Dislocation Defects and Diophantine Approximation
Jared C. Bronski
Zoi Rapti
University of Illinois, Department of Mathematics,

Abstract
In this paper we consider a Schrödinger eigenvalue problem with a potential consisting of a periodic part together with a compactly supported defect potential. Such problems arise as models in condensed matter to describe color in crystals as well as in engineering to describe optical photonic structures. We are interested in studying the existence of point eigenvalues in gaps in the essential spectrum, and in particular in counting the number of such eigenvalues. We use a homotopy argument in the width of the potential to count the eigenvalues as they are created. As a consequence of this we prove the following significant generalization of Zheludev’s theorem: the number of point eigenvalues in a gap in the essential spectrum is exactly 1 for sufficiently large gap number unless a certain Diophantine approximation problem has solutions, in which case there exists a subsequence of gaps containing 0, 1, or 2 eigenvalues. We state some conditions under which the solvability of the Diophantine approximation problem can be established.

1 Introduction

Periodic media with defects have long been studied in physics and applied mathematics. Such problems have been studied in quantum mechanics and condensed matter physics\cite{1} to model the effect of impurities on the color of a crystal. Since the development of photonic crystals\cite{10, 11, 12} and the ability of engineers to construct such defects in an optical context this area has received new attention. Most of these studies are concerned with the characterization of the spectrum of the medium due to the presence of the defect. More precisely, since a defect does not change the essential spectrum of the associated operators, the main problem is to study the creation of isolated point eigenvalues of finite multiplicity in the spectral gaps of the unperturbed problem.

There is a fairly extensive literature on the study of the existence and number of bound states with energies that lie in a spectral gap. Much of this literature\cite{2, 11, 12, 16} employs some variant of the Birman-Schwinger principle in order to count the number of gap modes. The Birman-Schwinger principle is, in essence, a homotopy argument in the coupling strength of the defect potential, where one tries to estimate the number of eigenvalues below a given value of the coupling strength. Weyl asymptotics and Dirichlet-Neumann bracketing have been used to produce asymptotic estimates for the number of defect eigenvalues in the spectral gap of Schrödinger operators in the large coupling limit. Other studies\cite{8} have used formal perturbation methods to investigate the origin and distribution of defect modes.

Perhaps the closest results to the ones presented here are due to Zheludev\cite{39, 40}, Rofe-Betekov\cite{27, 28} and Firsova\cite{13, 14} (see also the paper of Gesztesy...
and Simon[10], which gives a self contained derivation of these results). In these papers the following results are shown: given Schrödinger operator in one dimension with potential of the form \( q_{\text{per}}(x) + q_{\text{def}}(x) \), where \( q_{\text{per}}(x + a) = q_{\text{per}}(x) \) is periodic, \( q_{\text{per}} \in L^1_{\text{loc}}(\mathbb{R}) \), \((1 + |x|)q_{\text{def}}(x) \in L^1(\mathbb{R})\) then

i. There are a finite number of eigenvalues in each gap in the essential spectrum.

ii. There are at most two eigenvalues in each sufficiently large numbered gap.

iii. If \( \int q_{\text{def}}(x)dx \neq 0 \) there is precisely one eigenvalue in each sufficiently large numbered gap.

In this paper we will be concerned with the periodic Schrödinger eigenvalue problem with a compactly supported defect

\[
- u_{xx} + q(x) u = E u \quad x \in \mathbb{R}
\]

\[
q(x) = \begin{cases} 
q_{\text{per}}(x) & x \leq 0 \\
q_{\text{def}}(x) & x \in (0, 1) \\
q_{\text{per}}(x - 1) & x \geq 1
\end{cases}
\]

where the potential \( q_{\text{per}} \) has period \( a : q_{\text{per}}(x + a) = q_{\text{per}}(x) \). Note that we do not necessarily assume any particular relationship between the width of the defect (scaled for convenience to be 1) and the period of the potential \( q_{\text{per}}(x) \) (denoted by \( a \)) so there is a relative phase shift or dislocation in the potential between \(-\infty \) and \(+\infty \) if \( a^{-1} \) is not an integer. In engineering applications defects are created by cutting and layering materials with different properties, so the above form of the defect is actually extremely natural from the point of view of applications[37]. This asymptotic phase shift in the periodic potential will turn out to have very interesting physical and mathematical properties, and does not appear to have been previously considered.

An outline of the paper is as follows: we first give a simple topological argument relating the number of point eigenvalues in a gap to the number of connected components of the intersection of the gap with a certain set, essentially a resolvent set associated with the defect. Next we give necessary Diophantine condition for large-numbered gaps to intersect this resolvent set. In the end we establish the following result: Defining \( \Delta q \) to be the mean energy difference between the defect and periodic potentials

\[
\Delta q = \int_0^1 q_{\text{def}}(x)dx - \frac{1}{a} \int_0^a q_{\text{per}}(x)dx
\]

there is a set \( \mathcal{F}_a \) related to the distribution of errors in Diophantine approximation of \( a \) such that the following holds: if \( a\Delta q \notin \mathcal{F}_a \) then every sufficiently large numbered gap contains exactly one eigenvalue. If \( a\Delta q \in \mathcal{F}_a \) there exists a subsequence of gaps related to rational approximants of \( a \) which may contain 0, 1 or 2 eigenvalues. The set \( \mathcal{F}_a \) satisfies \( \mathcal{F}_a = \mathcal{F}_{a'} \) if \( a \) and \( a' \) are related by an element of the modular group \( \text{PSL}(2, \mathbb{Z}) \). The results of Zheludev, Firsova
and Rofe-Betekov are analogous to the case with no asymptotic phase shift, \( a^{-1} \equiv 0 \pmod 1 \), whose equivalence class is the rationals. For rational \( a \) the set \( F_a \) is simply the point 0, analogous to point (iii) above. For irrational \( a \), however, the set \( F_a \) is much more interesting. We characterize \( F_a \) for certain cases, and give an explicit example of a periodic potential and defect having a subsequence of gaps containing exactly 2 eigenvalues.

2 Preliminaries

In this section we define the important quantities for the defect eigenvalue calculation and present some technical results on the behavior of these quantities. Many of these are standard results which can be found in (for example) the text of Magnus and Winkler on Hill’s equation.

2.1 Basic Definitions and Equations

We will usually write equation (1) as a system

\[
\frac{d}{dx} \begin{pmatrix} u \\ p \end{pmatrix} = J \begin{pmatrix} E - q(x) & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = JH \begin{pmatrix} u \\ p \end{pmatrix}
\]

(3)

where the potential \( q \) is assumed to be piecewise \( C^1 \). This assumption could probably be weakened to allow Hamiltonians defined as quadratic forms, but we have not done this.

It is clear from a standard Weyl sequence argument that the essential spectrum of (1) is the same as the essential spectrum of the purely periodic problem

\[-u_{xx} + q_{\text{per}}(x)u = Eu\]

and, because the defect is compactly supported, there are no imbedded eigenvalues in the essential spectrum. See the general discussion in Reed and Simon\[25]\] and more specifically Theorem 6.28 in Rofe-Beketov and Kholkin\[26]\], which applies immediately to this case. Thus we need only understand the presence of point spectrum in the resolvent set of the periodic problem - the spectral gaps.

Let us recall some standard definitions and facts from Floquet theory.

We define \( M(E) \), the monodromy matrix for the periodic problem, to be

\[M(E) = U(E, a),\]

(4)

where the fundamental solution matrix \( U(E, x) \) satisfies

\[
U_x = J \begin{pmatrix} E - q_{\text{per}}(x) & 0 \\ 0 & 1 \end{pmatrix} U = JH_{\text{per}}(E, x)U
\]

(5)

\[U(E, 0) = I.\]
where $I$ is the identity matrix. The monodromy $M(E)$ satisfies the identity $M^tJM = J$ (i.e., $M(E)$ is a symplectic matrix). The Floquet discriminant associated to the periodic problem is defined to be

$$k(E) = \text{tr}(M(E))$$

The band edges $\{E_j\}_{j=0}^\infty$ are the roots of $k^2(E) = 4$ in increasing order and respecting multiplicity. The band edges $E_k$ are periodic points ($k(E_j) = 2$) if $j \equiv 0, 3 \mod 4$ and are antiperiodic points ($k(E_j) = -2$) if $j \equiv 1, 2 \mod 4$. An energy $E$ is said to belong to a band or a gap if $k^2(E) < 4$ or $k^2(E) > 4$ respectively. The bands are given by intervals of the form

$$k^2(E) < 4 \quad E \in (E_{2j}, E_{2j+1})$$

and the gaps by the intervals of the form

$$k^2(E) > 4 \quad E \in (E_{2j-1}, E_{2j}) = \mathcal{G}_j.$$ 

The slope of the Floquet discriminant in a band can be interpreted as the Krein signature\cite{20, 38, 4} of the eigenvalues of $M(E)$, although we will not exploit this here. The essential spectrum is the union of the bands and band edges:

$$\sigma_{\text{ess}} = \bigcup_{j=0}^\infty [E_{2j}, E_{2j+1}]$$

For energies in a gap, $E \in (E_{2j-1}, E_{2j})$, the monodromy matrix $M(E)$ has two distinct real eigenvalues,

$$M(E)v_\pm = \lambda_\pm v_\pm \quad |\lambda_-| < 1 < |\lambda_+|$$

one of modulus greater than one and one of modulus less than one. The resolvent set of the periodic problem

$$\mathcal{R}_{\text{per}} = \bigcup_{j=0}^\infty (E_{2j-1}, E_{2j})$$

will prove important. Here we use the convention that $E_{-1} = -\infty$ so the zeroth gap is the semi-infinite one $(-\infty, E_0)$.

Similarly $N(E, x)$ will denote the fundamental solution matrix associated to the defect

$$N_x = J \begin{pmatrix} E - q_{\text{def}}(x) & 0 \\ 0 & 1 \end{pmatrix} N = JH_{\text{def}}(E, x)N \quad (6)$$

$N(E, 0) = I$. 

4
We will define the Floquet discriminant for the defect to be

\[ k_{\text{def}}(E, x) = \text{tr} (N(E, x)) \]

We will refer to a point \((E, x)\) as belonging to a band, band-edge or gap for the defect problem if \(k_{\text{def}}^2(E, x) < 4\), \(k_{\text{def}}^2(E, x) = 4\), or \(k_{\text{def}}^2(E, x) > 4\) respectively.

The eigenvectors of \(N(x, E)\) in a gap will be denoted \(w_{\pm}\):

\[ N w_{\pm} = \tau_{\pm} w_{\pm}, \quad |\tau_-| < 1 < |\tau_+|. \]

We will often work with \(N(E, 1)\), the fundamental matrix evaluated at the end of the support of the defect potential, which with some small abuse of notation we refer to as the monodromy map for the defect. This will be denoted by \(N(E) = N(E, 1)\). We will also have occasion to fix either \(x\) or \(E\), and consider the the band-gap structure as the other quantity varies. In such cases we will refer to the gaps as being “in \(x\)” or “in \(E\)” as appropriate.

For the remainder of this discussion we consider a fixed energy \(E \in G_j\) in a gap of the essential spectrum. The eigenvectors \(v_{\pm}\) represent Jost-type solutions: \(v_+\) represents a solution to the periodic problem satisfying \(\lim_{n \to \infty} M^n v_+ = 0\), while \(v_-\) represents a solution to the periodic problem which satisfies \(\lim_{n \to \infty} M^n v_- = 0\). In order to have an \(L^2\) solution the solution which is decaying at \(-\infty\) must connect to the solution which is decaying at \(+\infty\). Since the defect potential is compactly supported this eigenvalue condition reduces to the following: \(N\), the transfer matrix for the defect mode, should map \(v_+\), the left Jost eigenvector for the periodic problem to a scalar multiple of \(v_-\), the right Jost eigenvector for the periodic problem. In other words for \(E \in G_j \subset \mathbb{R}_{\text{per}}\) and \(N(E)\) defined as above, the eigenvalue condition becomes

\[ N(E) v_+ = \mu v_. \quad (7) \]

Since we are in the \(2 \times 2\) case this is equivalent to the vanishing of the following inner product:

\[ \langle v_-, J N(E) v_+ \rangle = f(E) = 0, \quad (8) \]

where \(J\) is the standard skew-symmetric matrix \(J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\) defined previously. The function \(f(E)\) is the Evans function associated to the defect potential. Note that, by continuity \(f(E)\), can be defined uniquely at the band-edge: standard results (see Kato\[20\]) guarantee that the eigenvectors have a Puiseux series representation in powers of \((E - E_j)^{-\frac{1}{2}}\) in the neighborhood of a band edge \(E_j\). In a more general setting the Evans function is defined as a determinant of exponentially decaying Jost-type solutions, but throughout this paper we will make extensive use of the fact (obviously unique to the second order case) that the determinant can be written as the inner product with the standard skew-form \(J\). This, together with the fact that the Hamiltonian nature of the problem respects the skew-form, will simplify many of the calculations.

The zeros of the Evans function defined in Eq. (8) define the defect eigenvalues. However it is convenient to consider the width of the defect \(x\) as a
parameter. In this way we can make a homotopy argument in $x$, and count the roots of the above equation as they are created, with $x = 0$ corresponding to a purely periodic problem and $x = 1$ to the periodic problem with a defect. If $N(E, x)$ is the fundamental solution operator for the defect potential as defined in (6) we define a generalized Evans function to be

$$f(E, x) = \langle v_-, JN(E, x)v_+ \rangle, \quad x \in [0, 1].$$

(9)

The goal is to apply an implicit function argument to show that the zeros of the generalized Evans function lie on continuous curves $E(x)$, and thus can be tracked as functions of the homotopy parameter $x$.

Throughout this paper $G_j = (E_{2j+1}, E_{2j+2})$ will denote a gap in the essential spectrum, which is assumed to be non-empty. We will let $D_{G_j}$ represent the number of defect eigenvalues in $G_j$:

$$D_{G_j} = \#(E \in G_j \mid f(E) = 0).$$

Of course the goal of the paper is to understand $D_{G_j}$ for a general potential.

Finally $R_{def}$ will denote the set

$$R_{def} \{E \mid |\text{tr}(N(1, E))|^2 \geq 4\},$$

the energies for which the map across the defect has real eigenvalues. If one considers the periodic Schrödinger operator where the potential is the defect potential $q_{def}$ which is defined on $[0, 1]$ is extended to a 1-periodic function in the obvious way, then the set $R_{def}$ is the union of the resolvent set of this operator with the periodic and antiperiodic eigenvalues. Our count of the number of point eigenvalues in a gap can be expressed in terms of the number of components of the intersection of this set with the resolvent set of the periodic problem. Note that, despite the similarity in notation, $R_{def}$ is a closed set whereas $R_{per}$ is an open set, for reasons that should become clear.

### 2.2 Preliminary lemmas

We start with some facts about the dependence of the eigenvalues and eigenvectors of a $2 \times 2$ real symplectic matrix $M(E)$ on a real parameter $E$. We assume that $E \in R_{per}$, so that the eigenvalues are real and distinct. The eigenvectors $v_\pm$, while not orthogonal, are linearly independent and form a basis. We will normalize these vectors so that $\|v_+\| = \|v_-\| = 1$. It is convenient to define a second set of vectors, the dual basis, $v_+^tJ$, $v_-^tJ$. It is clear that these two sets are bi-orthogonal (though typically not orthonormal).

**Lemma 1.** Suppose that $M(E)$ is defined as in (8) has real distinct eigenvalues $|\lambda_-| < 1 < |\lambda_+|$ and eigenvectors $v_\pm$ ($|v_\pm| = 1$), and define $\alpha_\pm = \langle \frac{dv_\pm}{dE}, Jv_\pm \rangle$. Then we have

$$\alpha_\pm = \frac{\lambda_\pm \langle v_\pm, JM(E)v_\pm \rangle}{1 - \lambda_\pm^2}.$$  

(10)
Similarly if \( N(E, x) \) defined in (6) has real distinct eigenvalues \( \tau_{\pm} \) with \(|\tau_-| < 1 < |\tau_+|\) and associated eigenvectors \( w_{\pm} \) (\(|w_{\pm}| = 1\)) and we define

\[
\langle \frac{dw_+}{dx}, J w_\pm \rangle = \beta_\pm \tag{11}
\]

\[
\langle \frac{dw_+}{dx}, J w_\pm \rangle = \delta_\pm \tag{12}
\]

then the functions \( \beta_\pm, \delta_\pm \) satisfy

\[
\beta_\pm = \frac{\tau_+(w_+, J N_E w_\pm)}{1-\tau_\pm^2} \tag{13}
\]

\[
\delta_\pm = \frac{\tau_-(w_+, J N_x w_\pm)}{1-\tau_\pm^2} \tag{14}
\]

Note that the normalization \( \|w_{\pm}\| = 1 \) implies that

\[
\frac{dw_\pm}{dE} = \beta_\pm J w_\pm, \tag{15}
\]

\[
\frac{dw_\pm}{dx} = \delta_\pm J w_\pm, \tag{16}
\]

and similarly \( v_{\pm} \).

Proof. The eigenvalue equation is

\[
M v_+ = \lambda_+ v_+. \tag{17}
\]

Differentiation with respect to the parameter \( E \) gives

\[
\frac{dM}{dE} v_+ + M \frac{dv_+}{dE} = \frac{d\lambda_+}{dE} v_+ + \lambda_+ \frac{dv_+}{dE}. \tag{18}
\]

Taking the second equation and multiplying by \( J \) and dotting with \( v_{\pm} \), and using the fact that \( M \) is symplectic, gives

\[
\alpha_+(\lambda_+^{-1} - \lambda_+) = \langle v_+, J M_E v_+ \rangle
\]

\[
\alpha_-(\lambda_-^{-1} - \lambda_-) = \langle v_-, J M_E v_- \rangle
\]

Multiplying by \( J \) and dotting with \( v_\pm \) gives the equation for the change in the eigenvalue, and similar calculations give the equations for the other parameters. Note that all of the denominators are non-zero away from the band edges. \( \square \)

**Remark 1.** This is a slight modification of the Hellmann-Feynman lemma for self-adjoint matrices to the case of matrices in \( \text{Sp}(2, \mathbb{R}) \) with real distinct eigenvalues. Note that this result only uses the fact that the matrix \( M \) is in \( \text{Sp}(2, \mathbb{R}) \) with real eigenvalues, and does not use the fact that the monodromy matrices come from a specific second order self-adjoint eigenvalue problem.

The next two results exploit the fact that the monodromy matrices are derived from Schrödinger operators to show positivity/monotonicity of various quantities defined above. The first type of result is a Sturm oscillation type
result for the energy variable $E$, and shows that $\alpha_{\pm}, \delta_{\pm}, \beta_{\pm}$ are of a fixed sign. Since, by the above calculation, these parameters represent a sense of rotation of the eigenvectors, this result shows that (as a function of the energy) one eigenvector winds about the origin in a positive sense as the energy increases, and the other winds in a negative sense.

**Proposition 1.** The monodromy matrices $M(E), N(E,x)$ satisfy the differential equations (in $E$)

\[
M_E = MJ\Phi(E) \quad (19)
\]

\[
N_E = NJ\Theta(E,x) \quad (20)
\]

where the matrix $\Phi$ is positive definite, and $\Theta(E,0) = 0$ and $\Theta$ is positive definite for $x > 0$.

**Proof.** This calculation follows that given in Magnus and Winkler [22]. It is easy to see that $N_E$ satisfies the differential equation

\[
N_{x,E} = JHN_E + JH_E N_E(E,0) = 0 \quad (21)
\]

and a solution by variation of parameters gives the formula

\[
N_E = N \int_0^x N^{-1} JH_E N. \quad (22)
\]

Using the fact that $N^tJN = J$ the above becomes

\[
N_E = NJ \int_0^x N^tH_E N. \quad (23)
\]

It is clear that if $H_E$ is positive semi-definite then $\int N^tH_E N$ is also positive semi-definite, and in fact positive definite for $x > 0$ unless there exists a non-zero vector $v$ independent of $y$ such that $H_E N(E,y)v = 0$ for all $y$. For the equations considered here it is easy to see that no such $v$ can exist, and therefore $\int_0^x N^tH_E N(E,y)dy$ is positive-definite. Similarly $M(E)$ has the representation

\[
M_E = MJ \int_0^x U^t(E,y)H_E U(E,y)dy. \quad (24)
\]

**Remark 2.** The fact that $M_E = MJ\Phi$ (and similarly $N_E$) is simply the fact that the Lie algebra associated to the symplectic group is matrices of the form $JH$ with $H$ symmetric. The positivity of $\Phi$ is essentially the Sturm oscillation theorem.

**Corollary 1.** Let $v_{\pm}, w_{\pm}$ be the eigenvectors in a gap for the periodic and defect monodromy matrices respectively, and $\alpha_{\pm}, \beta_{\pm}, \delta_{\pm}$ be defined as in Eq.
\[
\frac{\partial v_\pm}{\partial E} = \alpha_\pm J v_\pm \quad (25)
\]
\[
\frac{\partial w_\pm}{\partial E} = \beta_\pm J w_\pm \quad (26)
\]
\[
\frac{\partial w_\pm}{\partial x} = \delta_\pm J w_\pm \quad (27)
\]

then \(\beta_+, \alpha_+ > 0\) and \(\beta_-, \alpha_- < 0\). Further, if the Hamiltonian matrix in the defect region \(H_{def}(E, x)\) is positive-definite, then \(\delta_+ > 0\) and \(\delta_- < 0\).

Proof. We know that the \(\beta_\pm\) satisfy
\[
\beta_+ = \frac{\lambda_+ \langle w_+, J N_E w_+ \rangle}{1 - \lambda_+^2} \\
\beta_- = \frac{\lambda_- \langle w_-, J N_E w_- \rangle}{1 - \lambda_-^2}
\]

Using the fact that \(N_E = NJ\Theta\) and \(N^T J N = J\) we have that
\[
\beta_+ = \frac{\lambda_+ \langle w_+, J N J \Theta w_+ \rangle}{1 - \lambda_+^2} \\
= \frac{-\lambda_+ \langle w_+, N^{-T} \Theta w_+ \rangle}{1 - \lambda_+^2} \\
= \frac{\langle w_+, \Theta w_+ \rangle}{\lambda_+^2 - 1} > 0
\]

and similarly \(\beta_-, \alpha_+, \alpha_-\). Using the fact that \(\Theta\) is positive-definite and \(|\lambda_+|^2 > 1\) we have that \(\alpha_+ > 0, \alpha_- < 0\).

The second part follows similarly: \(J N_x = -H_{def} N\), thus
\[
\delta_\pm = \frac{\lambda_\pm \langle w_+, -H_{def} N w_+ \rangle}{1 - \lambda_\pm^2} \quad (28)
\]
with \(H_{def}\) positive definite, and the above argument follows.

\[\square\]

3 Counting the Defects

In this section we present the main results, which allow us to estimate the number of gap eigenvalues created by a defect potential in terms of the winding number of the monodromy matrix at the band edge. Again the basic idea is to make a homotopy argument in \(x\) of the generalized Evans function \(f(E, x)\), and count the eigenvalues as the are created.

The first important result is the following:
Lemma 2. Suppose that $E \in \mathcal{R}_{def}$. The Evans function $f(E, x)$ and its first partial with respect to the energy $\frac{d f}{dE}$ cannot vanish simultaneously. For energies in the classically allowed region for the defect $\frac{\partial f}{\partial x}$ cannot vanish at a zero of the Evans function, and has the same sign as $\frac{\partial f}{\partial E}$.

Proof. Obviously we have the following expression for $f_E$:

$$f_E = \langle \frac{dv_-}{dE}, J N v_+ \rangle + \langle v_-, J N \frac{dv_+}{dE} \rangle + \langle v_-, J \frac{dN}{dE} v_+ \rangle. \quad (29)$$

Using the identities $\frac{dN}{dE} = NJ \Theta$ and $N^t J N = J$ the above expression reduces to

$$f_E = \alpha_- \langle v_-, N v_+ \rangle - \alpha_+ \langle v_-, N^{-1} v_+ \rangle - \langle v_-, N^{-1} \Theta v_+ \rangle. \quad (30)$$

We would like to compute the signs of the various terms above at a zero of the Evans function $f$. Note that, at a zero, we have $N v_+ = \mu v_-$, or $N + 1 v_- = \mu v_+$. Using this fact we have

$$f_E = \mu \alpha_- - \frac{\alpha_+}{\mu} - \frac{1}{\mu} \langle v_+, \Theta v_+ \rangle \quad (31)$$

Since $\Theta$ is positive definite, $\alpha_- < 0$ and $\alpha_+ > 0$ we have that $f_E$ cannot vanish at a zero of the Evans function and has the opposite sign from $\mu$. A similar but more straightforward calculation gives

$$f_x = \langle v_-, J N_x v_+ \rangle = \langle v_-, JJ H_{def} N v_+ \rangle \quad (32)$$
$$= -\mu \langle v_-, H_{def} v_- \rangle \quad (33)$$

where the last step assumes that one is at a zero of $f(E, x)$. Again $H_{def}$ is positive definite in the Schrödinger case for energies in the classically allowed region (for the defect) and in the other cases without restriction.

This result has a small technical drawback, in that the derivative of the Evans function with respect to energy diverges near the band edges of the periodic problem, since the spectral quantities have square-root type singularities near the band edges. These can easily be eliminated by choosing appropriate coordinates in the gap.

Lemma 3. For a given gap $G_j = (E_{2j+1}, E_{2j+2}) \subset \mathcal{R}_{per}$ define the new variable $\tilde{E}$ by the invertible map

$$\tilde{E} = \int_{E_{2j+1}}^{E} \frac{dE}{\sqrt{k^2(E) - 4}}$$

that maps $[E_{2j+1}, E_{2j+2}]$ to $[0, \omega_j]$, with $\omega_j = \int_{E_{2j+1}}^{E_{2j+2}} \frac{dE}{\sqrt{k^2(E) - 4}}$. Then $f$ is a $C^1$ function of $\tilde{E}$ in $[0, \omega_j]$, and $f$ and $f_{\tilde{E}}$ cannot vanish simultaneously in $[0, \omega_j]$. 

10
Proof. This is a straightforward chain-rule argument. The eigenvalue equation 
\[ \lambda^2 - k(E)\lambda + 1 = 0 \] is equivalent to
\[ \lambda^2 - 1 = \pm \lambda \pm \sqrt{k^2(E) - 4}. \]

From this together with the relation
\[ \frac{dE}{dE} = \frac{1}{\sqrt{k^2(E) - 4}} \]
we have that
\[ f(\bar{E}) = f(E) \frac{dE}{dE} = -\mu(M^{-1}v_-, \Phi v_-) - \frac{1}{\mu} (M^{-1}v_+, \Phi v_+) - \frac{1}{\mu} (v_+, \Theta v_+) \sqrt{k(E)^2 - 4}. \]

At the band edge, it holds \( k(E)^2 = 4 \) and \( Mv_\pm = \lambda_\pm v_\pm \) with \( |\lambda_\pm| = 1 \), and \( v_+(0) = v_-(0) \) so it follows that
\[ \lim_{\bar{E} \to 0} f(\bar{E}) = -\frac{\mu^2 + 1}{\mu} (v_+(0), \Phi(0)v_+(0)) \]
where \( v_+(0) \) is the (unique) eigenvector of \( M \) at the band-edge \( \bar{E} = 0 \), \( \mu \) is defined by \( N(0, x^*)v_+(0) = \mu v_+(0) \) which holds at a zero of \( f \), and \( \Phi \) is the positive-definite matrix defined in (20). A similar result holds for the upper band-edge \( \bar{E} = \omega_j \). \( \square \)

Remark 3. The above is the hyperelliptic integral associated to the spectral problem\([24, 3]\). Note that the integral is necessarily convergent, since the Floquet discriminant \( k(E) \) necessarily crosses \( \pm 2 \) transversely at the edge of a non-empty gap.

This lemma has the following obvious implication

Corollary 2. Suppose that the gap \( (G) = (0, \omega_j) \) is a gap (parameterized by \( \bar{E} \) as in lemma\([3]\)). A given zero level set of the generalized Evans function \( f(\bar{E}, x) \) is given by a function \( \bar{E}(x) \) which is either defined for all \( x \in [0, 1] \), or leaves the range \( (0, \omega_j) \) at some point(s). In the classically allowed region \( E > q_{def} \) this function is strictly monotone and thus invertible, \( \bar{x}(\bar{E}) \).

Proof. A standard implicit function argument. Local existence is obvious. Since the Evans function and its derivative with respect to energy cannot vanish simultaneously we have uniform control on the Lipschitz constant on \( [0, \omega_j] \times [0, 1] \), and thus the level set can be constructed for all \( x \) as long as \( \bar{E}(x) \) remains in \( [0, \omega_j] \).

From this it should be clear that in the classically allowed region for the defect the number of roots of the Evans function \( f(\bar{E}, 1) \) can be expressed in terms of the number of roots of the Evans function at the band edges 0 and 1. This is the content of the next proposition.
Proposition 2. Suppose that the gap \((0, \omega_j)\) is in the classically allowed region for the defect potential. Let \(N\) be the number of roots of \(f(\tilde{E}, 1)\) in the gap \(\tilde{E} \in (0, 1)\) \(n_1\) be the number of roots of \(f(0, x)\) for \(x \in (0, 1)\) and \(n_2\) be the number of roots of \(f(\omega_j, x)\) for \(x \in (0, 1)\). Then \(N = n_2 - n_1 + 1\).

Proof. This is a fairly standard lemma - that simple roots persist under a homotopy that fixes the endpoints.

Consider the region \((\tilde{E}, x) \in [0, \omega_j] \times [0, 1]\). It is easy to see that for \(x = 0\) the Evans function \(f(\tilde{E}, 0)\) is nonzero for \(\tilde{E} \in (0, \omega_j)\) and vanishes at the boundaries \(\tilde{E} = \{0, \omega_j\}\), since the monodromy map \(N(E, x)\) is the identity for \(x = 0\) and \(v_\pm\) are non-degenerate on the interior of the band and degenerate at the band edges. Since \(x(E)\) is decreasing the zero of \(f(\tilde{E}, x)\) at \((\tilde{E} = 0, x = 0)\) does not extend into the interior. If \(f(\tilde{E}, x)\) vanishes at the band edge \((\omega_j, 1)\) this zero also does not extend into the interior. By the above lemmas all other zeroes of the generalized Evans function can be continued to a zero level-set \(x(\tilde{E})\) that is a monotone decreasing function. Thus, each zero of the generalized Evans function on the right-hand boundary \(\tilde{E} = \omega_j\) extends to a unique curve that must intersect the left-hand boundary \(\tilde{E} = 0\) or the top boundary \(x = 1\). Thus we have \(n_2 + 1 = N + n_1\).

The first homotopy argument shows that the number of roots of the Evans function (in \(\tilde{E}\)) is equal to the difference in the number of roots (in \(x\)) on the band edges of the generalized Evans function. We would next like to be able to estimate the number of roots of the generalized Evans function in terms of the band-gap structure of the defect fundamental solution matrix. The next lemma shows that zeros of the Evans function on the boundary can only occur in gaps or band-edges for the fundamental matrix \(N(\tilde{E}, x)\) for the defect mode, but never in bands.

Lemma 4. Suppose that the generalized Evans function \(f(\tilde{E}, x)\) vanishes for an energy at a band-edge of the essential spectrum, \((\tilde{E}, x) = (0, x^*)\) or \((\tilde{E}, x) = (\omega_j, x^*)\). Then \(k_{def}^2(\tilde{E}, x^*) \geq 4\).

Proof. If \(\tilde{E} = 0\) or \(\tilde{E} = \omega_j\) the eigenvectors \(v_+\) and \(v_-\) are linearly dependent, and thus the condition that the Evans function implies that

\[
f(\tilde{E}, x) = 0 \iff \langle v_+, JNv_+ \rangle = 0 \iff Nv_+ = \mu v_+.
\]

Thus \(v_+\) is an eigenvector of \(N(\tilde{E}, x^*)\). Since \(v_+\) is a real vector it can be an eigenvector of \(N\) only if \(N\) has real eigenvalues, which is equivalent to \(k_{def}^2(\tilde{E}, x^*) \geq 4\).

The above shows that zeros of the Evans function on the boundary can only occur in gaps of \(N\). We would like to show that exactly one zero of the Evans function emerges from each gap. The next lemma, which will be needed to show this, says that gaps in \(x\) behave qualitatively like gaps in \(\tilde{E}\) for energies
in the classically allowed region, in the sense that in an open gap the Floquet discriminant necessarily crosses $\pm 2$ transversely. The analogous statement for gaps in $E$ is standard (see Magnus and Winkler) and will not be proven here.

Lemma 5. Suppose that $x_0$ is a periodic or anti-periodic point for the defect, $k_{def}(E, x_0) = \pm 2$ and that the energy $E$ is in the classically allowed region for the defect. Then either the Floquet discriminant crosses transversely, \( \frac{dk_{def}}{dx}(E, x_0) \neq 0 \), or $x_0$ is a double point $N(E, x_0) = \pm I$ and $k_{def} = \pm (2 - c(x - x_0)^2 + o((x - x_0)^2))$ with $c > 0$. In particular for an open gap the eigenvectors are degenerate only at the band edges.

Proof. We prove for the case $k_{def}(E, x_0) = 2$. The case $k_{def}(E, x_0) = -2$ follows similarly. If $k_{def}(E, x_0) = 2$ then $N$ takes the Jordan normal form $N = I + \kappa J$ where $v$ is the (non-zero) eigenvector of $N$. Note that $\kappa$ can vanish, in which case $N$ is the identity matrix. Taking the identity $\text{tr}(N^2) - (\text{tr}(N))^2 = -2 \det(N) = -2$, differentiating and substituting into the Jordan normal form gives $\frac{dk_{def}}{dx} = \kappa < v J N x v > - \kappa < v H_{def} v >$. Since the energy is in the classically allowed region for the defect the Hamiltonian is positive definite and the vanishing of $\text{tr}(N x)$ implies that $\kappa = 0$ and thus that the Jordan normal form is the identity. In this case we find that $\frac{d^2k_{def}}{dx^2} = \text{tr}(J H(E, x_0) J H(E, x_0)) = -2 \det(H(E, x_0)) < 0$. \(\square\)

The next lemma shows that the Evans function has exactly one zero in a gap (in $x$) of $N(\tilde{E}, x)$ if the Hamiltonian $H_{def}$ is positive-definite.

Lemma 6. Suppose $\tilde{E}$ is a fixed energy such that $H_{def}(E, x)$ is positive-definite, $v_+$ a fixed real vector, and $(x_{\text{low}}, x_{\text{high}})$ is an interval such that

- $k_{def}^2(\tilde{E}, x_{\text{low}}) = 4 = k_{def}^2(\tilde{E}, x_{\text{high}})$
- $k_{def}^2(\tilde{E}, x) > 4$ for $x \in (x_{\text{low}}, x_{\text{high}})$.

In other words $(x_{\text{low}}, x_{\text{high}})$ is a gap in $x$ of $N(\tilde{E}, x)$. Then the condition

$$\langle v_+ J N(\tilde{E}, x) v_+ \rangle = 0$$

has exactly one root in $x \in [x_{\text{low}}, x_{\text{high}}]$.

Proof. This follows from a simple monotonicity argument. We assume that the gap is not a double point, in which case the lemma is trivially true. The eigenvectors of $N(\tilde{E}, x)$ are degenerate at the band edges and (by the previous lemma) non-degenerate in the band interior. We can choose the eigenvectors $w_\pm$ in such a way that $w_+ = w_-$ at the lower band edge $x_{\text{low}}$. From Corollary 1 it follows that $w_+$ rotates clockwise and $w_-$ rotates counterclockwise until $w_+ = -w_-$, which (by the previous lemma) occurs at the upper band edge. By continuity it follows that the angle between $w_+$ and $w_-$ goes through $\pi$ radians. The eigenvalue condition is equivalent to either $w_+ = v_+$ or $w_- = v_+$. It follows that either $v_+$ is equal to a band-edge eigenvector of $N(\tilde{E}, x)$, in which case the
Figure 1: The picture of the band-gaps in the \((E, x)\) plane. The bands can touch at a double point, but cannot cross. Gaps, however, can disappear and reappear.

The above eigenvalue condition has a simple root at the appropriate band edge, or \(v_x\) is not a band edge eigenvector, in which case there is exactly one root of either \(w_+ = v_+\) or \(w_- = v_+\) (but not both). This is illustrated in Fig. (1).

Lemma 4 showed that the eigenvalue condition on the boundary of a gap in the essential spectrum could only have roots in the set \(k_{def}^2(E, x) \geq 4\). The above lemma shows that the eigenvalue equation has exactly one root in each interval of this form.

At this point we have shown that, for energies in the classically allowed region for the defect, eigenvalues persist under homotopy in \(x\). We have also shown that there are certain distinguished intervals in \(x\), \([x_{low}, x_{high}]\), where eigenvalues can enter the gap through the band edge \(E = E_{2j+2}\) or leave the gap through the band edge through the band edge \(E = E_{2j+1}\). Further we have exactly one eigenvalue entering or leaving the gap in each such interval. Thus the number of eigenvalues in the gap is equal to number which enter through \(E = E_{2j+2}\) minus the number which leave through \(E_{2j+1}\). This is not a particularly convenient characterization, since it requires us to count intervals in the homotopy parameter \(x\). Thus we give a second homotopy argument to count the number of gaps (in \(x\)) of \(N(E, x)\) in terms of the number of gaps (in \(E\)) for \(N(E, 1)\).

Lemma 7. For \(\delta\) sufficiently small the band gap structure of \(N(E, \delta)\) in \(E\) for

\[\begin{align*}
q(0) & \quad E \\
\end{align*}\]
Proposition 3. Suppose that $E$ is in a fixed interval about $q(0) \, \text{consists of}$

- Gap for $E < q(0) - o(1)$
- Band for $E > q(0) + o(1)$

Further there is a unique $E$ in $(q(0) - o(1), q(0) + o(1))$ where $\text{tr}(N(E, \delta) = 2$, and the crossing is transverse.

Proof. This result follows from Taylor expansion, self adjointness, and some elementary analytical considerations. First note that $N(E, 0) = I$. Differentiating gives $\text{tr} N_{xx}(E, 0) = -2(E - q(0))$, $\text{tr} N_{xE}(E, 0) = 0$ and $\text{tr} N_{EE}(E, 0) = 0$. So for small $x$ $k(E, x) = \text{tr} N(E, x) \approx 2 - (E-q(0))x^2 + O(x^3)$. Therefore, it is clear that for $x$ sufficiently small, $k(E, x) > 2$ for $E < q(0) - O(\delta)$ and $k(E, x) < 2$ for $E > q(0) + O(\delta)$. Next we need to show that there exists a single transverse crossing in $(q(0) - O(\delta), q(0) + O(\delta))$. To do this note that $N(E, x)$ is the monodromy map for a self-adjoint operator, and standard results (see Magnus and Winkler) show that the only possible band edges are a proper band edge, which crosses transversely (in this case $k(E, x) = 2, k_E(E, x) < 0$) or a double point (in this case $k(E, x) = 2, k_E(E, x) = 0, k_{EE}(E, x) < 0$). Thus the first crossing must be transverse. To show that this crossing is unique for sufficiently small $\delta$ we note that self-adjointness implies that the Floquet discriminant cannot have a critical point inside of a band. Suppose that there were two crossings in $(q(0) - O(\delta), q(0) + O(\delta))$. Then, since critical points inside of a band are disallowed, there must be a gap in $(q(0) - O(\delta), q(0) + O(\delta))$, and thus two antiperiodic points. Thus the Floquet discriminant must go from +2 to −2 in a distance of $O(\delta)$, and we have an estimate of the form $|k(E_1, \delta) - k(E_1 + \delta, \delta)| \geq O(\delta^{-1})$. Since the Floquet discriminant is continuous this cannot hold for $\delta$ arbitrarily small, and thus the crossing is unique for small $\delta$. 

Now we are in a position to prove the next result:

**Proposition 3.** Suppose that $E$ is in the classically allowed region for the defect mode. The number of bands of $N(E, x)$ in $x \in [0, 1]$ is the equal to the number of bands of $N(E, 1)$ for $E \in (-\infty, E]$. The number of gaps of $N(E, x)$ in $x \in [0, 1]$ is one less than the number of gaps of $N(E, 1)$ for $E \in (-\infty, E]$.

Proof. This again makes use of a homotopy argument. The basic observation is that, while the gaps can collapse to a point and thus cannot be continued by an implicit function argument the bands can be so continued.

It is somewhat more convenient to work on the the interval $[\delta, 1] \times [e, E]$ to avoid trouble with noncompactness in $\tilde{E}$ and the degeneracy at $x = 0$. Since $q_{def}$ is assumed to be piecewise $C^1$ we choose $e < \inf_{x\in[0,1]} g(x)$. In this case it is clear from the obvious lower bounds that there are no bands for energies less than or equal to $e$. From the above lemma we can choose $\delta$ sufficiently small such that $E < q(0) - o(1)$ is a gap, $E > q(0) + o(1)$ is a band, and there is a single periodic point at $x = \delta, E = q(0) + o(1)$. Since the bands are by definition open we can choose $\delta$ such that the number of bands for $x \in [0, 1]$ is the same as the number of bands for $x \in [\delta, 1]$. 

15
We define the bottom boundary $B$ to be $[e, \bar{E}] \times \delta$, the top boundary $T$ to be $[e, E) \times 1$, the right boundary $R$ to be $E \times [\delta, 1]$, and the left boundary $B$ to be $e \times [\delta, 1]$. Since $\frac{dk}{dE}$ cannot vanish on the interior of a band it follows from the implicit function theorem that a point in a band defines a local level set of the Floquet discriminant $E(x)$. Since we have global control of the Lipschitz constant this level set is defined for all $x$.

By construction the left boundary $L$ is chosen to be below the essential spectrum and has no bands. The bottom boundary $B$ has a single band ($q(0) + O(\delta), E$), and by construction $dk/dx < 0$ on this band. This band continues onto the right boundary $R$. Since $E$ is in the classically allowed region $dk/dx < 0$ for all bands on top boundary $R$. Thus all bands of the left and top boundaries move into the interior transversely as $x$ increases. Since a level set of $k(E, x)$ each point on a band interior on the top boundary moves into the interior as $x$ is increased, and can be followed until it intersects the right boundary. This defines a map of bands on the right boundary to bands on the top boundary. The converse argument defines the inverse map of bands on the top boundary to bands on the right boundary. Since we have an invertible map of band on the top boundary to bands on the right boundary the number of bands on the top boundary and on the right boundary must clearly be the same. Since the bands are open and disjoint the complements must also have the same number of components. The bottom boundary contains one gap, the semi-infinite one, and the remainder of the gaps occur on the right boundary, whence the gap count.

Remark 4. Note that the fact that the derivative $\partial k/\partial x$ is of the same sign as $\partial k/\partial E$ is critical to this argument, and depends crucially on being in the classically allowed region for the defect. Without control on the sign of $\partial k/\partial x$ (or equivalently $dx/dE$) there is no guarantee that a band could not enter and leave the region repeatedly. Physically this seems to be a non-resonance condition.

From this it follows that we have the following bounds on the number of defect eigenvalues.

**Theorem 1.** Suppose that a gap $\mathcal{G}$ is in the classically allowed region for the defect mode. Define the set

$$\mathcal{R}_{def} = \{ E | (\text{tr}(M(E)))^2 \geq 4 \}$$

and the integers $n_{\mathcal{G}}$ and $n_{\partial \mathcal{G}}$ to be the number of connected components of the sets $\mathcal{R}_{def} \cap \mathcal{G}$ and $\mathcal{R}_{def} \cap \partial \mathcal{G}$ respectively. Then, the number of defect modes $D_{\mathcal{G}}$, satisfies the inequality

$$n_{\mathcal{G}} + 1 - n_{\partial \mathcal{G}} \leq D_{\mathcal{G}} \leq n_{\mathcal{G}} + 1.$$  \hspace{1cm} (34)

Proof. We’ll prove the case $n_{\partial \mathcal{G}} = 0$ first, in which case the count is exact. If $n_{\partial \mathcal{G}} = 0$, i.e., neither edge lies in a gap for the defect monodromy matrix, then
from the previous proposition and lemma 8 it follows that the number of gaps of \( N(\tilde{E}, x) \) in \( x \) is the equal to the number of gaps of \( N(0, x) \) in \( x \) for \( x \in [0, 1] \) plus \( n_G \). But, since in each gap (in \( x \)) there is a unique eigenvalue, we obtain that (in the terminology of Proposition 1) \( n_2 - n_1 = n_G \), and therefore \( D_G = n_G + 1 \).

On the other hand, for each of the edges \( 0, 1 \) that lie in a gap for the defect monodromy, the defect modes can be reduced by 1. This is true, since the zero level curves for the Evans function might not exit the \( x \)-interval \( [0, 1) \) in the case where \( E_{\text{low}} \) lies in a gap, or the defect mode might be generated outside of \( [0, 1) \) in the case where \( E_{\text{high}} \) lies in a gap. \( \square \)

**Remark 5.** It is worth making a number of remarks about this result. First we note that one could easily find upper and lower bounds on the number of defect eigenvalues generated in a gap by counting Dirichlet eigenvalues of the defect. However using this method there seems to be no clear criterion for guaranteeing that the count is exact, which will be necessary for the main result of this paper, the large gap number estimate.

As noted earlier the set \( R_{\text{def}} \) is the union of the resolvent set and the periodic and anti-periodic eigenvalues of the periodic Schrödinger operator with potential given by the periodization of the defect potential. Thus the above result, roughly speaking, gives an estimate of the number of defect eigenvalues in terms of the number of connected components of the intersection of the resolvent sets.

The above calculation can also be interpreted as a Maslov index calculation. Given a curve \( N(E) \) in the symplectic group and a Lagrangian subspace \( L \) (in this case any one dimensional subspace) the Maslov index is a signed count of the number of intersections of \( N(E)L \) with \( L \). In our case lemma ?? guarantees that the index is always positive, so the Maslov index actually counts intersections. This count depends, of course, on the Lagrangian subspace chosen but in the special case \( n_{\partial G} = 0 \) the Maslov index \( \mu_L \) is the same for all Lagrangian subspaces and the number of defect eigenvalues is one plus the Maslov index of \( N(E) \) for \( E \in (E_{2j+1}, E_{2j+2}) \).

Finally we remark that, in the case of defect potentials which are constant the set \( R_{\text{def}} \) consists of single points. In this case it is easy to see that the count is exactly \( n_G + 1 \) regardless of whether or not \( n_{\partial G} = 0 \).

### 3.1 Large gap number asymptotics

In this section we present results for the high gap-number behavior of the number of defect eigenvalues. It is known [7] that the \( n \)-th Dirichlet eigenvalue for the problem

\[-u_{xx} + V(x)u = \lambda_n u, \quad u(0) = u(L) = 0\]

behaves asymptotically as

\[\lambda_n \sim \frac{n^2 \pi^2}{L^2} + \frac{1}{L} \int_0^L V(x)dx + o(1).\]

We have established previously bounds for the number of eigenvalues in each gap. In particular we have that if the gaps of the (periodically extended) defect
problem do not intersect a gap of the periodic problem, then that gap has exactly one defect eigenvalue. Further we know the following standard facts:

- The $n^{th}$ Dirichlet eigenvalue is contained in the $n^{th}$ gap.
- The width of the $n^{th}$ gap goes to zero for large $n$. In particular if $V \in L_2$ then the sequence of widths is in $l_2$, with stronger decay estimates if $V$ has additional smoothness properties.

Thus, if we denote the $n^{th}$ Dirichlet eigenvalue of the periodic problem by $\mu_n$ and the $m^{th}$ Dirichlet eigenvalue for the defect problem by $\tilde{\mu}_m$ then we can expect to have one eigenvalue in each gap, unless $\mu_n \approx \tilde{\mu}_m$, for some integers $m, n$. To quantify this we first define the following set of exceptional energies, which detects possible overlaps between the Dirichlet spectra of the periodic potential and the defect potential:

**Definition 1.** For a real number $a$ we define the set $F_a$ as follows: a number $y$ belongs to $F_a$ if for every $\delta > 0$ there exists an infinite, strictly increasing sequence of pairs of integers $\{N_k, M_k\}_{k=1}^{\infty}$ such that

$$|y - M_k(N_k - M_k a)| < \delta$$

In other words, the set $F_a$ represents the (appropriately scaled) asymptotic distribution of errors in rational approximations of $a$. In the next lemma we note some simple properties of the set $F_a$.

**Lemma 8.** The set $F_a$ has the following properties:

- The set $F_a$ is never empty. If $a$ is rational then $F_a$ contains only the point $y = 0$.
- If $a$ is irrational then there are at least countably many points in $F_a$.
- The set $F_a$ is invariant under the modular group $\text{PSL}(2, \mathbb{Z})$: if $y \in F_a$ with $M_k(N_k - a M_k) \rightarrow y$ and $a = \frac{n_1 b + n_2}{n_3 b + n_4}$ with $n_1 n_4 - n_2 n_3 = 1$ then $y \in F_b$.

**Proof.** The first property is obvious, since it is easy to see that a given non-zero integer can be written as a difference of squares in at most a finite number of ways. For the irrational case note that from elementary number theory if $a$ is irrational there exists an infinite sequence of pairs $(N, M)$ such that $|\frac{N}{M} - a| < \frac{1}{M^2}$, thus an infinite sequence of pairs $(N, M)$ such that $M(N - Ma) \in (-1, 1)$, and by compactness a limit point. Note that if $y \in F_a$ then $j^2 y \in F_a$ for all integers $j$, so the number of points in $F_a$ is at least countably infinite. Finally to see the invariance of $F_a$ under the modular group note that a straightforward calculation shows that if the sequence $(N_k, M_k)$ satisfies $M_k(N_k - a M_k) \rightarrow y$ then the sequence $N'_k = n_4 N_k - n_2 M_k, M'_k = n_1 M_k - n_3 N_k$ satisfies $M'_k(N'_k - b M'_k) \rightarrow y$.

Finally, we characterize the set $F_a$ for some classes of real numbers $a$. 18
Proposition 4. Suppose \( a \) has the continued fraction expansion \( a = [a_0, a_1, a_2 \ldots] \).

- If \( \{a_j\}_{j=0}^\infty \) is eventually periodic (in other words if \( a \) is a quadratic irrational) then \( F_a \) is a discrete set of point.
- If \( \{a_{2j}\}_{j=0}^\infty \) is unbounded then \( F_a \) contains the negative half-line \((-\infty, 0] \).
- If \( \{a_{2j+1}\}_{j=0}^\infty \) is unbounded then \( F_a \) contains the positive half-line \([0, \infty) \).
- If \( \{a_j\}_{j=1}^\infty \) is bounded then \( F_a \) does not contain some interval about the origin.

In particular for Lesbesgue almost every \( a \) both the even and the odd terms in the continued fraction expansion are unbounded and thus we have \( F_a = \mathbb{R} \), the whole real line.

Proof. In the case of quadratic irrationals it is relatively easy to compute explicitly what \( F_a \) is. Let \( f(x) = n_1x^2 + n_2x + n_3 \) with \( n_{1,2,3} \in \mathbb{Z} \) relatively prime be the quadratic polynomial with root \( a \). Then \( F_a \) consists of all numbers of the form \( f(\alpha) = \frac{n_1 \alpha^2 + n_2 \alpha + n_3}{M_j} \), where \( j \) is any integer which can be represented in the form \( n_1N^2 + n_2NM + n_3M^2 = j \).

To see this note that standard results in the theory of quadratic Diophantine equations show that the existence of one solution guarantees the existence of a family of solutions. Let \( N_k, M_k \) be increasing sequences of integers such that \( N_k/M_k \rightarrow a \). Obviously \( n_1N_k^2 + n_2N_kM_k + n_3M_k^2 = j \) for some integer \( j \). Since \( f(\alpha) = 0 \), it follows by the mean value theorem that

\[
f(\alpha) = f(N_k/M_k) = f'(x_0)(a - N_k/M_k),
\]

for some \( x_0 \) between \( a \) and \( N_k/M_k \), and so we obtain \( f'(x_0)(a - N_k/M_k) = -j/M_k^2 \). Therefore

\[
M_k(N_k - aM_k) = \frac{j}{f'(x_0)}
\]

for \( x_0 \in (a, N_k/M_k) \). Thus all elements of \( F_a \) are of the stated form. To see that all such numbers are actually arise note that the existence of one solution to \( n_1N^2 + n_2NM + n_3M^2 = j \) implies the existence of a family of such solutions, which by the above must satisfy

\[
M_k(N_k - aM_k) = \frac{j}{f'(x_0)}
\]

To see the second and third claims we consider the following doubly indexed sequence: \( N_{j,k} = jP_k, M_{j,k} = jQ_k \), where \( \frac{P_k}{Q_k} \) are the continued fraction approximants to \( a \). Standard results show that \( |P_k^2 - a^2Q_k^2| \leq \frac{\epsilon_k}{a} \), so if \( \epsilon_k \) is unbounded there exists a subsequence such that \( P_k^2 - Q_k^2a^2 = \epsilon_k \rightarrow 0 \). Further \( \epsilon_k \) is negative (resp. positive) if \( k \) is even (resp. odd). Note that for a fixed integer \( j \) we have that \( j^2P_k^2 - a^2j^2Q_k^2 = j^2\epsilon_k \). It is clear that for any \( y \) having the same sign as \( \epsilon_k \) if we take \( j_k = \lfloor \frac{y}{\epsilon_k} \rfloor \) we have \( |j_k^2\epsilon_k - y| \leq O(\epsilon_k^j) \).
The fourth observation follows from the well-known fact that a number with a bounded continued fraction cannot be approximated by rationals to better than quadratic order: if the continued fraction coefficients satisfy $a_i < m$ then one has a lower bound of the form

$$|N/M - a| \geq f(m)/M^2$$

with $f(m) > 0$, from which it follows that the interval $|y| < f(m)$ is not in the set $F_a$.

The last assertion follows from a trivial modification of the proof in Hardy and Wright that the set of numbers with bounded continued fraction coefficients has measure zero. 

**Remark 6.** The case which is still incompletely understood is that for which the continued fraction expansion has bounded coefficients but is not periodic. It would be interesting, although likely very difficult, to classify $F_a$ based on the distribution of the continued fraction coefficients.

Now we are in a position to state the main result, which relates the asymptotic number of eigenvalues in a gap to the properties of the set $F_a$.

**Theorem 2.** Assume that the width of the defect is normalized to 1, and as before denote the period of the periodic potential by $a$. Define the energy difference $\Delta q$ to be the mean of periodic potential minus the mean of the defect potential:

$$\Delta q = \int_0^1 q_{def}(y)dy - \frac{1}{a} \int_0^a q_{per}(y)dy.$$  

Then:

- If the energy difference does not belong to the set of exceptional energies, $\frac{\Delta q}{\pi^2} \notin F_a$, then every sufficiently large numbered gap contains exactly one defect eigenvalue.

- If $\frac{\Delta q}{\pi^2} \in F_a$ then there exists a sequence of exceptional gaps. Every sufficiently large numbered gap which is not in the sequence of exceptional gaps contains exactly one eigenvalue. Every sufficiently large numbered gap which is in the sequence of exceptional gaps contains 0, 1, or 2 defect eigenvalues.

**Proof.** Denote the $n$-th Dirichlet eigenvalue of the periodic problem by $\mu_n$ and the $m$-th Dirichlet eigenvalue for the defect problem by $\tilde{\mu}_m$. Then,

$$\mu_n - \tilde{\mu}_m \sim \frac{n^2 \pi^2}{a^2} - m^2 \pi^2 - \Delta q + o(1)$$

(35)

$$\sim \frac{1}{a^2 \pi^2} (n + am)(n - am) - \Delta q + o(1).$$

(36)
For $n, m$ large this is clearly bounded away from zero unless $n = am + o(1)$, in which case this becomes

$$
\mu_n - \tilde{\mu}_m \sim \frac{2\pi^2}{a} m(n - am) - \Delta q + o(1).
$$

(37)

If $\Delta q$ does not belong to the set of exceptional energies $\mathcal{F}_a$ then this quantity is eventually uniformly bounded away from zero. Thus all sufficiently large Dirichlet eigenvalues of the periodic problem and the defect problem are bounded away from each other. Since the Dirichlet eigenvalues are contained in the gaps, and the width of the gaps is approaching zero, it follows that the gaps are eventually non-intersecting. From the count in Theorem 1 it follows that each gap contains exactly one eigenvalue.

If $\Delta E \in \mathcal{F}_a$ then it is clear that at most one of the gaps of the defect problem can intersect a gap of the periodic problem. Hence the gap of contains either 0, 1 or 2 defect eigenvalues according to Theorem 1.

To close we construct an example to show that the exceptions considered in the previous theorem are real. In particular we construct a combination of periodic and defect potentials such that a particular (infinite) subsequence of gaps contains two defect eigenvalues.

**Example 1.** In order to construct this example we would like to choose the periodic and defect potentials in such a way that the gaps in the essential spectrum of the periodic problem are comparatively wide. For this reason we choose a piecewise constant (Kronig-Penney) potential. We choose the period to be a quadratic irrational since this guarantees that we have a clean description of the set $\mathcal{F}_a$. For reasons of tradition we take $a = \phi$ the golden mean, although any quadratic irrational would serve. We take the defect potential to be constant, $q_{def}(x) = q_{def}$, so the set $\mathcal{R}_{def}$ consists of a union of points, and the eigenvalue count is guaranteed to be exact. In particular for the periodic potential we take the Kronig-Penney potential

$$
q_{per}(x) = \begin{cases} 
-A & \text{for } 0 \leq x < \phi/2 \\
A & \text{for } \phi/2 \leq x < \phi
\end{cases}
$$

where $A$ is a constant to be determined later. The gaps grow in size with $A$, and our strategy is to choose $A$ sufficiently large so that appropriate points of $\mathcal{R}_{def}$ are eventually contained in the appropriate gaps, as this will guarantee two eigenvalues.

The transfer matrix for $-u_{xx} + q_{per}(x)u = Eu$ can be easily calculated to be

$$
M_{KP} = \begin{pmatrix}
\cos(\frac{\phi\sqrt{E-A}}{2}) & \sin(\frac{\phi\sqrt{E-A}}{2}) \\
-\sin(\frac{\phi\sqrt{E-A}}{2}) & \cos(\frac{\phi\sqrt{E-A}}{2})
\end{pmatrix}
\begin{pmatrix}
\cos(\frac{\phi\sqrt{E+A}}{2}) & \sin(\frac{\phi\sqrt{E+A}}{2}) \\
-\sin(\frac{\phi\sqrt{E+A}}{2}) & \cos(\frac{\phi\sqrt{E+A}}{2})
\end{pmatrix}
.$$
From this, the location of the band-edges is given by roots of the equation
\[ \text{tr}(M_{K'}) = 2 \cos \left( \frac{\sqrt{E-A}}{2} \right) \cos \left( \frac{\sqrt{E+A}}{2} \right) - \left( \frac{\sqrt{E-A}}{2} + \frac{\sqrt{E+A}}{2} \right) \sin \left( \frac{\sqrt{E-A}}{2} \right) \times \sin \left( \frac{\sqrt{E+A}}{2} \right) = \pm 2. \]

From some straightforward asymptotic analysis it can be seen that the location of the \( j \)th gap is approximately
\[ G_j = \begin{cases} \left( \frac{j^2 \pi^2}{\sigma^2} - \frac{\phi A}{2 \pi j} + O(j^{-2}) \right) & \text{for } j \gg 1 \text{ odd} \\ \left( \frac{j^2 \pi^2}{\sigma^2} - \frac{\phi^2 A^2}{4 \pi^2 j^2} + O(j^{-3}) \right) & \text{for } j \gg 1 \text{ even} \end{cases} \] (38)

Since the defect potential is constant the periodization is constant. Thus the gaps close to double points and the set \( R_{\text{def}} \) is given by
\[ R_{\text{def}} = \bigcup_{j=0}^{\infty} \mu_j \quad \mu_j = \pi^2 j^2 + q_{\text{def}}. \]

The set \( F_\phi \) consists of real numbers of the form
\[ F_\phi = \left\{ \frac{j}{\sqrt{5}} \right\} \quad j \in \pm \{1, 4, 5, 9, 11, 16, 19, 20, 25, 29, 31, 36\ldots\} \] (39)

where the sequence is all positive integers \( j \) which are representable in the form \( j = n^2 - nm - m^2 \) (sequence A031363 in Sloane’s encyclopedia[33]). The mean of the periodic potential is zero, so if the mean of the defect potential is chosen to be in the set \( \frac{2\pi}{\sigma} F_\phi \) then there is an infinite sequence of gaps which potentially have more than one defect eigenvalue. We will, somewhat arbitrarily, focus on the \( j = 11 \) term of \( F_\phi \). This term is interesting since it admits two distinct families of solutions to the Diophantine equation \( n_k^2 - n_km_k - m_k^2 = 11 \). These two families are given by the following sequences:
\[ m_k = \{1, 5, 14, 37, 97\ldots\} \quad n_k = \{4, 9, 23, 60\ldots\} \] (40)
\[ m_k = \{2, 7, 19, 50, 131\ldots\} \quad n_k = \{5, 12, 31, 81\ldots\}. \] (41)

Each of the sequences \( n_k, m_k \) satisfies the recurrence \( a_{k+1} = 3a_k - a_{k-1} \) and \( n_k^2 - n_km_k - m_k^2 = 11 \). It is straightforward to compute that the \( n_k, m_k \) satisfy the following asymptotic relation
\[ m_k(n_k - \frac{1 + \sqrt{5}}{2} m_k) = \frac{11}{\sqrt{5}} - \frac{121}{m_k^2 \sqrt{125}} + O(m_k^{-4}). \]

(This is easiest to see if one notes that \( n_k^2 - n_km_k - m_k^2 = 11 \) can be factored over \( \mathbb{Q}(\sqrt{5}) \) as \( (n_k - \phi m_k)(n_k + \phi^{-1} m_k) = 11 \) and proceed from there.)

We look at the \( G_{n_k} \), the \( n_k \)th gap in the essential spectrum with \( n_k \) an element of one of \( \{11\} \) or \( \{11\} \), and the \( m_k \)th point in \( R_{\text{def}} \), which is located at \( \pi^2 m_k^2 + \)
The distance between the center-point of \( G_{n_k} \) and \( \pi^2 m_k^2 + q_{def} \) is given by

\[
\pi^2 m_k^2 + q_{def} - \frac{n_k^2 \pi^2}{\phi^2} = \pi^2 (m_k + \frac{n_k}{\phi})(m_k - \frac{n_k}{\phi}) \\
\approx q_{def} - \frac{22\pi^2}{\sqrt{5}\phi} + \frac{121\pi^2}{5\phi^2m_k^2} + o(m_k^{-2}).
\]

Choosing \( q_{def} = \frac{22\pi^2}{\sqrt{5}\phi} \) (again this is the \( j = 11 \) element of \( \frac{2m^2}{\phi}F^2 \)) causes the leading order terms to cancel. Given the gap asymptotics in (38) it is clear that for \( n_k \) odd the point \( \mu_{m_k} \) is always eventually contained in the gap \( G_{n_k} \), since the width of the gaps \( G_{n_k} \) decays more slowly that the above error. For \( m_k \) even the point \( \mu_{m_k} \) will eventually be contained in the gap \( G_{n_k} \) if \( A \) is chosen to be sufficiently large. If we choose

\[
\frac{3\phi^2 A^2}{4\pi^2 n_k^2} > \frac{121\pi^2}{5m_k^2\phi^2}
\]

or equivalently

\[
A > \frac{22\pi^2}{\sqrt{15}\phi}
\]

then the radius of the \( n_k \) gap is asymptotically larger than the distance between the \( m_k \) point in \( R_{def} \) and the center of the gap, and thus the \( m_k \) point in \( R_{def} \) is contained in the \( n_k^{th} \) gap. Thus \( n_G = 1, n_{\partial G} = 0 \) and the gap \( G_{n_k} \) contains precisely 2 eigenvalues.

Note that this example is fairly robust. For any positive \( A \) the odd gaps \( G_{n_k} \) for \( n_k \) in the sequences (10) or (11) get exactly two eigenvalues: the lower bound on \( A \) is necessary only to insure that the even gaps (which are asymptotically narrower) get two eigenvalues. Also note that the choice of \( q_{def}(x) \) is not particularly important: as long as \( q_{def} \) is smooth enough that the intervals in \( R_{def} \) decay at least as fast as the gaps in the essential spectrum then (for sufficiently large contrast \( A \)) the above example can be made to work. Similarly, as noted above, the above construction goes through for any quadratic irrational (in fact \( \phi \) is in some sense the worst example since it is the least well approximated by rationals). For a general irrational \( a \) and general potentials \( q_{def}(x) \) and \( q_{per}(x) \) there is a somewhat delicate interplay between the size of the intervals in \( R_{def} \) and \( R_{per} \) and the error in the rational approximations of \( a \), and while it is clear that the sequence of extraordinary gaps can contain at most two eigenvalues it is difficult to determine the exact number.

### 4 Conclusion

In this paper, we analyzed in detail the emergence and distribution of defect eigenvalues in the gaps of the essential spectrum of the linear one-dimensional Schrödinger equation, with a potential consisting of a periodic part plus a compactly supported defect part. We used an Evans function technique that reduces
the problem to that of finding the zeros of an analytic function, and by means of a homotopy argument we were able to count the eigenvalues as they emerge from the band edges. It is found that if a gap is in the classically allowed region for the defect potential, then the number of defect modes in the gap can be expressed in terms of the number of roots of the Evans function at its band edges. It is shown that for a gap in the classically allowed region for the defect potential, the number of zeros of the generalized Evans function is no larger than the number of gaps of the defect problem in terms of the homotopy parameter $x$. In addition, this number was found to be the same as that of the gaps in terms of the eigenvalue parameter $E$. As a result, bounds for the defect modes are given in terms of the gaps of the defect monodromy matrix that intersect the gap. Finally, we proved the following significant generalization of Zheludev’s theorem: the number of point eigenvalues in a gap in the essential spectrum is exactly 1 for sufficiently large gap number unless a certain Diophantine approximation problem has solutions, in which case there exists a subsequence of gaps containing 0, 1, or 2 eigenvalues. We stated some conditions under which the solvability of the Diophantine approximation problem can be established, and we included an example where a particular (infinite) subsequence of gaps contains two defect eigenvalues.

There are a number of interesting open questions. It would be interesting to understand the structure of the set $F_a$ for a irrational with bounded coefficients but not a quadratic irrational, although this would likely depend in a sensitive way on the distribution of the continued fraction coefficients. Also, since the bounds are expressed in terms of the intersection of resolvent sets it would be interesting to understand how these are effected by isospectral flows on the potential(s), which obviously leave these sets invariant. We believe, although we have not yet checked this, that by flowing the periodic potential according to the Korteweg-DeVries hierarchy (which obviously leaves $R_{per}$ invariant) one should be able to force any particular gap to achieve any of the possibilities allowed by (34).

**References**

[1] Microcavities and Photonic Band Gap: Physics and Applications. 1996.

[2] S. Alama, P. A. Deift, and R. Hempel. Eigenvalue branches of the Schrödinger operator $H - \lambda W$ in a gap of $\sigma(H)$. *Comm. Math. Phys.*, 121(2):291–321, 1989.

[3] E.D. Beolokolos, A.I. Bobenko, V.Z. Enol’skii, A.R. Its, and V.B Matveev. Algebro-geometric approach to nonlinear integrable equations. Springer-Verlag, Berlin, 1994.

[4] J. C. Bronski and Z. Rapti. Modulational instability for nonlinear Schrödinger equations with a periodic potential. *Dyn. Partial Differ. Equ.*, 2(4):335–355, 2005.
[5] G. Chrystal. "Algebra," volume II. Chelsea, sixth edition, 1959.

[6] P. Dzhakov and B. S. Mityagin. Instability zones of one-dimensional periodic Schrödinger and Dirac operators. Uspekhi Mat. Nauk, 61(4(370)):77–182, 2006.

[7] M. S. P. Eastham. The spectral theory of periodic differential equations. Scottish Academic Press, 1973.

[8] F. Fedele, J. Yang, and Z. Chen. Properties of defect modes in one-dimensional optically induced photonic lattices. Stud. Appl. Math., 115(2):279–301, 2005.

[9] A. Figotin and A. Klein. Localized classical waves created by defects. J. Statist. Phys., 86(1-2):165–177, 1997.

[10] A. Figotin and A. Klein. Midgap defect modes in dielectric and acoustic media. SIAM J. Appl. Math., 58(6):1748–1773 (electronic), 1998.

[11] A. Figotin and P. Kuchment. Band-gap structure of spectra of periodic dielectric and acoustic media. I. Scalar model. SIAM J. Appl. Math., 56(1):68–88, 1996.

[12] A. Figotin and P. Kuchment. Band-gap structure of spectra of periodic dielectric and acoustic media. II. Two-dimensional photonic crystals. SIAM J. Appl. Math., 56(6):1561–1620, 1996.

[13] N.E. Firsova. Trace formula for a perturbed one-dimensional Schrödinger operator with a periodic potential i. Problemy Mat. Fiz., 7:162–177, 1974.

[14] N.E. Firsova. Trace formula for a perturbed one-dimensional Schrödinger operator with a periodic potential i. Problemy Mat. Fiz., 8:158–171, 1976.

[15] F. Gesztesy and B. Simon. On a theorem of Deift and Hempel. Comm. Math. Phys., 116(3):503–505, 1988.

[16] F. Gesztesy and B. Simon. A short proof of Zheludev’s theorem. Trans. Am. Math. Soc., 335(1):329–340, 1993.

[17] I. C. Gohberg and M. G. Krein. Introduction to the theory of linear non-selfadjoint operators. Translated from the Russian by A. Feinstein. Translations of Mathematical Monographs, Vol. 18. American Mathematical Society, Providence, R.I., 1969.

[18] J.D. Joannopoulos, S.G. Johnson, J. N. Winn, and R.D. Meade. Photonic Crystals: Molding the Flow of Light. Princeton University Press, 2008.

[19] T. Kapitula and B. Sandstede. Eigenvalues and resonances using the Evans function. Discrete Contin. Dyn. Syst., 10(4):857–869, 2004.
[20] T. Kato. *Perturbation theory for linear operators*. Springer-Verlag, Berlin, second edition, 1976. Grundlehren der Mathematischen Wissenschaften, Band 132.

[21] P. Kuchment and B. Vainberg. On absence of embedded eigenvalues for Schrödinger operators with perturbed periodic potentials. *Comm. Partial Differential Equations*, 25(9-10):1809–1826, 2000.

[22] W. Magnus and S. Winkler. *Hill’s equation*. Interscience Tracts in Pure and Applied Mathematics, No. 20. Interscience Publishers John Wiley & Sons New York-London-Sydney, 1966.

[23] D. McDuff and D. Salamon. *Introduction to symplectic topology*. Oxford Mathematical Monographs. The Clarendon Press Oxford University Press, New York, second edition, 1998.

[24] H. P. McKea and P. van Moerbeke. The spectrum of Hill’s equation. *Invent. Math.*, 30(3):217–274, 1975.

[25] Michael Reed and Barry Simon. *Methods of modern mathematical physics. I-IV*. Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1978.

[26] Fedor S. Rofe-Beketov and Aleksandr M. Kholkin. *Spectral analysis of differential operators*, volume 7 of *World Scientific Monograph Series in Mathematics*. World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2005. Interplay between spectral and oscillatory properties, Translated from the Russian by Ognjen Milatovic and revised by the authors, With a foreword by Vladimir A. Marchenko.

[27] F.S Rofe-Beketov. A test for the finiteness of the number of discrete levels introduced into gaps in the continuous spectrum by perturbations of a periodic potential. *Soviet Math. Doklady*, 5:689–692, 1964.

[28] F.S Rofe-Beketov. Perturbation of a Hill operator having a first moment and non-zero integral creates one discrete level in distant spectral gaps. *Mat. Fizika i Funkts. Analiz.*, 19:158–159, 1973.

[29] O. L. Safronov. The discrete spectrum in the gaps of the continuous one for non-signdefinite perturbations with a large coupling constant. *Comm. Math. Phys.*, 193(1):233–243, 1998.

[30] O. L. Safronov. The amount of discrete spectrum of a perturbed periodic Schrödinger operator inside a fixed interval $(\lambda_1, \lambda_2)$. *Int. Math. Res. Not.*, 9:411–423, 2004.

[31] O.L. Safronov. The discrete spectrum of the perturbed periodic Schrödinger operator in the large coupling constant limit. *Comm. Math. Phys.*, 218(1):217–232, 2001.
[32] L. Schiff. *Quantum Mechanics*. McGraw-Hill, 1955.

[33] N. J. A. Sloane and Simon Plouffe. *The encyclopedia of integer sequences*. Academic Press Inc., San Diego, CA, 1995. With a separately available computer disk.

[34] A. V. Sobolev. *Weyl asymptotics for the discrete spectrum of the perturbed Hill operator*, volume 7 of *Adv. Soviet Math*. Amer. Math. Soc., Providence, RI, 1991.

[35] A.M. Stoneham. *Theory of Defects in Solids*. Oxford University Press, 1975.

[36] P.D. Townsend and J.C. Kelly. *Colour Centres and imperfections in insulators and semiconductors*. Chatto and Windus/Sussex University Press, 1973.

[37] E. Yablonovich. Inhibited spontaneous emission in solid-state physics and electronics. *Physical Review Letters*, 58:2059–2062, 1987.

[38] V.A. Yakubovich and V.M. Starzhinskii. *Linear Differential Equations with Periodic Coefficients I,II*. Wiley, 1975.

[39] V.A. Zheludev. Eigenvalues of the perturbed Schrodinger operators with a periodic potential. *Topics in Mathematical Physics*, 2:87–101, 1968.

[40] V.A. Zheludev. Perturbation of the spectrum of the one-dimensional self-adjoint Schrodinger operator with a periodic potential. *Topics in Mathematical Physics*, 4:55–75, 1971.