Journal of Mathematical Analysis and Applications **266,** 127–148 (2002)
doi:10.1006/jmaa.2001.7716, available online at http://www.idealibrary.com on IDEAL®

Spectral Asymptotics for Schrödinger Operators with Periodic Point Interactions

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Submitted by Fritz Gesztesy

Received February 13, 2001

Spectrum of the second-order differential operator with periodic point interactions in $L_2(\mathbf{R})$ is investigated. Classes of unitary equivalent operators of this type are described. Spectral asymptotics for the whole family of periodic operators are calculated. It is proven that the first several terms in the asymptotics determine the class of equivalent operators uniquely. It is proven that the spectrum of the operators with anomalous spectral asymptotics (when the ratio between the lengths of the bands and gaps tends to zero at infinity) can be approximated by standard periodic "weighted" operators with step-wise density functions. It is shown that this sequence of periodic weighted operators converges in the norm resolvent sense to the formal (generalized) resolvent of the periodic "Schrödinger operator" with certain energy-dependent boundary conditions. The operator acting in an extended Hilbert space such that its resolvent restricted to $L_2(\mathbf{R})$ coincides with the formal resolvent is constructed explicitly.

Key Words: point interactions; spectral asymptotics; self-adjoint extensions.

1. INTRODUCTION, DEFINITION OF THE OPERATOR

Differential and pseudodifferential operators with point interactions are widely used in applications to quantum and atomic physics to produce exactly solvable models of complicated physical phenomena [3, 4, 10]. Applications of this method to solid-state physics is of particular interest, since these models reproduce the geometry of the problem extremely well. The first model of this type is due to Kronig and Penney [20] and can be described by a Hamiltonian in $L_2(\mathbf{R})$,

$$H = -\frac{d^2}{dx^2} + \sum_{n\in\mathbf{Z}} \alpha_n \delta(x-n),$$

0022-247X/02 $35.00

where δ is the Dirac's delta function and α_n are real coupling constants describing each of the point interactions. If all coupling constants are equal $\alpha_n = \alpha$, one obtains a periodic operator modeling a particle moving in a one-dimensional periodic potential. This model, known as the Kronig–Penney model, became classical and is included in many textbooks on quantum mechanics. One can prove that the functions from the domain of the operator H satisfy the following boundary conditions at each point $x = n$:

$$\begin{pmatrix} \psi(n^+) \\ \psi'(n^+) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix} \begin{pmatrix} \psi(n^-) \\ \psi'(n^-) \end{pmatrix}.$$

Different models with point interactions can be obtained by considering more general boundary conditions at the singular points. Consider first one point interaction at the origin. A mathematically rigorous description of such point interaction can be obtained by considering all possible self-adjoint extensions of the symmetric operator $H^0 = -d^2/dx^2$ with the domain

$$\mathrm{Dom}(H^0) = \{\psi \in W_2^2(\mathbf{R}) : \psi(0) = \psi'(0) = 0\}.$$

One can prove that self-adjoint extensions can be divided into two classes: connected and separated extensions. Separated extensions are described by two independent boundary conditions on the half-axes and are equal to the orthogonal sum of two self-adjoint operators acting in $L_2(\mathbf{R}_-)$ and $L_2(\mathbf{R}_+)$, respectively. Such extensions are not interesting in our studies and will be excluded from our consideration. Connected extensions of the operator H^0 can be described by the boundary conditions at the origin,

$$\begin{pmatrix} \psi(0^+) \\ \psi'(0^+) \end{pmatrix} = e^{i\theta} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \psi(0^-) \\ \psi'(0^-) \end{pmatrix}, \tag{1}$$

where the parameters a, b, c, d are real, $ad - bc = 1$, and $\theta \in [0, 2\pi)$. These point interactions are well described in the literature [3, 4, 15, 23, 29, 30]. The problem of approximating these contact interactions by standard operators of mathematical physics with short-range interactions attracted the attention of many researchers. Approximations of δ and δ'-interactions[1] have been constructed in [2, 3, 12, 28]. Another approximation of the δ'-potential using "geometric scatterers" appeared in [17].

[1]These interactions are described by the boundary conditions with

$$\theta = 0, \qquad \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix}$$

and

$$\theta = 0, \qquad \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 1 & \beta \\ 0 & 1 \end{pmatrix},$$

respectively.

Different approximations of the whole four-parameter family of point interactions have been constructed in [7–9, 23, 31].

In the current paper we are going to study the operator $L = L(A, \theta)$, the second-derivative operator with periodic local point interactions determined by

DEFINITION 1.1. Let $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}(2, \mathbf{R})$ and let $\theta \in [0, 2\pi)$. Then the operator $L \equiv L(A, \theta)$ is the second-derivative operator $L = -d^2/dx^2$ acting in the Hilbert space $L_2(\mathbf{R})$ defined on the functions from $W_2^2(\mathbf{R}\backslash\{n\}_{n\in\mathbf{Z}})$ satisfying the boundary conditions

$$\begin{pmatrix} u(n^+) \\ u'(n^+) \end{pmatrix} = e^{i\theta} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} u(n^-) \\ u'(n^-) \end{pmatrix}, \qquad n \in \mathbf{Z}. \tag{2}$$

Each operator L is a self-adjoint extension of the unperturbed second-derivative operator $L_0 = -d^2/dx^2$ restricted to the set of functions from $W_2^2(\mathbf{R})$ vanishing in a neighborhood of the points $x = n$. We do not study all periodic self-adjoint extensions of L_0. In particular, nonlocal operators and operators described by separated boundary conditions are excluded from our consideration. The spectrum of the operator L can be investigated using Bloch's theorem. The first application of Bloch's theorem to point interactions other than the standard Kronig–Penney model was discussed by Gesztesy and Holden in [13], where the so-called δ'-interactions were first treated (see also [3]). Another three-parameter class of periodic point interactions was considered in [16]. The authors are grateful to the referee for pointing out that the whole four-parameter family of periodic point interactions in $\mathbf{R}^1$ was considered by Exner and Grosse in [11], where explicit formulas for the spectral bands have been presented. The same problem has been discussed in [32], but the result has never been published. Therefore we start our presentation by proving the spectral asymptotics for the second-derivative operator with different periodic boundary conditions leading to self-adjoint operators.

The aim of the current paper is to study the spectral asymptotics for the operator L. In particular we are interested in approximations of these operators with contact interactions by standard operators of mathematical physics. We are going to study the positive part of the spectrum. The spectrum of this operator is pure absolutely continuous and fills in an infinite number of bands separated by gaps. In Section 2 we discuss the classes of unitary equivalent operators with periodic point interactions. The monodromy matrix and dispersion relation are obtained in Section 3. This relation is used to calculate the spectral bands. At this point our approach is different from that of [16]. In addition, the whole four-parameter family of periodic operators is studied.[2] The character of the spectral asymptotics depends on the parameters appearing in (2) and is described by Propositions 1–3. These propositions correspond to three different asymptotic pictures observed for periodic operators. In particular it is proven that if the parameter $b \neq 0$, then the ratio between the lengths of the bands and gaps tends to zero at high energies (Theorem 4.1). This behavior is different from those for the periodic Schrödinger operator with less singular interactions. Therefore periodic operators of this type attracted the attention of several scientists [3, 5, 14]. It is shown in Section 6 that such a spectrum can be obtained as a limit of the spectrum of the periodic "weighted" operator, which corroborates another one-time approach developed in [6, 23]. We study the norm resolvent convergence of this operator sequence. It is proven that this sequence converges to the resolvent of the formal differential expression defined on the functions satisfying the energy-dependent boundary conditions (46). Since this expression does not define any operator, we construct another self-adjoint operator acting in a certain extended Hilbert space such that its resolvent restricted to the original space $L_2(\mathbf{R})$ is just the formal resolvent obtained as the limit of the operator sequence. Section 5 is devoted to the inverse spectral problem for the singular periodic operator. It is proven that the first few terms in the spectral asymptotics determine the class of unitary equivalent operators uniquely.

2. UNITARY EQUIVALENCE AND REDUCTION OF THE PARAMETERS

The parameters a, b, c, d, and θ do not parameterize the operators L uniquely. Actually the operator determined by the matrix $-A$ and the phase $\theta + \pi$ coincides with the operator determined by A and θ, since these parameters determine just the same boundary conditions (2). Therefore without loss of generality we reduce our studies to operators determined by matrices A with positive trace,

$$t \equiv a + d \geq 0. \tag{3}$$

Since our goal is to study the spectrum of the operators L, let us describe the classes of unitary equivalent operators.

We note first that the operators determined by the same matrices A and different phases θ are unitary equivalent. Consider the unimodular function

$$U(x) = e^{in(\theta_2 - \theta_1)}, \qquad x \in [(n-1), n).$$

[2]Our result is partially covered by [11], but to establish the uniqueness of the solution of the inverse spectral problem we need to calculate the spectral asymptotics in more detail.

Then the unitary equivalence between the operators $L(A, \theta_1)$ and $L(A, \theta_2)$ follows from

$$L(A, \theta_1) = U^{-1} L(A, \theta_2) U.$$

Consider the reflection operator $(\mathbf{I}f)(x) = f(-x)$. Then the unitary equivalence between the operators $L\big(\big(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\big), \theta\big)$ and $L\big(\big(\begin{smallmatrix} d & b \\ c & a \end{smallmatrix}\big), -\theta\big)$ follows from[3]

$$L\left(\begin{pmatrix} d & b \\ c & a \end{pmatrix}, -\theta\right) = \mathbf{I}^{-1} L\left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \theta\right) \mathbf{I}.$$

Definition 2.1. The operators $L(A_1, \theta_1)$ and $L(A_2, \theta_2)$ are called **equivalent** if and only if at least one of the following two equalities is satisfied[4]:

$$\begin{matrix} a_1 = a_2 \\ b_1 = b_2 \\ c_1 = c_2 \\ d_1 = d_2 \end{matrix} \quad \text{or} \quad \begin{matrix} a_1 = d_2 \\ b_1 = b_2 \\ c_1 = c_2 \\ d_1 = a_2 \end{matrix}. \tag{4}$$

The classes of equivalent operators can be described by three independent real parameters (instead of four independent real parameters describing the operators L),

$$t = a + d, \quad b, \quad \text{and} \quad c,$$

subject to the inequality

$$t \geq 2\sqrt{1 + bc}. \tag{5}$$

Taking into account that $ad - bc = 1$, the parameter a can be determined from the second-order algebraic equation $a^2 - at + 1 + bc = 0$, which has two real solutions due to (5). The two different solutions correspond to the two equivalent operators, which one gets by interchanging the parameters a and d.

The class of operators described by the parameters $a = 1$, $b = 0$, $c = 0$, $d = 1$ is equivalent to the second-derivative operator in $L_2(\mathbf{R})$ with the domain $W_2^2(\mathbf{R})$. The spectrum of this operator is pure absolutely continuous and covers the interval $[0, \infty)$. This trivial case will be excluded from our consideration.

[3]One has to take into account that the first derivative changes sign under reflection $\frac{d}{dx}(\mathbf{I}f)(x) = -\frac{d}{dx} f(-x)$.

[4]We have already restricted our consideration to the set of operators described by matrices with nonnegative traces (3).

3. THE MONODROMY MATRIX AND DISPERSION RELATION

The monodromy matrix for the interval $0^- \to 1^-$ is given by

$$\mathbf{M}^\lambda(0^-, 1^-) = \begin{pmatrix} \cos k & \frac{1}{k}\sin k \\ -k\sin k & \cos k \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$
$$= \begin{pmatrix} a\cos k + \frac{c}{k}\sin k & b\cos k + \frac{d}{k}\sin k \\ -ak\sin k + c\cos k & -bk\sin k + d\cos k \end{pmatrix}, \tag{6}$$

where $k = \sqrt{\lambda}$. The characteristic determinant of the monodromy matrix is

$$\det(\mathbf{M}^\lambda - \lambda \mathbf{I}) = \lambda^2 - \lambda \mathrm{Tr}\mathbf{M}^\lambda + \det \mathbf{M}^\lambda$$
$$= \lambda^2 - \lambda \mathrm{Tr}\mathbf{M}^\lambda + 1, \tag{7}$$

since $\det \mathbf{M}^\lambda = 1$. The spectrum of the operator L coincides with the set of λ for which the zeroes of the characteristic determinant are nonreal, i.e., $|\mathrm{Tr}\,\mathbf{M}^\lambda| \leq 2$,

$$\left|(a+d)\cos k + \left(\frac{c}{k} - bk\right)\sin k\right| \leq 2. \tag{8}$$

The last equation describes the spectrum of the periodic operator with the interaction given by (1). We introduce the function f,

$$f(k) = t\cos k + \left(\frac{c}{k} - bk\right)\sin k. \tag{9}$$

Then the spectrum of L is described by the equation

$$|f(k)| \leq 2. \tag{10}$$

Solving this inequality, we will get the spectrum of the periodic operator L in the following section. The spectrum consists of an infinite number of bands of the absolutely continuous spectrum. Depending on the parameters t, b, and c, the asymptotics of this spectrum are different. The graph of the function f and the spectrum of the corresponding periodic operator are plotted in Fig. 1.

4. SPECTRAL ASYMPTOTICS FOR THE PERIODIC OPERATOR

The spectrum of the operators L is pure absolutely continuous and consists of an infinite number of bands tending to $+\infty$ [3, 16, 25].[5] In this

[5]Note that we do not consider operators described by separated boundary conditions, which lead to eigenvalues of infinite multiplicity.

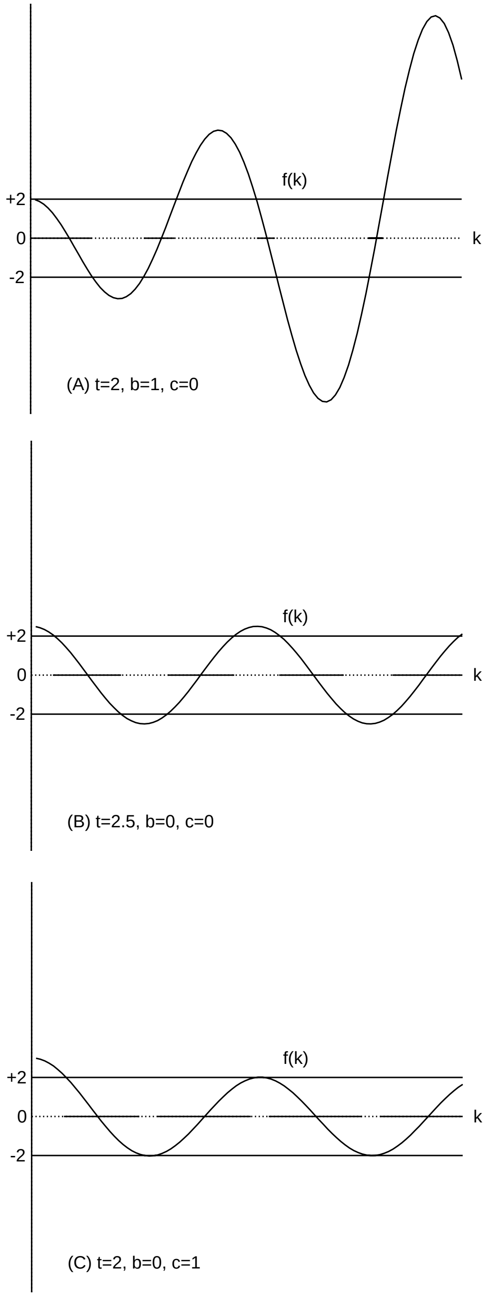

FIG. 1. The function $f(k) = t\cos(k) + (c/k - bk)\sin(k)$ and the positive spectrum of the periodic operator.

section the spectral asymptotics of these operators will be studied in detail. The following three cases covering all possible values of the parameters t, b, and c will be considered separately:

A. $b \neq 0$, t and c arbitrary satisfying (5);

B. $b = 0$, $t > 2$, c arbitrary;

C. $b = 0$, $t = 2$, $c \neq 0$ arbitrary.

Case A is generic, but the spectral asymptotics in this case are different from those for the standard Schrödinger operator in dimension one. Case C corresponds to periodic delta interactions that have been well studied in the literature.

The following three propositions describe the spectrum of the operator L in the three outlined cases.

Case A.

PROPOSITION 4.1. *Let $b \neq 0$; then the spectrum of the operator L consists of an infinite number of bands $\Delta_n = [a_n^2, b_n^2]$ situated for large values of n on the intervals $[(\pi n - \pi/2)^2, (\pi n + \pi/2)^2]$. The asymptotics of the band edges when $\lambda \to \infty$ is*

$$a_n = \pi n + \frac{1}{\pi}\left[\frac{t}{b} - \frac{2}{|b|}\right]\frac{1}{n} + \left[-\frac{t^3}{3b^3\pi^3} - \left(1 - \frac{1}{|b|}\right)\frac{t^2}{b^2\pi^3} + \left(\frac{c}{b^2\pi^3} + \frac{4|b|}{b^3\pi^3}\right)t - \frac{4}{3|b|^3\pi^3} - \frac{2}{b^3\pi^3}\left(2b + c|b|\right)\right]\frac{1}{n^3} + O\left(\frac{1}{n^5}\right), \qquad \text{as } n \to \infty;$$

$$b_n = \pi n + \frac{1}{\pi}\left[\frac{t}{b} + \frac{2}{|b|}\right]\frac{1}{n} + \left[-\frac{t^3}{3b^3\pi^3} - \left(1 + \frac{1}{|b|}\right)\frac{t^2}{b^2\pi^3} + \left(\frac{c}{b^2\pi^3} - \frac{4|b|}{b^3\pi^3}\right)t + \frac{4}{3|b|^3\pi^3} - \frac{2}{b^3\pi^3}(2b - c|b|)\right]\frac{1}{n^3} + O\left(\frac{1}{n^5}\right), \qquad \text{as } n \to \infty. \tag{11}$$

The length $|\Delta_n|$ and the middle point m_n of the band Δ_n are asymptotically given by

$$|\Delta_n| = \frac{8}{|b|} + \frac{4}{\pi^2}\left(-\frac{1}{|b|\,b^2}t^2 - \frac{2}{b\,|b|}t + \frac{4}{3\,|b|^3} + \frac{2c}{b\,|b|}\right)\frac{1}{n^2} + O\left(\frac{1}{n^4}\right), \qquad \text{as } n \to \infty, \tag{12}$$

and

$$m_n = \pi^2 n^2 + \frac{2t}{b} + \frac{1}{\pi^2}\left(-\frac{2}{3b^3}t^3 - \frac{1}{b^2}t^2 + \frac{2c}{b^2}t - \frac{4}{b^2}\right)\frac{1}{n^2} + O\left(\frac{1}{n^4}\right), \qquad \textit{as} \quad n \to \infty, \tag{13}$$

respectively.

Proof. We first prove that exactly one band Δ_n of the absolutely continuous spectrum is situated in each interval $l_n = [(\pi n - \pi/2)^2, (\pi n + \pi/2)^2]$ for large enough values of k.[6] The values of the function f at the end points of each interval l_n

$$\begin{aligned} f(\pi n + \pi/2) &= (-1)^n \left(\frac{c}{\pi n + \pi/2} - b(\pi n + \pi/2)\right) \\ &= (-1)^{n+1} b\pi n + O(1), \qquad \text{as } n \to \infty, \end{aligned}$$

have alternating signs and an absolute value of >2 if n is sufficiently large. Taking into account that the function $f(k)$ is continuous, we conclude that each considered interval contains at least one spectral band.

The zeroes of $f'(k) = -(t + c/k^2 + b)\sin k + (\frac{c}{k} - bk)\cos k$ are determined by the equation

$$\tan k = \frac{k(c - bk^2)}{(t+b)k^2 + c}. \tag{14}$$

The function $k(c - bk^2)/((t+b)k^2 + c)$ is rational and tends to $\pm\infty$ as $k \to \infty$ as follows:

$$\frac{k(c-bk^2)}{(t+b)k^2+c} = \begin{cases} -\dfrac{b}{t+b}k + \dfrac{c(t+2b)}{(t+b)^2}\dfrac{1}{k} + O\left(\dfrac{1}{k^2}\right), & t+b \neq 0\,; \\ k - \dfrac{b}{c}k^3, & t+b = 0,\ c \neq 0. \end{cases}$$

In the special case where $t + b = 0,\ c = 0$, the relation (14) takes the form $-bk\cos k = 0$ and has solutions $k = \frac{\pi}{2} + \pi n$. Therefore each interval l_n contains exactly one extreme point for the function f when $n \to \infty$. Since f is continuous and monotonous between the extreme points, it follows that there is precisely one interval where $|f(k)| \leq 2$ in each l_n if n is sufficiently large.

The end points of each band $\Delta_n = [a_n^2, b_n^2]$ can be calculated by solving the equation $|f(k)| = 2$. Consider first the case $b > 0$. Then the left

[6] We find it convenient to count the band of the continuous spectrum by the number n, so that the band Δ_n is situated near the point $\pi^2 n^2$ for large values of the energy.

and right end points of the intervals Δ_n satisfy the following equations, respectively:

$$t\cos a_n + \left(\frac{c}{a_n} - b\, a_n\right)\sin a_n = (-1)^n 2; \tag{15}$$

$$t\cos b_n + \left(\frac{c}{b_n} - b\, b_n\right)\sin b_n = -(-1)^n 2. \tag{16}$$

Since the points a_n and b_n are close to πn for large n, we use the asymptotic representations

$$\begin{aligned} a_n &= \pi n + \frac{\alpha}{n} + \frac{\alpha'}{n^3} + O\left(\frac{1}{n^5}\right), \\ & \qquad\qquad\qquad\qquad n \to \infty. \\ b_n &= \pi n + \frac{\beta}{n} + \frac{\beta'}{n^3} + O\left(\frac{1}{n^5}\right), \end{aligned}$$

Substituting these representations into (15) and (16), we get

$$\begin{aligned} a_n = \pi n &+ \frac{t-2}{b\pi}\frac{1}{n} + \left(-\frac{1}{3b^3\pi^3}t^3 + \frac{1-b}{b^3\pi^3}t^2\right. \\ &\left.+\frac{c+4}{b^2\pi^3}t - \frac{4}{3b^3\pi^3} - \frac{4+2c}{b^2\pi^3}\right)\frac{1}{n^3} + O\left(\frac{1}{n^5}\right), \qquad \text{as } n \to \infty; \\ b_n = \pi n &+ \frac{t+2}{b\pi}\frac{1}{n} + \left(-\frac{1}{3b^3\pi^3}t^3 - \frac{1+b}{b^3\pi^3}t^2\right. \\ &\left.+\frac{c-4}{b^2\pi^3}t + \frac{4}{3b^3\pi^3} + \frac{2c-4}{b^2\pi^3}\right)\frac{1}{n^3} + O\left(\frac{1}{n^5}\right), \qquad \text{as } n \to \infty. \end{aligned} \tag{17}$$

Similar analysis in the case where $b < 0$ leads to formula (11).

The length and the middle point of the band Δ_n are given by

$$|\Delta_n| = b_n^2 - a_n^2, \qquad m_n = \frac{a_n^2 + b_n^2}{2}. \tag{18}$$

Then formulas (12) and (13) are straightforward corollaries of (17). The proposition is proven. ∎

The length of the gap G_n between the bands with the numbers n and $n+1$ can be calculated as follows:

$$|G_n| = a_{n+1}^2 - b_n^2 = 2\pi^2 n + \pi^2 - \frac{8}{|b|} + O\left(\frac{1}{n^2}\right). \tag{19}$$

The ratio between the lengths of the bands and forbidden gaps tends to zero as follows:

$$\frac{|\Delta_n|}{|G_n|} = \frac{4}{\pi^2|b|}\frac{1}{n} + O\left(\frac{1}{n^3}\right), \qquad \text{as } n \to \infty. \tag{20}$$

Case B.

PROPOSITION 4.2. *Let $b = 0$ and let $t > 2$; then the spectrum of the operator L consists of an infinite number of bands $\Delta_n = [a_n^2, b_n^2]$ situated for sufficiently large n inside the intervals $[\pi^2 n^2, \pi^2(n+1)^2]$. The asymptotics of the band edges are given by*

$$\begin{aligned} a_n &= \pi n + \arccos\frac{2}{t} + \frac{c}{\pi t n} + O\left(\frac{1}{n^2}\right), \qquad \textit{as } n \to \infty; \\ b_n &= \pi(n+1) - \arccos\frac{2}{t} + \frac{c}{\pi t n} + O\left(\frac{1}{n^2}\right), \qquad \textit{as } n \to \infty. \end{aligned} \tag{21}$$

The length $|\Delta_n|$ and the middle point m_n of the band Δ_n are asymptotically given by

$$\begin{aligned} |\Delta_n| = 2\pi\left(\pi - 2\arccos\frac{2}{t}\right)n + \left(\pi^2 - 2\pi\arccos\frac{2}{t}\right) \\ + O\left(\frac{1}{n}\right), \qquad \textit{as } n \to \infty, \end{aligned} \tag{22}$$

and

$$\begin{aligned} m_n = \pi^2\left(n + \frac{1}{2}\right)^2 + \left(\arccos\frac{2}{t} - \frac{\pi}{2}\right)^2 + \frac{2c}{t} \\ + O\left(\frac{1}{n}\right), \qquad \textit{as } n \to \infty\,. \end{aligned} \tag{23}$$

Proof. The function f looks as follows in the considered case:

$$f(k) = t\cos k + \frac{c}{k}\sin k. \tag{24}$$

The proof of the fact that exactly one band of the absolutely continuous spectrum is situated in each interval $l_n = [\pi^2 n^2, \pi^2(n+1)^2]$ is similar to that of Proposition 1. Actually the values of the function f at the end points of each interval l_n

$$f(\pi n) = (-1)^n t,$$

have alternating signs and an absolute value of >2 for sufficiently large n. The equation for extreme points,

$$\tan k = \frac{ck}{k^2 t + c},$$

has exactly one solution in each interval, since the function $ck/(k^2 t + c)$ is decreasing if k is sufficiently large.

Solutions to the equation $t \cos k = \pm 2$ are situated at the points

$$k = \pm \arccos \frac{2}{t} + \pi n.$$

Since $0 < \frac{2}{t} < 1$, $\arccos \frac{2}{t}$ satisfies

$$0 < \arccos \frac{2}{t} < \pi/2.$$

Since the points a_n and b_n are close to $\pi n + \arccos \frac{2}{t}$ and $\pi(n+1) - \arccos \frac{2}{t}$, respectively, the following representations can be used:

$$a_n = \pi n + \arccos \frac{2}{t} + \alpha_n, \qquad b_n = \pi(n+1) - \arccos \frac{2}{t} + \beta_n.$$

The equation for the left end point,

$$t \cos\left(\pi n + \arccos \frac{2}{t} + \alpha_n \right) + \frac{c}{\pi n + \arccos(2/t) + \alpha_n} \sin\left(\pi n + \arccos \frac{2}{t} + \alpha_n \right) = (-1)^n 2,$$

implies that

$$t\left(\frac{2}{t} \cos \alpha_n - \sin\left(\arccos \frac{2}{t} \right) \sin \alpha_n \right) + \frac{c}{\pi n + \arccos(2/t) + \alpha_n} \left(\sin\left(\arccos \frac{2}{t} \right) \cos \alpha_n + \frac{2}{t} \sin \alpha_n \right) = 2.$$

Keeping the first terms of the perturbation theory, we get

$$\alpha_n = \frac{c}{\pi t n} + O\left(\frac{1}{n^2} \right), \qquad n \to \infty,$$

and formula (21). The representation for b_n can be proven similarly. Formulas (22) and (23) follow directly from the asymptotic representations (21) and definition (18). The proposition is proven. ∎

The length of the gap between the spectral bands Δ_n and Δ_{n+1} is

$$|G_n| = 4\pi\left(\arccos \frac{2}{t} \right) n + 4\pi \arccos \frac{2}{t} + O\left(\frac{1}{n} \right), \qquad \text{as } n \to \infty. \tag{25}$$

Both the gaps and the bands are growing approximately linearly with the number n. The ratio between the lengths of the bands and gaps tends to the finite nonzero limit depending on the parameter t only,

$$\frac{|\Delta_n|}{|G_n|} = \frac{\pi/2 - \arccos(2/t)}{\arccos(2/t)} + O\left(\frac{1}{n} \right), \qquad \text{as } n \to \infty. \tag{26}$$

Case C.

PROPOSITION 4.3. *Let $b = 0$, $t = 2$, and $c \neq 0$; then the spectrum of the operator L consists of an infinite number of bands $\Delta_n = [a_n^2, b_n^2]$ situated for sufficiently large n inside the intervals $[\pi^2 n^2, \pi^2 (n+1)^2]$. The asymptotics of the band edges are*

$$\left.\begin{aligned} a_n &= \pi n + \frac{c}{\pi n} + O\left(\frac{1}{n^2}\right), \quad \text{as } n \to \infty, \\ b_n &= \pi(n+1), \end{aligned}\right\} \quad \text{if } c > 0;$$
$$\left.\begin{aligned} a_n &= \pi n, \\ b_n &= \pi(n+1) - \frac{|c|}{\pi n} + O\left(\frac{1}{n^2}\right), \quad \text{as } n \to \infty, \end{aligned}\right\} \quad \text{if } c < 0; \tag{27}$$

The length $|\Delta_n|$ and the middle point m_n of the band Δ_n are asymptotically given by

$$|\Delta_n| = 2\pi^2 n + (\pi^2 - 2|c|) + O\left(\frac{1}{n}\right), \qquad \text{as } n \to \infty; \tag{28}$$

$$m_n = \pi^2 n^2 + \pi^2 n + \frac{\pi^2}{2} + c + O\left(\frac{1}{n}\right), \qquad \text{as } n \to \infty. \tag{29}$$

Proof. The proof of this proposition follows the same lines as those of propositions 1 and 2. It can be found in many textbooks (see, e.g., [3]). ∎

The length of the gap between the bands is given by

$$|G_n| = 2|c| + O\left(\frac{1}{n}\right), \qquad n \to \infty. \tag{30}$$

The ratio between the length of the nth band and the width of the nth gap tends to infinity as follows:

$$\frac{|\Delta_n|}{|G_n|} = \frac{\pi^2}{|c|} n + O(1), \qquad n \to \infty. \tag{31}$$

In the case $t = 2$, $b = c = 0$, the operator L coincides with the unperturbed second-derivative operator. The gaps between the spectral bands disappear when $c \to 0$, and the absolutely continuous spectrum fills the whole interval $[0, \infty)$.

Our results concerning the spectral asymptotics for the periodic operator with point interactions can be summarized as follows:

THEOREM 4.1. *The spectrum of the operator L with periodic point interactions consists of an infinite number of bands Δ_n of the absolutely continuous spectrum separated by an infinite number of gaps G_n (if the operator is not equivalent to the unperturbed second-derivative operator). The lengths of the bands and gaps and the ratio between them are given by*

- *if* $b \neq 0$

$$\begin{aligned} |\Delta_n| &= \frac{8}{|b|} + O\left(\frac{1}{n^2}\right), \\ |G_n| &= 2\pi^2 n + O(1), \qquad \text{as } n \to \infty; \\ \frac{|\Delta_n|}{|G_n|} &= \frac{4}{\pi^2 |b|}\frac{1}{n} + O\left(\frac{1}{n^2}\right), \end{aligned} \tag{32}$$

- *if* $b = 0,\ t > 2$

$$\begin{aligned} |\Delta_n| &= 2\pi\left(\pi - 2\arccos\frac{2}{t}\right)n + O(1), \\ |G_n| &= 4\pi\left(\arccos\frac{2}{t}\right)n + O(1), \qquad \text{as } n \to \infty; \\ \frac{|\Delta_n|}{|G_n|} &= \frac{\pi/2 - \arccos(2/t)}{\arccos(2/t)} + O\left(\frac{1}{n}\right), \end{aligned} \tag{33}$$

- *if* $b = 0,\ t = 2,\ c \neq 0$

$$\begin{aligned} |\Delta_n| &= 2\pi^2 n + O(1), \\ |G_n| &= 2|c| + O\left(\frac{1}{n}\right), \qquad \text{as } n \to \infty. \\ \frac{|\Delta_n|}{|G_n|} &= \frac{\pi^2}{|c|} n + O(1), \end{aligned} \tag{34}$$

5. INVERSE SPECTRAL PROBLEM FOR A SINGULAR PERIODIC OPERATOR

The spectral asymptotics determine the class of equivalent operators uniquely.

THEOREM 5.1. *The spectral asymptotics for the operator L with periodic point interactions determine uniquely the class of equivalent operators; that is, the parameters $t = a + d$, b, and c can uniquely be determined either from* *the asymptotics of the band edges or from the asymptotics of the lengths and middle points of the spectral bands.*

Proof. Let us consider the three cases described by Propositions 1–3 separately. These cases can easily be distinguished from the spectral asymptotics, since the ratio between the lengths of the bands and gaps has different behaviors for large values of the energy.

In Case A the terms of order $\frac{1}{n}$ in formulas (11) determine the parameters b and t uniquely, since the parameter t is positive. Then the parameter c is determined by the third-order term. Similarly the first two terms in the asymptotics of $|\Delta_n|$ and the first three terms in the asymptotics of m_n determine the three parameters t, b, and c as well.

Cases B and C are similar. The theorem is proven. ∎

The theorem implies that the spectral asymptotics generally do not determine uniquely the parameters of the periodic operator L. The set of operators having the same spectral asymptotics coincides with the set of equivalent operators.

6. SPECTRAL ASYMPTOTICS FOR A PERIODIC OPERATOR AND A "WEIGHTED" OPERATOR

The spectral asymptotics calculated in Section 4 can be compared with the spectral asymptotics for nonsingular periodic one-dimensional operators. The asymptotics in Case C resemble the asymptotics for a periodic Schrödinger operator,

$$-\frac{d^2}{dx^2} + U(x), \qquad U(x+1) = U(x), \qquad U \in C(\mathbf{R}).$$

We would like to point out that this operator has an absolutely continuous spectrum filling up the bands separated by a finite or an infinite number of gaps. The ratio between the lengths of the bands and gaps increases as $\lambda \to \infty$, and the rate depends on the regularity of the interaction.

The spectral asymptotics obtained in Case A differ drastically from those for the periodic Schrödinger operator. In this case the ratio between the lengths of the bands and gaps tends to zero as $\lambda \to \infty$. In this section we show that such spectral asymptotics appear naturally during the investigation of the periodic "weighted" operator

$$\mathbf{W\Psi} = -\frac{1}{\rho}\frac{d}{dx}\left(\rho\frac{d}{dx}\psi\right), \tag{35}$$

with $\rho > 0$. This operator was investigated recently by Korotyaev (see [18, 19] for references and historical remarks). Consider the periodic weighted operator

$$\mathbf{W}_\epsilon \boldsymbol{\Psi} = -\frac{1}{\rho_\epsilon(x)} \frac{d}{dx}\left(\rho_\epsilon(x)\frac{d}{dx}\boldsymbol{\Psi}\right), \tag{36}$$

where the density function

$$\rho_\epsilon(x) = 1 + \sum_{n=-\infty}^{\infty} h\frac{1}{\epsilon}\chi_\epsilon(x-n), \qquad h \in \mathbf{R}_+ \tag{37}$$

is defined using the characteristic function

$$\chi_\epsilon(x) = \begin{cases} 1, & x \in [0,\epsilon] \\ 0, & x \notin [0,\epsilon]. \end{cases} \tag{38}$$

The density function ρ_ϵ is chosen so that it converges to the sum of delta functions plus 1 as $\epsilon \to 0$.

Let us study the spectrum of the operator $\mathbf{W}_\epsilon$. Since the function ρ_ϵ is discontinuous at $x = n$, $x = n+\epsilon$, the functions from the domain of the operator $\mathbf{W}_\epsilon$ satisfy the boundary conditions

$$\begin{aligned} \Psi(n^+) &= \Psi(n^-), \\ \left(1+h\frac{1}{\epsilon}\right)\Psi'(n^+) &= \Psi'(n^-), \\ \Psi((n+\epsilon)^+) &= \Psi((n+\epsilon)^-), \\ \Psi'((n+\epsilon)^+) &= \left(1+h\frac{1}{\epsilon}\right)\Psi'((n+\epsilon)^-). \end{aligned} \tag{39}$$

These conditions guarantee that the functions $\boldsymbol{\Psi}$ and $\rho_\epsilon\boldsymbol{\Psi}'$ are continuous. The monodromy matrix for the operator $\mathbf{W}$ is equal to the product of four matrices: two monodromy matrices for the second-derivative operator on the intervals $(0^+,\epsilon^-)$ and $(\epsilon^+,1^-)$ and two monodromy matrices corresponding to discontinuities at $x=0$ and $x=\epsilon$,

$$\begin{aligned} &\mathbf{M}^\lambda_{\mathbf{W}_\epsilon}(0^-,1^-) \\ &\quad= \mathbf{M}^\lambda_{-\frac{d^2}{dx^2}}(\epsilon^+,1^-)\begin{pmatrix} 1 & 0 \\ 0 & 1+\frac{h}{\epsilon}\end{pmatrix}\mathbf{M}^\lambda_{-\frac{d^2}{dx^2}}(0^+,\epsilon^-)\begin{pmatrix} 1 & 0 \\ 0 & 1-\frac{h}{\epsilon+h}\end{pmatrix} \\ &\quad= \begin{pmatrix} \cos k - \frac{1}{\epsilon}\sin(1-\epsilon)k\sin\epsilon k & \frac{1}{k}\sin k - \frac{1}{k(\epsilon+h)}\cos(1-\epsilon)k\sin\epsilon k \\ -k\sin k - \frac{k}{\epsilon}\cos(1-\epsilon)k\sin\epsilon k & \cos k + \frac{1}{\epsilon+h}\sin(1-\epsilon)k\sin\epsilon k \end{pmatrix}. \end{aligned} \tag{40}$$

Since the determinant of the monodromy matrix $\mathbf{M}^{\lambda}_{\mathbf{W}_\epsilon}$ is equal to one, the spectrum of the operator is determined by the trace of the monodromy matrix

$$|\mathrm{Tr}\mathbf{M}^{\lambda}_{\mathbf{W}_\epsilon}| = \left|2\cos k - \frac{h}{\epsilon(\epsilon+1)}\sin[(1-\epsilon)k]\sin[k\epsilon]\right| \leq 2. \tag{41}$$

Consider the limit $\epsilon \to 0$; then the last equation transforms into the equation

$$|2\cos k - hk\sin k| \leq 2, \tag{42}$$

which coincides with the dispersion equation for the operator with periodic point interactions determined by the parameters

$$a = 1, \qquad b = h, \qquad c = 0, \qquad d = 1. \tag{43}$$

It follows that each band of the absolutely continuous spectrum of the operator $\mathbf{W}_\epsilon$ as $\epsilon \to 0$ converges to a certain band of the absolutely continuous spectrum of the operator L with the parameters chosen as above. This calculation shows again that the singular second-derivative operator described by the boundary conditions (1) with $\theta = 0$ and $a = d = 1$, $c = 0$, $b \neq 0$ can be interpreted as the operator with singular density. This fact was observed for the first time in [23], where singular interactions for the second-derivative operator in $L_2(\mathbf{R})$ were investigated.

We have shown that the behavior of the spectral bands for the operator with periodic point interactions in Case A resembles those for the operator W_ϵ as $\epsilon \to 0$. Let us study the norm resolvent convergence of the operator sequence W_ϵ. One can easily prove that the resolvents of W_ϵ do not converge to a resolvent of any operator acting in the Hilbert space $L_2(\mathbf{R})$. The limit is given by a so-called generalized resolvent—restriction to $L_2(\mathbf{R})$ of the resolvent of a certain self-adjoint operator acting in a certain extended Hilbert space [1]. Obviously the extended operator is not uniquely defined. One such self-adjoint operator can be constructed using the method of generalized point interactions [4, 22, 24, 26, 27]. Consider the Hilbert space $\mathbf{H} = L_2(\mathbf{R}) \oplus l_2$ and the self-adjoint operator $\mathbf{A}$ defined by following formula

$$\mathbf{A}\begin{pmatrix}\Psi\\ \psi\end{pmatrix} = \begin{pmatrix}-\dfrac{d^2}{dx^2}\Psi\\ \{[\Psi']\}/\sqrt{h}\end{pmatrix} \tag{44}$$

on functions $(\Psi, \psi) \in W_2^2(\mathbf{R}\backslash\mathbf{Z}) \oplus l_2$ satisfying the boundary conditions

$$\begin{cases}\Psi(n^+) = \Psi(n^-),\\ \psi_n = -\sqrt{h}\{\Psi\}_n,\end{cases} \qquad n \in \mathbf{Z}, \tag{45}$$

where $\{[\Psi']\}$ and $\{\Psi\}$ denote the vectors from l_2 with the coordinates $\Psi'(n^+) - \Psi'(n^-)$ and $\Psi(n)$, respectively. The self-adjointness of the operator $\mathbf{A}$ so defined can be proven by noting that the operator is symmetric and the range of $\mathbf{A} - \lambda$ coincides with $\mathbf{H}$ if $\Im\lambda \neq 0$ (for details see [4, 21, 24]). The resolvent of the operator $\mathbf{A}$ restricted to the space $L_2(\mathbf{R})$ coincides with the resolvent of the differential operator $-d^2/dx^2$ with the energy-dependent boundary conditions at the points $x = n$,

$$\begin{pmatrix} \Psi(n^+) \\ \Psi'(n^+) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -hk^2 & 1 \end{pmatrix} \begin{pmatrix} \Psi(n^-) \\ \Psi'(n^-) \end{pmatrix}. \tag{46}$$

To calculate the restricted resolvent one has to solve the following equation for any function $F \in L_2(\mathbf{R})$:

$$(\mathbf{A} - \lambda)\begin{pmatrix} \Psi \\ \psi \end{pmatrix} = \begin{pmatrix} F \\ 0 \end{pmatrix} \Rightarrow \begin{cases} -\dfrac{d^2}{dx^2}\Psi(x) - \lambda\Psi(x) = F(x), & x \notin \mathbf{Z} \\ \dfrac{1}{\sqrt{h}}\{[\Psi']\} - \lambda\psi = 0. \end{cases}$$

Excluding the vector ψ from this system of equations, using the second boundary condition (45), we get an energy-dependent boundary condition for the component Ψ,

$$\{[\Psi']\} = -\lambda h\{\Psi\},$$

which is exactly the second equation in (46).

THEOREM 6.1. *Let $h > 0$; then as $\epsilon \to 0^+$ the resolvents of the operators W_ϵ converge to the restriction to $L_2(\mathbf{R})$ of the resolvent of A.*

Proof. The operator W_ϵ commutes with the shift operator. Hence it is natural to use the (Bloch) decomposition of the Hilbert space $L_2(\mathbf{R})$ into the orthogonal integral over the spaces of quasi-periodic functions H^θ [3],

$$L_2(\mathbf{R}) \sim \int_{\theta\in[-\pi,\pi)}^{\oplus} H^\theta \, d\theta, \qquad H^\theta = L_2([0,1]), \tag{47}$$

where $\sim$ denotes the unitary equivalence. Similarly the operator W_ϵ is equal to the orthogonal integral of the operators W_ϵ^θ, each acting in the space $H^\theta = L_2([0,1])$ of quasi-periodic functions. The domain of each operator W_ϵ^θ consists of functions ψ from $W_2^2([0,1])$ satisfying the boundary conditions at the point $x = \epsilon$ and at the end points of the interval $[0,1]$

$$\begin{aligned} \psi(0^+) &= q\psi(1) \\ (1 + h/\epsilon)\psi'(0^+) &= q\psi'(1^-) \\ \psi(\epsilon^+) &= \psi(\epsilon^-) \\ \psi'(\epsilon^+) &= (1 + h/\epsilon)\psi'(\epsilon^-), \end{aligned} \tag{48}$$

where we introduced for convenience the parameter $q = e^{i\theta}$.

The kernel $r_{\theta,\epsilon}(x,y)$ of the resolvent $(W_\epsilon^\theta - \lambda)^{-1}$ can be calculated for arbitrary λ, $\Im\lambda \neq 0$, using the representation

$$r_{\theta,\epsilon}(x,y) = r_\theta^0(x,y) + \begin{cases} \alpha\cos kx + \beta kx; \\ \quad 0 < x < \epsilon, \\ A\cos kx + B\sin kx; \\ \quad \epsilon < x < 1, \end{cases} \qquad k^2 = \lambda, \tag{49}$$

where $r_\theta^0(x,y)$ is the kernel of the resolvent of the second-derivative operator $-d^2/dx^2$ defined in H^θ by the quasi-periodic boundary conditions

$$\psi(0) = q\psi(1), \qquad \psi'(0) = q\psi'(1).$$

The parameters α, β, A, B appearing in (49) depend on y and λ. Substituting the kernel $r_{\theta,\epsilon}(x,y)$ into the boundary conditions (48), one gets the following 4×4 linear system:

$$\begin{aligned} \alpha &= q(A\cos k + B\sin k) \\ (1+h/\epsilon)(r_x^0(0,y) + \beta k) &= q(r_x^0(1,y) - Ak\sin k + Bk\cos k) \\ A\cos k\epsilon + B\sin k\epsilon &= \alpha\cos k\epsilon + \beta k\sin k\epsilon \\ r_x^0(\epsilon) - Ak\sin k\epsilon + Bk\cos k\epsilon &= (1+h/\epsilon)(r_x^0(\epsilon,y) - \alpha k\sin k\epsilon \\ &\qquad + \beta k\sin\cos k\epsilon). \end{aligned}$$

The first two equations imply that

$$\begin{aligned} \alpha &= q\cos kA + q\sin kB, \\ \beta &= \frac{1}{k(1+h/\epsilon)}(-h/\epsilon r_x^0(0,y) - qk\sin\, kA + qk\cos kB). \end{aligned} \tag{50}$$

Substituting α and β into the second pair of equations, one gets a 2×2 linear system which has the solution

$$\begin{aligned} A &= h\frac{r_x^0(0,y)(-q\sin k + \frac{h}{\epsilon h}\cos k\epsilon\sin k\epsilon) + r_x^0(\epsilon,y)(-\sin k\epsilon + q\cos k\epsilon\sin k + \frac{\epsilon q}{\epsilon+h}\sin k\epsilon\cos k)}{\epsilon k(1+q[-2\cos k\epsilon\cos k(1-\epsilon) + (\frac{\epsilon}{\epsilon+h} + \frac{\epsilon+h}{\epsilon})\sin k\epsilon\sin k(1-\epsilon)] + q2)}; \\ B &= h\frac{r_x^0(0,y)(q\cos k - 1 + \sin^2 k\epsilon\frac{h}{\epsilon+h}) + r_x^0(\epsilon,y)(\cos k\epsilon - q\cos k\epsilon\cos k + \frac{\epsilon q}{\epsilon+h}\sin k\epsilon\sin k)}{\epsilon k(1+q[-2\cos k\epsilon\cos k(1-\epsilon)(\frac{\epsilon}{\epsilon+h} + \frac{\epsilon+h}{\epsilon})\sin k\epsilon\sin k(1+\epsilon)] + q^2)}. \end{aligned} \tag{51}$$

As $\epsilon \to 0^+$ these parameters tend to the following limits, respectively:

$$\begin{aligned} A_0 &= \frac{-khq\sin kr^0(0,y)}{1 - 2q\cos k + hkq\sin k + q^2}, \\ B_0 &= \frac{-kh(1-q\cos k)r^0(0,y)}{1 - 2q\cos k + hkq\sin k + q^2}. \end{aligned} \tag{52}$$

This convergence is uniform with respect to θ. It follows that the coefficients α and β are uniformly bounded with respect to θ. Consider the integral operator with the kernel

$$\rho_\theta(x, y) = r^0(x, y) + A_0 \cos kx + B_0 \sin kx.$$

The difference between the operators with the kernels $r_{\theta,\epsilon}$ and ρ_θ tends to zero as $\epsilon \to 0$ in the Hilbert–Schmidt norm uniformly with respect to θ.

The function $\rho_\theta(x, y)$ solves the equation $-(d^2/dx^2)\rho(x, y) - \lambda\rho(x, y) = \delta(x - y)$ and satisfies the following boundary conditions:

$$\rho_\theta(0^+, y) = q\rho_\theta(1, y),$$
$$\frac{\partial}{\partial x}\rho_\theta(0^+, y) = -hk^2 q\rho_\theta(1, y) + q\frac{\partial}{\partial x}\rho_\theta(1, y).$$

It follows that the operators with the kernels $\rho_\theta(x, y)$ determine via Bloch decomposition (47) exactly the resolvent of the operator $\mathbf{A}$ restricted to the space $L_2(\mathbf{R})$. Since the convergence is uniform with respect to θ, we have proven that the resolvent of W_ϵ converges in the operator norm to the resolvent of the operator $\mathbf{A}$ restricted to the subspace $L_2(\mathbf{R}) \subset \mathbf{H}$. The theorem is proven. ∎

For negative values of h one can easily construct a similar self-adjoint operator acting in a certain Krein space (with indefinite metrics).

ACKNOWLEDGMENTS

The author thanks S. Albeverio, J. Boman, E. Korotyaev, and B. Pavlov for fruitful discussions. Financial support from the Swedish Royal Academy of Sciences is gratefully acknowledged. The authors thank the referee for important remarks on the literature, encouragement to prove Theorem 6.1, and valuable comments.

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