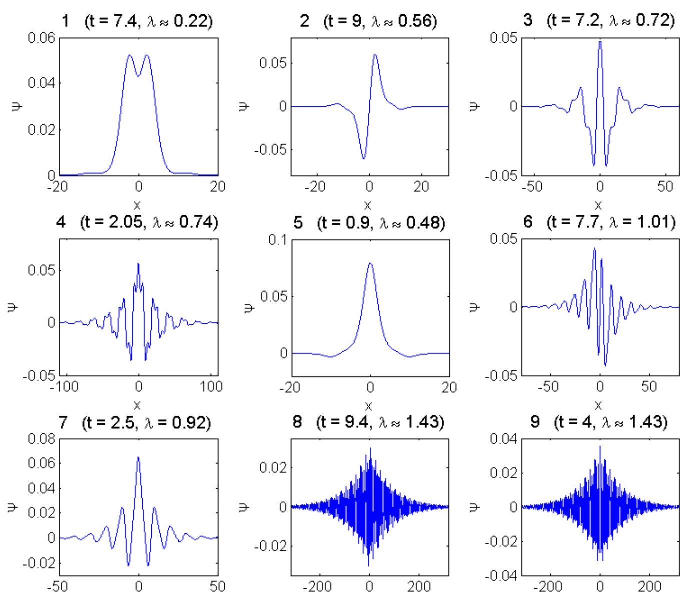

Figure 8: Eigenfunctions corresponding to the 9 labeled eigenvalues in Figure 7.

where $\psi_-^0(x; \lambda)$ and $\psi_+^t(x; \lambda)$ are those Bloch functions of L_0 and $L_t = -\partial_x^2 + V_0(x+t)$, which decay on $\mathbb{R}^-$ and $\mathbb{R}^+$, respectively. The matching condition (3.14) now becomes

$$R_+^0(t; \lambda) = R_-^0(0; \lambda),$$

where $R_-^0(0;\lambda)$ is the same as $R_-(\lambda)$ defined in (3.4).

Because $R_-^0(0;\lambda)$ is decreasing and continuous in each gap (Lemma 3.1) and given the analysis of $R_+^0(t;\lambda)$ in Section 3.2.1, determining intersections of $R_+^0(t;\lambda)$ and $R_-^0(0;\lambda)$ in G_0 and G_1 is now straightforward.

Lemma 3.14. *For $s=0$ the number of dislocation eigenvalues in any gap $G_n, n \geq 0$, is $0, 1$ or 2.*

Proof. $R_+^0(t;\lambda)$ is strictly increasing and continuous in λ on each continuity segment and its continuity can be broken only at one point (pole) in G_n, see Lemma 3.8. As $R_-^0(0;\lambda)$ is continuous and decreasing throughout G_n, only up to 2 intersections of $R_+^0(t;\lambda)$ and $R_-^0(0;\lambda)$ can occur. □

Theorem 3.15. *Suppose V_0 satisfies the basic assumptions, i.e., continuous, even and d-periodic and $s=0$ in (1.3), and consider the semi-infinite gap $G_0=(-\infty, s_1)$.*

(a) If V_0 is strictly increasing on $[0,d/2]$, then there is exactly zero/one dislocation eigenvalue in G_0 for $t \in (0,d/2]$ / $(d/2,d)$ respectively.

(b) If V_0 is strictly decreasing on $[0,d/2]$, then there is exactly one/zero dislocation eigenvalue in G_0 for $t \in (0,d/2)$ / $[d/2,d)$ respectively.

Proof. We, once again, present the proof only of (a) as (b) follows by shifting the potential in x (or t) by $d/2$. As explained in the proof of Theorem 3.11, s_1 is a Neumann eigenvalue and the corresponding eigenfunction can be taken positive and strictly decreasing on $[0,d/2]$ with a point of even symmetry at $x=d/2$.

By Lemmas 3.1, 3.2 and 3.3 the function $R_-^0(0;\lambda)$ decreases continuously from ∞ at $\lambda \to -\infty$ to 0 at $\lambda = s_1$. The behavior of $R_+^0(t;\lambda)$ is explained in the proof of Theorem 3.11. It follows that $R_-^0(0;\lambda)$ and $R_+^0(t;\lambda)$ intersect in G_0 exactly once for $t \in (d/2,d)$ and do not intersect for $t \in (0,d/2]$. □

Theorem 3.16. *Suppose V_0 is an even, d-periodic C^1-function, let $s=0$ in (1.3) and consider the first finite gap $G_1=(s_2,s_3)$.*

(a) If V_0 is strictly increasing on $[0,\frac{d}{2}]$, so that $G_1=(\nu_2,\mu_1)$, then there is exactly one dislocation-eigenvalue in G_1 for all $t \in (0,d)$.

(b) If V_0 is strictly decreasing on $[0,\frac{d}{2}]$, so that $G_1=(\mu_1,\nu_2)$, then we have the following alternative for the second Neumann-eigenfunction u:

  (b1) u is strictly monotone on $[0,\frac{d}{2}]$. Then there is exactly one dislocation-eigenvalue in G_1 for all $t \in (0,d)$.

  (b2) u changes monotonicity on $[0,\frac{d}{2}]$ exactly once at the extremal point $d_0 \in (0,\frac{d}{2})$. Then the number of dislocation-eigenvalues in G_1 is as follows:

dislocation parameter	$t \in (0,d_0)$	$t \in [d_0, d-d_0)$	$t \in [d-d_0, d)$
number of eigenvalues	2	1	0

Proof. Case (a): As explained in the proof of part (a) of Theorem 3.12, for $t \in (0, d/2]$ we have $R_+^0(t; s_2) < 0$ and $R_+^0(t; \lambda)$ continuous and increasing in $\lambda \in G_1$. Therefore, $R_+^0(t; \lambda)$ intersects exactly once $R_-^0(0; \lambda)$, which decreases continuously from 0 at $\lambda = s_2$ to $-\infty$ at $\lambda \to s_3-$, see Lemmas 3.1, 3.2.

Next, as the proof of Theorem 3.12 (a) shows, for $t \in (d/2, d)$ the function $R_+^0(t; \lambda)$ has a pole at some $\lambda_0 \in G_1$ and increases continuously on the interval (s_2, λ_0) with $R_+^0(t; s_2) > 0, R_+^0(t; \lambda_0-) = \infty$ and on the interval (λ_0, s_3) with $R_+^0(t; \lambda_0+) = -\infty, R_+^0(t; s_3) < R_+^0(t; s_2)$. The functions $R_+^0(t; \lambda)$ and $R_-^0(0; \lambda)$, therefore, intersect exactly once on $\lambda \in (\lambda_0, s_3)$ and they do not intersect on $\lambda \in (s_2, \lambda_0)$.

Case (b): In the case of V_0 strictly decreasing on $[0, d/2]$ the function $R_-^0(0; \lambda)$ is continuous and strictly decreasing from ∞ at $\lambda \to s_2+$ to 0 at $\lambda = s_3$, see Lemmas 3.1, 3.2. We obtain below the behavior of $R_+^0(t; \lambda)$ from that of $R(t; \lambda)$ in the proof of Theorem 3.12 (a) by the shift of $d/2$ in t and switching of the roles of μ_1 and ν_2.

Case (b1): For $t \in (0, d/2)$ we have $R_+^0(t; \mu_1) > 0 > R_+^0(t; \nu_2)$ and $R_+^0(t; \lambda)$ has one pole in λ within G_1. $R_-^0(0; \lambda)$ thus intersects $R_+^0(t; \lambda)$ exactly once on G_1. For $t \in [d/2, d)$ the function $R_+^0(t; \lambda)$ is continuous on G_1 and $R_+^0(t; \mu_1) \leq 0 < R_+^0(t; \nu_2)$. Exactly one intersection of $R_+^0(t; \lambda)$ and $R_-^0(0; \lambda)$ thus exists.

Case (b2): For $t \in (0, d_0)$ the function $R_+^0(t; \lambda)$ behaves in λ like $R(t; \lambda)$ on $t \in (d/2, d - d_0)$ in the proof of Theorem 3.12 (a2). Namely, we get $R_+^0(t; \mu_1) > R_+^0(t; \nu_2) > 0$ and a pole of $R_+^0(t; \lambda)$ at some $\lambda \in G_1$. Two intersections of $R_+^0(t; \lambda)$ and $R_-^0(0; \lambda)$ thus exist. For $t \in [d_0, d - d_0)$ the behavior of the eigenfunction and hence of $R_+^0(t; \lambda)$ is qualitatively the same as in (b1) of this proof and precisely one eigenvalue thus appears in G_1. Finally, for $t \in [d - d_0, d)$ the function $R_+^0(t; \lambda)$ behaves in λ like $R(t; \lambda)$ on $t \in [d_0, d/2)$ in the proof of Theorem 3.12 (a2). Therefore, $R_+^0(t; \mu_1) < R_+^0(t; \nu_2) \leq 0$ and $R_+^0(t; \lambda)$ is continuous throughout G_1. No intersections of $R_+^0(t; \lambda)$ and $R_-^0(0; \lambda)$ thus occur. □

Numerical Results Results of numerical eigenvalue computations with the dislocation interface (1.3) with $s = 0$ and $V_0 = \sin^2(\pi x/10)$ are in Figure 9. They agree with Theorems 3.15 and 3.16. Figure 10 shows the eigenfunctions corresponding to the 6 labeled eigenvalues in Figure 9. As expected, they lack symmetry in contrast with the eigenfunctions of the symmetric dislocation in Figure 8.

The results for $V_0(x) = \cos^2(\pi x/10)$, as an example of a potential that falls in the case (b) of Theorem 3.16, appear in Figures 11 and 12. As we know from Section 3.2.1, the potential $\cos^2(\pi x/10)$ falls into the case (b2) and the second Neumann eigenfunction thus changes monotonicity on $(0, d/2)$, see Figure 11 top. Agreement of the numerics with Theorems 3.15 and 3.16 is, once again, observed.

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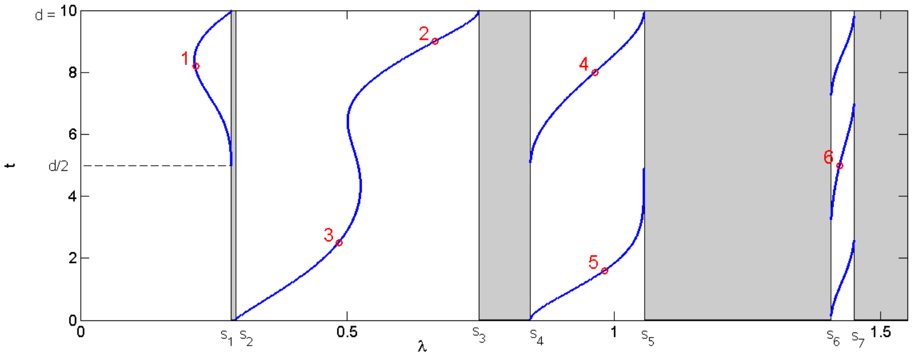

Figure 9: Point spectrum of L for (1.3) with $s = 0$ and $V_0 = \sin^2(\pi x/10)$. Eigenfunctions for the labeled points are plotted in Figure 10.

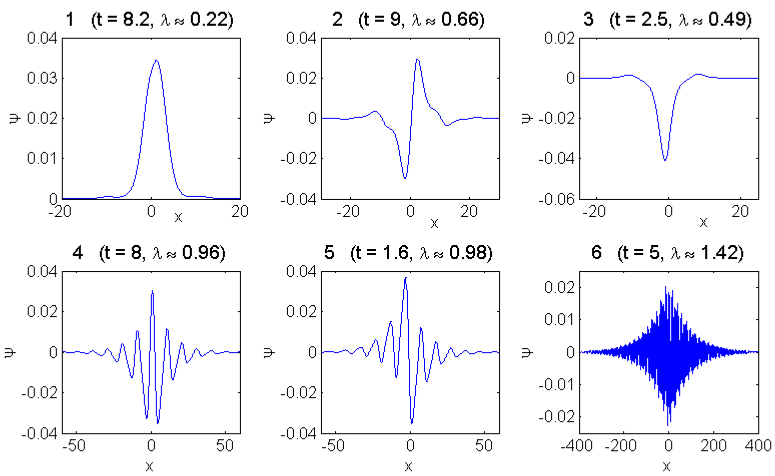

Figure 10: Eigenfunctions corresponding to the 6 labeled eigenvalues in Figure 9.

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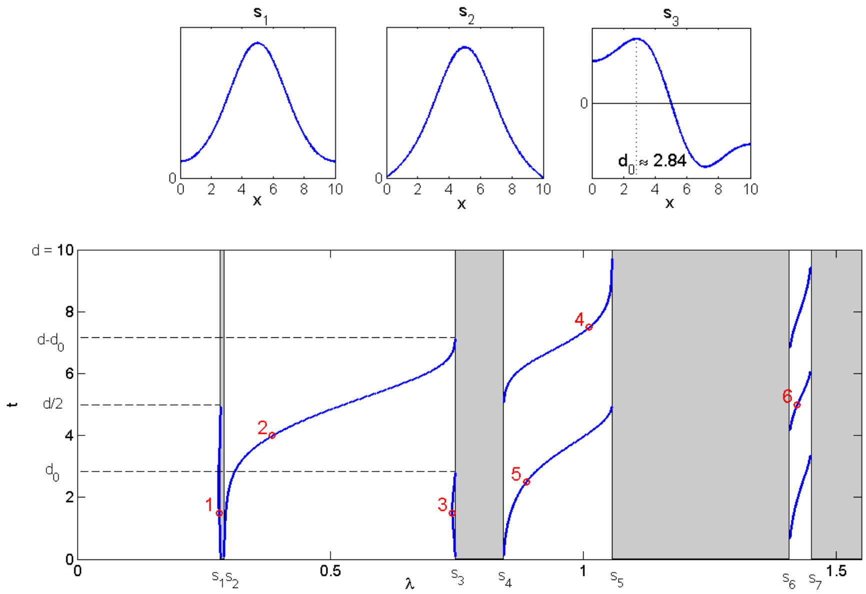

Figure 11: top: the first three band edge Bloch functions of L_0 with $V_0(x) = \cos^2(\pi x/10)$; bottom: point spectrum of L for (1.3) with $s = 0$ and $V_0 = \cos^2(\pi x/10)$ for $t \in [0, d)$. The spectral bands of L are shaded. Eigenfunctions for the labeled points are plotted in Figure 12.

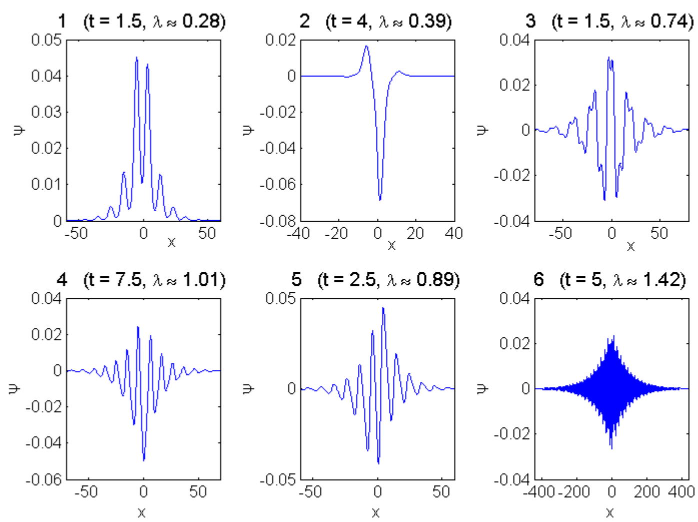

Figure 12: Eigenfunctions corresponding to the 6 labeled eigenvalues in Figure 11.

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