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Spectral asymptotics for Schrödinger operators with periodic point interactions

P.Kurasov and J.Larson

Abstract. Spectrum of the second order differential operator with periodic point interactions in $L_2(\mathbf{R})$ is investigated. Classes of unitary equivalent operator of this type are described. Spectral asymptotics for the whole family of periodic operators are calculated. It is proven that the first several terms of 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.

1. Introduction, definition of the operator.

Differential and pseudodifferential operators with points interaction are widely used in applications to quantum and atomic physics to produce exactly solvable models of complicated physical phenomena [**1, 5**]. 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 R. de L. Kronig and W.G.Penney [**11**] and can be described by the following Hamiltonian in $L_2(\mathbf{R})$

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

where δ is 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 periodic operator modelling particle moving in a one-dimensional periodic potential. This model known as Kronig-Penney model became classical and is included in many text books 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. Mathematically rigorous description of such point interaction can be obtained by considering all possible self-adjoint extensions of the symmetric operator $H^0 = -\frac{d^2}{dx^2}$ with the domain

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

One can prove that the self-adjoint extensions can be divided into two classes: connected and separated extensions. Separated extensions are described by two independent boundary conditions on the the half axes and are equal to the orthogonal sum of the two self-adjoint in $L_2(\mathbf{R}_-)$ and $L_2(\mathbf{R}_+)$. 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 following 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 [**1, 2, 7, 12, 13, 14**].

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

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

Each operator L is a self-adjoint extension of the unperturbed second derivative operator $L_0 = -\frac{d^2}{dx^2}$ restricted to the set of functions from $W_2^2(\mathbf{R})$ vanishing in a neighborhood of the points $x = n$. The spectrum of the operator L can be investigated using Bloch's theorem (see [**8**], where Bloch's theorem has been applied to point interaction models).

The aim of the current paper is to study the spectral asymptotics for the operator L. Since all operators L are bounded from below, the positive part of the spectrum will be investigated. The spectrum of this operator is pure absolutely continuous and fills in 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 [**8**]. In addition the whole 4-parameter family of periodic operators is studied.[1] 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 1). This behavior is different from those for the periodic Schrödinger operator. Therefore periodic operators of this type attracted attention of several scientists [**1, 3, 6**]. It is shown in Section 6 that such spectrum can be obtained as a limit of the spectrum of the periodic "weighted" operator, which corroborates another one time approach developed in [**4, 12**]. 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 parametrize the operators L uniquely. Really 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

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

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 $L\left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \theta\right)$ and $L\left(\begin{pmatrix} d & b \\ c & a \end{pmatrix}, -\theta\right)$ follows

[1] To our surprise the whole family of operators with periodic point interactions have not been studied in details.

from[2]

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

DEFINITION 2. 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[3]

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

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

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

subject to the inequality

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

Really 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 corresponds to the two equivalent operators which one gets 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. The monodromy matrix and dispersion relation.

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

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

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

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

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

$$\begin{aligned} \det\left(\mathbf{M}^\lambda - \lambda \mathbf{I}\right) &= \lambda^2 - \lambda \mathrm{Tr}\mathbf{M}^\lambda + \det \mathbf{M}^\lambda \\ &= \lambda^2 - \lambda \mathrm{Tr}\mathbf{M}^\lambda + 1, \end{aligned} \tag{7}$$

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. $|\mathrm{Tr}\, \mathbf{M}^\lambda| \leq 2$

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

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 infinite number of bands of the absolutely continuous spectrum. Depending on the parameters t, b and c the asymptotics of this spectrum is different. The graph of the function f and the spectrum of the corresponding periodic operator are plotted on Figure 1.

4. Spectral asymptotics for the periodic operator.

The spectrum of the operators L is pure absolutely continuous and consists of infinite number of bands tending to $+\infty$[**1, 8**]. In this section the spectral asymptotics of these operators will be studied in details. 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.

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

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

Case A.

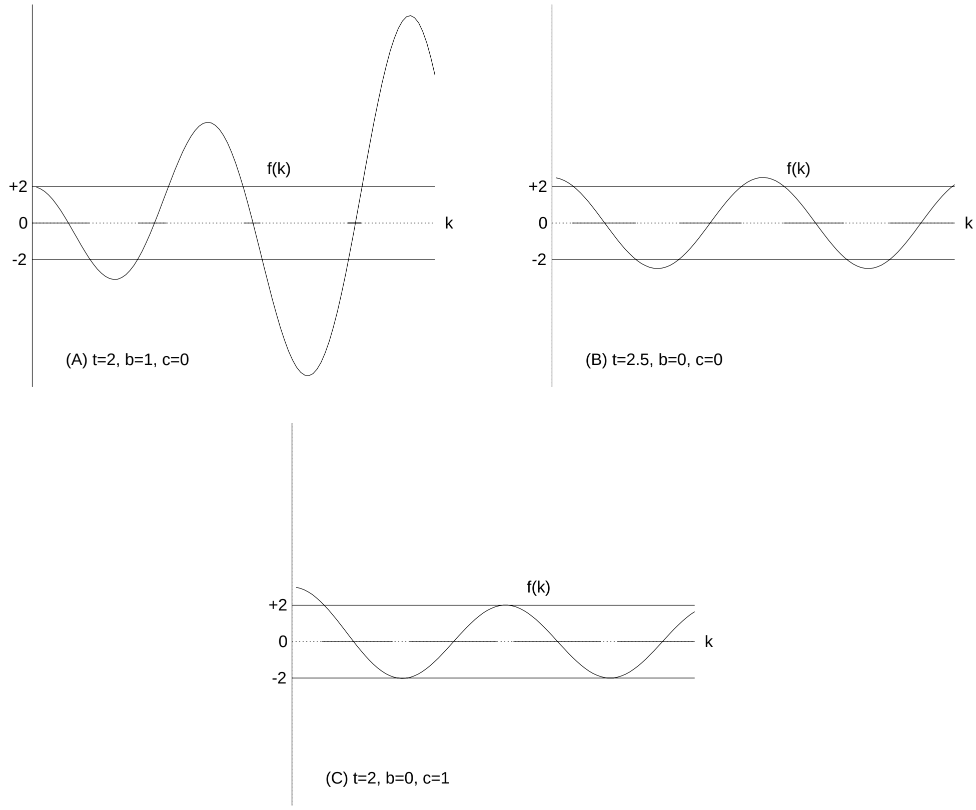

FIGURE 1. The function $f(k) = t\cos(k) + (c/k - bk)\sin(k)$ and the positive spectrum of the periodic operator.

PROPOSITION 1. Let $b \neq 0$, then the spectrum of the operator L consists of 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 when $\lambda \to \infty$ of the band edges is

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

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

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

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

and

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

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.[4] The values of the function f at the end points of each interval l_n

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

have alternating signs and absolute value > 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.

[4]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.

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

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

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

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

In the special case $t+b = 0, c = 0$ 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 solving the equation $|f(k)| = 2$. Consider first the case $b > 0$. Then the left 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

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

Substituting these representations into (15) we get

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

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

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

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

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

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

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

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

Case B.

Proposition 2. Let $b=0$ and $t>2$, then the spectrum of the operator L consists of 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 is given by

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

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

$$|\Delta_n| = 2\pi(\pi - 2\arccos\frac{2}{t})n + (\pi^2 - 2\pi\arccos\frac{2}{t}) + O(\frac{1}{n}), \quad \text{as } n \to \infty, \tag{22}$$

and

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

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. Really 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 absolute value > 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 $\frac{ck}{k^2t+c}$ 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

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

The equation for the left end point

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

implies that

$$t\left(\frac{2}{t}\cos\alpha_n - \sin\left(\arccos\frac{2}{t}\right)\sin\alpha_n\right)$$

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

Keeping the first terms of the perturbation theory we get

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

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

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

Both the gaps and the bands are growing approximately linear 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

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

Case C.

Proposition 3. Let $b = 0$, $t = 2$, and $c \neq 0$, then the spectrum of the operator L consists of 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 is

$$\begin{array}{lll} a_n &=& \pi n + \frac{c}{\pi n} + O(\frac{1}{n^2}),\ \text{as } n\to\infty, \\ b_n &=& \pi(n+1), \end{array} \quad \text{if } c>0;$$

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

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

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

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

PROOF. The proof of this proposition follows the same lines as those of propositions 1 and 2. It can be found in many text books (See e.g. [**1**]). □

The length of the gap between the bands is given by

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

The ratio between the length of the n-th band and the width of the n-th gap tends to infinity as follows

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

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 1. *The spectrum of the operator L with periodic point interactions consists of infinite number of bands Δ_n of the absolutely continuous spectrum separated by 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 $b \neq 0$*

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

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

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

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

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

5. The inverse spectral problem for the periodic operator.

The spectral asymptotics determine the class of equivalent operators uniquely.

THEOREM 2. *The spectral asymptotics for the operator L with periodic point interactions determine uniquely the class of equivalent operators, namely 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 behavior for large values of the energy.

In the 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.

The cases B and C are similar. The Theorem is proven. □

The theorem implies that the spectral asymptotics generally does 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 periodic operator and "weighted" operator

The spectral asymptotics calculated in Section 4 can be compared with the spectral asymptotics for non singular periodic one dimensional operators. The asymptotics in Case C resembles the asymptotics for periodic Schrödinger operator

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

We would like to remind that this operator has absolutely continuous spectrum filling up the bands separated by finite or infinite number of gaps. The ratio between the lengths of the bands and gaps is increasing as $\lambda\to\infty$.

The spectral asymptotics obtained in Case A differs from those for the periodic Schrödinger operator drastically. 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 appears 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 $\rho\in W_2^1$, $\rho>0$. This operator was investigated recently by E.Korotyaev (See [**9, 10**] for references and historical remarks). Consider the following periodic weighted operator

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

where the density function

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

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 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

$$\left\{ \begin{array}{rcl} \Psi(n^+) & = & \Psi(n^-), \\ (1 + h\frac{1}{\epsilon})\Psi'(n^+) & = & \Psi'(0^-), \end{array} \right.$$
$$\left\{ \begin{array}{rcl} \Psi\left((n+\epsilon)^+\right) & = & \Psi\left((n+\epsilon)^-\right), \\ \Psi'\left((n+\epsilon)^+\right) & = & (1 + h\frac{1}{\epsilon})\Psi'\left((n+\epsilon)^-\right). \end{array} \right. \tag{39}$$

These condition guarantee that the functions Ψ and $\rho_\epsilon \Psi'$ 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 $x = \epsilon$

$$\mathbf{M}^\lambda_{\mathbf{W}}(0^-, 1^-) = \mathbf{M}^\lambda_{-\frac{d^2}{dx^2}}(\epsilon^+, 1^-) \begin{pmatrix} 1 & 0 \\ 0 & 1 + \frac{h}{\epsilon} \end{pmatrix} \mathbf{M}^\lambda_{-\frac{d^2}{dx^2}}(0^+, \epsilon^-) \begin{pmatrix} 1 & 0 \\ 0 & 1 - \frac{h}{\epsilon + h} \end{pmatrix}$$

$$= \begin{pmatrix} \cos k - \frac{1}{\epsilon}\sin(1-\epsilon)k \sin \epsilon k & \frac{1}{k}\sin k - \frac{1}{k(\epsilon+h)}\cos(1-\epsilon)k\sin\epsilon k \\ -k\sin k - \frac{k}{\epsilon}\cos(1-\epsilon)k\sin\epsilon k & \cos k + \frac{1}{\epsilon+h}\sin(1-\epsilon)k\sin\epsilon k \end{pmatrix} \tag{40}$$

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

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

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

$$a = 1,\ b = h,\ c = 0,\ d = 1.$$

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. These calculation shows another one time 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 [**12**], where singular interactions for the second derivative operator in $L_2(\mathbf{R})$ were investigated.

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