Explicit Estimates for the Energy Bands and Forbidden Gaps of the One-dimensional Schrodinger Operator and the Kronig-Penney Model

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OUTLINE

The present talk deals with the spectrum of the one-dimensional Schrödinger operator $L(q)$ generated in $L_2(-\infty, \infty)$ by the differential expression

$$l(y) = -y'' + qy, \tag{1}$$

where q is 1-periodic integrable on $[0, 1]$ and a real-valued potential. Without loss of generality, it is assumed that

$$\int_0^1 q(x)dx = 0. \tag{2}$$

It is well known that the spectrum $\sigma(L(q))$ of $L(q)$ is the union of the spectra $\sigma(L_t(q))$ of the operators $L_t(q)$ for $t \in (-\pi, \pi]$ generated in $L_2[0,1]$ by (1) and the boundary conditions

$$y(1) = e^{it} y(0), \qquad y'(1) = e^{it} y'(0). \tag{3}$$

Moreover, $\sigma(L(q))$ consists of the closed intervals (called bands of the spectrum) whose end points are the eigenvalues of $L_t(q)$ for $t = 0, \pi$ (see (3)). Therefore, to study the spectrum of the self adjoint operator $L(q)$ it is enough to investigate the eigenvalues of $L_0(q)$ and $L_\pi(q)$, which are called the periodic and antiperiodic eigenvalues, respectively.

The first periodic eigenvalue is denoted by λ_0. The other eigenvalues of $L_0(q)$ and the eigenvalues of $L_\pi(q)$ are denoted by $\lambda_{n,j}$ and $\mu_{n,j}$, respectively, for $n \in \mathbb{N}$, $j = 1, 2$, where $\mathbb{N}$ is the set of positive integers. Without loss of generality, it is assumed that $\lambda_{n,1} \leq \lambda_{n,2}$ and $\mu_{n,1} \leq \mu_{n,2}$, for $n \in \mathbb{N}$.

It is known that (see [4, Eastham, 1973]), the spectrum of the Schrödinger operator $L(q)$ consists of the real intervals

$$\Gamma_1 := [\lambda_0, \mu_{1,1}], \quad \Gamma_2 := [\mu_{1,2}, \lambda_{1,1}], \quad \Gamma_3 := [\lambda_{1,2}, \mu_{2,1}], \quad \Gamma_4 := [\mu_{2,2}, \lambda_{2,1}],$$

The bands Γ_1, Γ_2, ... of the spectrum $\sigma(L(q))$ of $L(q)$ are separated by the gaps

$$\Delta_1 := (\mu_{1,1}, \mu_{1,2}), \quad \Delta_2 := (\lambda_{1,1}, \lambda_{1,2}), \quad \Delta_3 := (\mu_{2,1}, \mu_{2,2}), \quad \Delta_4 := (\lambda_{2,1}, \lambda$$

In this work, we obtain explicit formulas for the large eigenvalues of $L_0(q)$ and $L_\pi(q)$ and estimate the small eigenvalues of these operators. We also give explicit and sharp estimations for the lengths of the bands and gaps in the spectrum of the operator $L(q)$. Moreover, we take the Kronig-Penney model as an example and illustrate asymptotic formulas and estimations with this example.

In [2, Dernek and Veliev, 2005], the following equalities were established:

$$
\begin{aligned}
&(\lambda_{n,j} - (2\pi n)^2 - A_m(\lambda_{n,j}))(\Psi_{n,j}(x), e^{i2\pi nx}) \\
&\quad - (q_{2n} + B_m(\lambda_{n,j}))(\Psi_{n,j}(x), e^{-i2\pi nx}) = R_m(\lambda_{n,j}),
\end{aligned} \tag{4}
$$

where $\Psi_{n,j}(x)$ is an eigenfunction corresponding to the eigenvalue $\lambda_{n,j}$, $q_k = (q(x), e^{i2\pi kx})$,

$$
A_m(\lambda_{n,j}) = \sum_{k=1}^{m} a_k(\lambda_{n,j}), \quad B_m(\lambda_{n,j}) = \sum_{k=1}^{m} b_k(\lambda_{n,j}),
$$

$$
a_k(\lambda_{n,j}) = \sum_{n_1, n_2, \ldots, n_k} \frac{q_{n_1} q_{n_2} \ldots q_{n_k} q_{-n_1-n_2-\ldots-n_k}}{\prod_{s=1}^{k} (\lambda_{n,j} - (2\pi(n - n_1 - n_2 - \ldots - n_s))^2)},
$$

$$
b_k(\lambda_{n,j}) = \sum_{n_1, n_2, \ldots, n_k} \frac{q_{n_1} q_{n_2} \ldots q_{n_k} q_{2n-n_1-n_2-\ldots-n_k}}{\prod_{s=1}^{k} (\lambda_{n,j} - (2\pi(n - n_1 - n_2 - \ldots - n_s))^2)},
$$

and

$$R_m(\lambda_{n,j}) = \sum_{n_1, n_2, \ldots, n_{m+1}} \frac{q_{n_1} q_{n_2} \ldots q_{n_m} q_{n_{m+1}} (q(x)\Psi_{n,j}(x), e^{i2\pi(n-n_1-\ldots-n_{m+1})x})}{\prod_{s=1}^{m+1} (\lambda_{n,j} - (2\pi(n - n_1 - n_2 - \ldots - n_s))^2)}.$$

The summations in these formulas are taken over the indices satisfying the conditions

$$n_s \neq 0, \quad n_1 + n_2 + \ldots + n_s \neq 0, 2n,$$

for $s = 1, 2, \ldots, m+1$.

In [17, Veliev, 2024], the terms $a_1(\lambda_{n,j})$ and $a_2(\lambda_{n,j})$ were investigated in detail and the following estimations were proved:

$$a_1(\lambda_{n,j}) = a_1((2\pi n)^2) + o(n^{-2}) = o(n^{-1})$$

and

$$a_2(\lambda_{n,j}) = a_2((2\pi n)^2) + o(n^{-3}\ln n),$$

where $a_1((2\pi n)^2)$ and $a_2((2\pi n)^2)$ are obtained from $a_1(\lambda_{n,j})$ and $a_2(\lambda_{n,j})$ by changing $\lambda_{n,j}$ to $(2\pi n)^2$ in the corresponding formulas and $q \in L_1[0,1]$.

Similarly, in [13, Shkalikov and Veliev, 2009], the following relations were obtained:

$$b_1(\lambda_{n,j}) = b_{1,n}((2\pi n)^2) + o\left(n^{-2}\right), \qquad b_2(\lambda_{n,j}) = o\left(n^{-2}\right),$$
$$b_{1,n}((2\pi n)^2) = 2Q_0 Q_{2n} - S_{2n},$$

where $b_1((2\pi n)^2)$ is obtained from $b_1(\lambda_{n,j})$ by changing $\lambda_{n,j}$ to $(2\pi n)^2$, $Q_k = (Q, e^{2\pi ikx})$ and $S_k = (S, e^{2\pi ikx})$ are the Fourier coefficients of the following functions:

$$Q(x) = \int_0^x q(t)\,dt, \qquad S(x) = Q^2(x).$$

To obtain explicit formulas for the large eigenvalues, we use the following lemmas.

Lemma

If $q \in L_1[0,1]$, then the following formula holds:

$$a_1((2\pi n)^2) = \frac{|q_{2n}|^2}{-16\pi^2 n^2} + D(2n),$$

where

$$D(k) =: \frac{i}{2\pi k} \int_0^1 q(x)(Q(x,k) - Q_{k,0}))e^{-i2\pi kx}\,dx,$$

$$Q(x,k) = \int_0^x q(t)e^{i2\pi kt}\,dt - q_{-k}x, \;\; Q_{k,0} = \int_0^1 Q(x,k)dx.$$

Now we consider $a_2((2\pi n)^2)$. We obtain that

$$a_2((2\pi n)^2) = \frac{1}{16\pi^2 n^2}(I_1 + I_2 + I_3 + I_4),$$

where

$$I_1(q) = \sum_{k,l} \frac{q_k q_l q_{-k-l}}{2\pi k(2\pi k + 2\pi l)},$$

$$I_2(n,q) = \sum_{k,l} \frac{q_k q_l q_{-k-l}}{(4\pi n - 2\pi k)(2\pi k + 2\pi l)},$$

$$I_3(n,q) = \sum_{k,l} \frac{q_k q_l q_{-k-l}}{2\pi k(4\pi n - 2\pi k - 2\pi l)},$$

and

$$I_4(n,q) = \sum_{k,l} \frac{q_k q_l q_{-k-l}}{(4\pi n - 2\pi k)(4\pi n - 2\pi k - 2\pi l)}.$$

We estimate $I_1(q)$ and $I_j(n,q)$, for $j = 2, 3, 4$, in the following lemma:

Lemma

$I_1(q) = 0$ and $I_j(n,q) = o(n^2)$, for $j = 2, 3, 4$.

We have the following asymptotic formulas for the periodic eigenvalues:

Theorem

If

$$|q_k - S_k + 2Q_0 Q_k| \geq \varepsilon k^{-2},$$

for $k = 2n$, holds, then the eigenvalues $\lambda_{n,j}$, for $n > N$ and $j = 1, 2$, are simple and satisfy the asymptotic formula

$$\lambda_{n,j} = (2\pi n)^2 + D(2n) + (-1)^j |q_{2n} - S_{2n} + 2Q_0 Q_{2n}| + o(n^{-2})$$

as $n \longrightarrow \infty$, where

$$D(k) = \frac{i}{2\pi k} \int_0^1 q(x)(Q(x,k) - Q_{k,0}) e^{-i2\pi kx}\, dx,$$

$$Q(x,k) = \int_0^x q(t) e^{i2\pi kt}\, dt - q_{-k} x, \;\; Q_{k,0} = \int_0^1 Q(x,k) dx.$$

The corresponding results for the antiperiodic problem can be carried out in a similar way.

Theorem

If

$$|q_k - S_k + 2Q_0Q_k| \geq \varepsilon k^{-2},$$

for $k = 2n-1$, *holds, then the eigenvalues* $\mu_{n,j}$ *of the operator* $L_\pi(q)$, *for* $n > N$ *and* $j = 1, 2$, *are simple and satisfy the asymptotic formula*

$$\mu_{n,j} = (2\pi n - \pi)^2 + D(2n-1) + (-1)^j \left|q_{2n-1} - S_{2n-1} + 2Q_0Q_{2n-1}\right| + o(n^{-$$

as $n \longrightarrow \infty$.

Now, we take the Kronig-Penney model as an example and use this example to illustrate the obtained asymptotic formulas.
The Kronig-Penney model is a simplified model of an electron in a one-dimensional periodic potential and has been studied in many works (see, for example, [1, Kronig and Penney, 1931], [2, Brown, Eastham, and Schmidt, 2013], [3, Titchmarsh, 1958], [4, Veliev, 2024] and references therein).

In this case, the potential $q(x)$ has the form

$$q(x) = \begin{cases} a & \text{if } x \in [0, c] \\ b & \text{if } x \in (c, d], \end{cases}$$

and $q(x + d) = q(x)$, where $c \in (0, d)$. For simplicity of notation and without loss of generality, we assume that $d = 1$, $a < b$ and

$$\int_0^1 q(x)dx = 0.$$

Then, we have

$$q(x) = \begin{cases} a & \text{if } x \in [0, c] \\ b & \text{if } x \in (c, 1], \end{cases} \tag{5}$$

where $a < 0 < b$ and

$$ac + (1 - c)b = 0.$$

The following equalities were obtained in [17, Veliev, 2024]:

$$q_k = \frac{a-b}{2\pi ki}(1 - e^{-2\pi kic}),$$

$$Q_k = \frac{q_k}{2\pi ki} = \frac{a-b}{(2\pi k)^2}(e^{-2\pi kic} - 1), \qquad Q_0 = \frac{1}{2}b(c-1),$$

$$S_k = \frac{a^2}{\pi ki}\left(\frac{e^{-2\pi ikc} - 1}{(2\pi k)^2} - \frac{ce^{-2\pi ikc}}{2\pi ik}\right) + \frac{b^2}{\pi ki}\left(\frac{1 - e^{-2\pi ikc}}{(2\pi k)^2} + \frac{ce^{-2\pi ikc} - 1}{2\pi ik}\right) - \frac{b^2}{\pi ki}\left(\frac{e^{-2\pi ikc} - 1}{2\pi ik}\right),$$

where $Q_k = (Q, e^{2\pi ikx})$ and $S_k = (S, e^{2\pi ikx})$ are the Fourier coefficients of the following functions:

$$Q(x) = \int_0^x q(t)\,dt, \qquad S(x) = Q^2(x).$$

We need to calculate the term $D(2n)$ where

$$D(k) =: \frac{i}{2\pi k} \int_0^1 q(x)(Q(x,k) - Q_{k,0}))e^{-i2\pi kx}\, dx,$$

$$Q(x,k) = \int_0^x q(t)e^{i2\pi kt}\, dt - q_{-k}x, \qquad Q_{k,0} = \int_0^1 Q(x,k)dx.$$

By direct calculations we obtain

$$Q(x,k)=\begin{cases}\dfrac{a}{i2\pi k}(e^{i2\pi kx}-1)-q_{-k}x & \text{if } x\in[0,c]\\ \dfrac{b}{i2\pi k}(e^{i2\pi kx}-1)-q_{-k}x+q_{-k} & \text{if } x\in(c,1].\end{cases}$$

Therefore, we have

$$Q_{k,0}=\int_0^1 Q(x,k)dx=\frac{(b-a)(e^{i2\pi kc}-1)}{4\pi^2k^2}+\frac{(a+b)(e^{i2\pi kc}-1)}{4\pi ki}$$

and

$$\begin{aligned}D(k)&=\frac{i}{2\pi k}\int_0^1 q(x)Q(x,k)e^{-i2\pi kx}\,dx-\frac{iQ_{k,0}}{2\pi k}\int_0^1 q(x)e^{-i2\pi kx}\,dx\\&=\frac{i}{2\pi k}\left(\int_0^c q(x)Q(x,k)e^{-i2\pi kx}\,dx+\int_c^1 q(x)Q(x,k)e^{-i2\pi kx}\,dx\right)\\&-\frac{iQ_{k,0}q_k}{2\pi k}.\end{aligned}$$

Simplifying a bit, we obtain

$$D(k) = \frac{-ab}{4\pi^2 k^2} + O(\frac{1}{k^3}).$$

and

$$\begin{aligned} q_k - S_k + 2Q_0 Q_k &= \frac{a-b}{2\pi ki}(1 - e^{-2\pi kic}) + \frac{ba}{(2\pi k)^2}(e^{-2\pi ikc} + 1) + O(k^{-3}) \\ &= e^{-\pi kic}\left(\frac{a-b}{\pi k}\sin(\pi kc) + \frac{ba}{2(\pi k)^2}\cos(\pi kc)\right) + O(k^{-3}). \end{aligned}$$

In Theorem 2.1.11 of [17, Veliev, 2024], it was proved that if $c \in \mathbb{Q}$, then $|q_k - S_k + 2Q_0Q_k| > c_0 k^{-2}$, for some positive constant c_0, where $\mathbb{Q}$ is the set of rational numbers. Therefore the following theorems follow from Theorem 3 and Theorem 4, respectively.

Theorem

If $c \in \mathbb{Q}$, then the periodic eigenvalues $\lambda_{n,j}$, for $n > N$ and $j = 1, 2$, are simple and satisfy the asymptotic formula

$$\lambda_{n,j} = (2\pi n)^2 + \frac{-ab}{16\pi^2 n^2} + (-1)^j |q_{2n} - S_{2n} + 2Q_0Q_{2n}| + o(n^{-2})$$

as $n \longrightarrow \infty$.

and

Theorem

If $c \in \mathbb{Q}$, then the antiperiodic eigenvalues $\mu_{n,j}$ of the operator $L_\pi(q)$, for $n > N$ and $j = 1, 2$, are simple and satisfy the asymptotic formula

$$\mu_{n,j} = (2\pi n - \pi)^2 + \frac{-ab}{4\pi^2(2n-1)^2} + (-1)^j \left| q_{2n-1} - S_{2n-1} + 2Q_0 Q_{2n-1} \right| + c$$

as $n \to \infty$.

Now, let us consider the general case $c \in \mathbb{R}$. We show that if there exists $\varepsilon > 0$ such that the inequality

$$|\sin(\pi k c + \theta)| > \frac{\varepsilon}{k} \tag{6}$$

is satisfied, then $|q_k - S_k + 2Q_0 Q_k| \geq \varepsilon k^{-2}$ holds. Thus the following theorems follow from Theorem 3 and Theorem 4, respectively.

Theorem

If (6) is satisfied for $k = 2n$, then the periodic eigenvalues $\lambda_{n,j}$, for $n > N$ and $j = 1, 2$, are simple and satisfy asymptotic formula

$$\lambda_{n,j} = (2\pi n)^2 + \frac{-ab}{16\pi^2 n^2} + (-1)^j \left| q_{2n} - S_{2n} + 2Q_0 Q_{2n} \right| + o(n^{-2})$$

as $n \longrightarrow \infty$.

and

Theorem

If (6) is satisfied for $k = 2n - 1$, then the antiperiodic eigenvalues $\mu_{n,j}$ of the operator $L_\pi(q)$, for $n > N$ and $j = 1, 2$, are simple and satisfy asymptotic formula

$$\mu_{n,j} = (2\pi n - \pi)^2 + \frac{-ab}{4\pi^2 (2n-1)^2} + (-1)^j \left| q_{2n-1} - S_{2n-1} + 2Q_0 Q_{2n-1} \right| + o$$

as $n \longrightarrow \infty$.

Now we consider the small periodic and antiperiodic eigenvalues of the Schrödinger operator $L(q)$ with potential (5). We shall focus on the operator $L_0(q)$ with potential (5). The investigation of $L_\pi(q)$ is similar.

Basically, we use the following iteration formula [2, Dernek and Veliev, 2005]:

$$\left(\lambda_{n,j} - (2\pi n)^2 - \sum_{k=1}^{m} a_k(\lambda_{n,j})\right)(\Psi_{n,j}(x), e^{i2\pi nx}) - \left(q_{2n} + \sum_{k=1}^{m} b_k(\lambda_{n,j})\right)(\Psi_{n,j}(x), e^{-i2\pi nx}) = R_m(\lambda_{n,j}), \qquad (7)$$

where

$$a_k(\lambda_{n,j}) = \sum_{n_1,n_2,\ldots,n_k} \frac{q_{n_1}q_{n_2}\ldots q_{n_k}q_{-n_1-n_2-\ldots-n_k}}{\prod_{s=1}^{k}(\lambda_{n,j} - (2\pi(n-n_1-n_2-\ldots-n_s))^2)},$$

$$b_k(\lambda_{n,j}) = \sum_{n_1,n_2,\ldots,n_k} \frac{q_{n_1}q_{n_2}\ldots q_{n_k}q_{2n-n_1-n_2-\ldots-n_k}}{\prod_{s=1}^{k}(\lambda_{n,j} - (2\pi(n-n_1-n_2-\ldots-n_s))^2)},$$

and

$$R_m(\lambda_{n,j}) = \sum_{n_1,n_2,\ldots,n_{m+1}} \frac{q_{n_1} q_{n_2} \ldots q_{n_m} q_{n_{m+1}} (q(x)\Psi_{n,j}(x), e^{i2\pi(n-n_1-\ldots-n_{m+1})x})}{\prod_{s=1}^{m+1} (\lambda_{n,j} - (2\pi(n - n_1 - n_2 - \ldots - n_s))^2)}.$$

The summations in these formulas are taken over the indices satisfying the conditions

$$n_s \neq 0, \quad n_1 + n_2 + \ldots + n_s \neq 0, 2n,$$

for $s = 1, 2, \ldots, m+1$.

Before stating the main results, we write the following relations:

$$a_1((2\pi n)^2) = \frac{-ab}{16\pi^2 n^2} + \frac{(b^2 - a^2)\sin(4\pi nc)}{64\pi^3 n^3} + \frac{3(b-a)^2(\cos(4\pi nc) - 1)}{128\pi^4 n^4}$$

and

$$\begin{aligned} q_{2n} + b_1((2\pi n)^2) &= q_{2n} + 2Q_0 Q_{2n} - S_{2n} \\ &= \frac{(a-b)(1 - e^{-i4\pi nc})}{4\pi n i} + \frac{ab(1 + e^{-i4\pi nc})}{16\pi^2 n^2} + \frac{(a^2 - b^2)(1 - e^{-i4\pi nc})}{32\pi^3 n^3 i}. \end{aligned}$$

Now we state the following interesting remark:

Remark

We have the formulas $q_{-k} = e^{i2\pi kc} q_k$ *and* $q_{-k} = \overline{q_k}$. *These give, respectively,*

$$\arg q_{-k} = \arg q_k + 2\pi kc \text{ and } \arg q_{-k} = -\arg q_k$$

and hence $\arg q_k = -\pi kc$, $q_k = e^{-i\pi kc} |q_k|$, *from which we obtain*

$$q_{2n} = e^{-i2\pi nc} |q_{2n}|$$

and

$$q_{n_1} q_{n_2} \ldots q_{n_k} q_{2n-n_1-n_2-\ldots-n_k} = |q_{n_1} q_{n_2} \ldots q_{n_k} q_{2n-n_1-n_2-\ldots-n_k}| \, e^{-i2\pi nc}.$$

It means that $e^{i2\pi nc} \left(q_{2n} + \sum_{k=1}^{\infty} b_k(\lambda) \right)$ *is a real number.*

Using this remark and letting m tend to infinity in equation (7), we obtain the following main results. First, we consider the case $n \geq 1$:

Theorem

(a) *If* $M \leq \dfrac{4\pi^2(2n-1)}{3}$*, then* $\lambda_{n,j}$ *is an eigenvalue of* $L_0(q)$ *if and only if it is either the root of the equation*

$$\lambda - (2\pi n)^2 - \sum_{k=1}^{\infty} a_k(\lambda) - e^{i2\pi nc}\left(q_{2n} + \sum_{k=1}^{\infty} b_k(\lambda)\right) = 0 \qquad (8)$$

or the root of

$$\lambda - (2\pi n)^2 - \sum_{k=1}^{\infty} a_k(\lambda) + e^{i2\pi nc}\left(q_{2n} + \sum_{k=1}^{\infty} b_k(\lambda)\right) = 0 \qquad (9)$$

in the set $D_n := [(2\pi n)^2 - M, (2\pi n)^2 + M]$*, where* $n = 1, 2, \ldots$*. Moreover, the roots of (8) and (9) in* D_n*, coincide with the* $(2n)$*th and* $(2n+1)$*st periodic eigenvalues* $\lambda_{n,1}$ *and* $\lambda_{n,2}$*.*

Now, we consider the case $n = 0$.

Theorem

If $M \leq 4\pi^2/3$, then the first periodic eigenvalue λ_0 is the root of the equation

$$\lambda - \sum_{k=1}^{\infty} a_k(\lambda) = 0, \tag{10}$$

in the set $D_0 = [-M, M]$. Moreover, (10) has exactly one root (counting multiplicity) in the set D_0 and this root coincides with the first eigenvalue λ_0 of L_0.

Now, we can use numerical methods by taking finite sums instead of the infinite series obtained. In this case, we write

$$\lambda - (2\pi n)^2 - \sum_{k=1}^{r} a_{s,k,n}(\lambda) + (-1)^j e^{i2\pi nc}\left(q_{2n} + \sum_{k=1}^{r} b_{s,k,n}(\lambda)\right) = 0,$$

for $j = 1$ and $j = 2$, and

$$\lambda - \sum_{k=1}^{r} a_{s,k,0}(\lambda) = 0,$$

where

$$a_{s,k,n} = \sum_{n_1,n_2,\ldots,n_k=-s}^{s} \frac{q_{n_1} q_{n_2} \cdots q_{n_k} q_{-n_1-n_2-\cdots-n_k}}{[\lambda - (2\pi(n-n_1))^2] \cdots [\lambda - (2\pi(n-n_1-\cdots-n_k))^2]}$$

$$b_{s,k,n} = \sum_{n_1,n_2,\ldots,n_k=-s}^{s} \frac{q_{n_1} q_{n_2} \cdots q_{n_k} q_{2n-n_1-n_2-\cdots-n_k}}{[\lambda - (2\pi(n-n_1))^2] \cdots [\lambda - (2\pi(n-n_1-\cdots-n_k))^2]}$$

We define the functions

$$K_{n,j}(\lambda) := \lambda - (2\pi n)^2 - g_{n,j}(\lambda)$$

and

$$K_0(\lambda) := \lambda - g_0(\lambda),$$

where

$$g_{n,j}(\lambda) = \sum_{k=1}^{r} a_{s,k,n}(\lambda) - (-1)^j e^{i2\pi nc}\left(q_{2n} + \sum_{k=1}^{r} b_{s,k,n}(\lambda)\right)$$

and

$$g_0(\lambda) = \sum_{k=1}^{r} a_{s,k,0}(\lambda).$$

Then,

$$\lambda = (2\pi n)^2 + g_{n,j}(\lambda), \tag{11}$$

for $j = 1$ and $j = 2$, and $n \geq 1$.
Now we state another main result.

Theorem

If $M \leq \dfrac{4\pi^2(2n-1)}{3}$, *then for all* x *and* y *from the interval* $D_n = [(2\pi n)^2 - M, (2\pi n)^2 + M]$, *the relations*

$$|g_{n,j}(x) - g_{n,j}(y)| \leq C_n |x - y|,$$

$$C_n = \frac{4(b-a)^2}{\pi(4\pi^2(2n-1) - M)[\pi(4\pi^2(2n-1) - M) - (b-a)]} \leq \frac{4}{\pi(\pi - 1)},$$

hold for $j = 1, 2$, *and equation* (11) *has a unique solution* $\rho_{n,j}$ *in* D_n, *for each* j, *where* $n = 1, 2, \ldots$. *Moreover*

$$|\lambda_{n,j} - \rho_{n,j}| < \frac{6(b-a)^2}{\pi^2(s+1)^2[4\pi^2(s+1)|s+1-2n| - M](1 - C_n)} + \frac{3(b-a)^{r+2}}{2\pi^{r+1}(4\pi^2(2n-1) - M)^r[\pi(4\pi^2(2n-1) - M) - (b-a)](1 - C_n)}$$

for $j = 1, 2$.

An analogous theorem can be given for the case $n = 0$.
Now let us approximate $\rho_{n,j}$ by the fixed point iterations:

$$x_{n,i+1} = (2\pi n)^2 + g_{n,1}(x_{n,i}), \tag{12}$$

and

$$y_{n,i+1} = (2\pi n)^2 + g_{n,2}(y_{n,i}), \tag{13}$$

where $g_{n,j}(x) = \sum_{k=1}^{r} a_{s,k,n}(\lambda) - (-1)^j e^{i2\pi nc}\left(q_{2n} + \sum_{k=1}^{r} b_{s,k,n}(\lambda)\right)$
$(j = 1, 2)$.

We state the following result:

Theorem

If $M \leq \dfrac{4\pi^2(2n-1)}{3}$, *then the following estimations hold for the sequences* $\{x_{n,i}\}$ *and* $\{y_{n,i}\}$ *defined by* (12) *and* (13):

$$|x_{n,i} - \rho_{n,1}| < (C_n)^i \left(\frac{(b-a)}{2\pi n(1-C_n)} + \frac{3(b-a)^2}{2\pi[4\pi^3(2n-1)-(b-a)](1-C_n)} \right)$$

$$|y_{n,i} - \rho_{n,2}| < (C_n)^i \left(\frac{(b-a)}{2\pi n(1-C_n)} + \frac{3(b-a)^2}{2\pi[4\pi^3(2n-1)-(b-a)](1-C_n)} \right)$$

for $i = 1, 2, 3, \ldots$, *where* C_n *is defined in Theorem 11 and* $n = 1, 2, \ldots$.

An analogous theorem can be given for the case $n = 0$.

We present a numerical example:

Example

For $a = -\pi^2$, $b = \pi^2$, and $c = 1/2$, we have the following approximations for the first periodic eigenvalues λ_0, $\lambda_{1,1}$, $\lambda_{1,2}$, $\lambda_{2,1}$, $\lambda_{2,2}$ and antiperiodic eigenvalues $\mu_{1,1}$, $\mu_{1,2}$, $\mu_{2,1}$, $\mu_{2,2}$:

$$\begin{aligned}
\lambda_0 &= -0.100720167503\pi^2, & & \\
\lambda_{1,1} &= 3.953707280198\pi^2, & \lambda_{1,2} &= 3.976894161836\pi^2, \\
\lambda_{2,1} &= 15.974913551204\pi^2, & \lambda_{2,2} &= 15.983422370241\pi^2, \\
\mu_{1,1} &= 0.317539742073\pi^2, & \mu_{1,2} &= 1.578063115969\pi^2, \\
\mu_{2,1} &= 8.768711027230\pi^2, & \mu_{2,2} &= 9.180457181326\pi^2.
\end{aligned}$$

In our calculations, we take $r = s = 5$. Usually it takes $8 - 10$ iterations with the tolerance $1e - 18$ by the fixed point iteration method, even if we choose an initial value that is not too close to the exact value, which means that convergence is quite fast.

Example

As noted in the introduction, the above estimates determine the bands and gaps as well as their lengths. For example, we have the following estimations for the first 4 gaps:

$$
\begin{aligned}
|\Delta_1| &:= \mu_{1,2} - \mu_{1,1} = 1.260523373896\pi^2 = 12.440867038680 \\
|\Delta_2| &:= \lambda_{1,2} - \lambda_{1,1} = 0,023186881638\pi^2 = 0.228845349062 \\
|\Delta_3| &:= \mu_{2,2} - \mu_{2,1} = 0.411746154096\pi^2 = 4.063771654597 \\
|\Delta_4| &:= \lambda_{2,2} - \lambda_{2,1} = 0.008508819037\pi^2 = 0.083978677816.
\end{aligned}
$$

B. M. Brown, M. S. P. Eastham, K. M. Schmidt, Periodic Differential Operators, Springer Basel (2013).

N. Dernek, O. A. Veliev, On the Riesz basisness of the root functions of the non-selfadjoint Sturm-Liouville operator. Isr. J. Math. 145, 113–123 (2005).

N. Dunford, J. T. Schwartz, Linear Operators, Part 2. Spectral Theory, Self Adjoint Operators in Hilbert Space. John Wiley & Sons, New York (1988).

M. S. P. Eastham, The Spectral Theory of Periodic Differential Equations. Scotting Academic Press, Edinburgh (1973).

I. M. Gelfand, Expansions in series of eigenfunctions of an equation with periodic coefficients, Sov. Math. Dokl. 73 (1950), 1117–1120.

T. Kato, Perturbation Theory for Linear Operators, Berlin. Springer-Verlag, Germany (1980).

R. de L. Kronig, W. G. Penney, Quantum mechanics in cristal lattices, Proc. Roy. Soc. 130 (1931), 499-513.

- W. Magnus, S. Winkler, Hill's Equation. Interscience Publishers, New York (1966).
- V. A. Marchenko, Sturm-LiouvilleOperators andApplications. BirkhauserVerlag, Basel (1986).
- D. C. McGarvey, Differential operators with periodic coefficients in $L_p(-\infty, \infty)$. Journal of Mathematical Analysis and Applications 11 (1965), 564-596.
- M. A. Naimark, Linear Differential Operators. George G. Harap & Company, London (1967).
- F. S. Rofe-Beketov, The spectrum of non-self-adjoint differential operators with periodic coefficients, Soviet Math. Dokl. 4 (1963), 1563-1566.
- A. A. Shkalikov, O. A. Veliev, On the Riesz basis property of the eigen- and associated functions of periodic and antiperiodic Sturm-Liouville Problems, Mathematical Notes,Vol 85, No. 5, pp.647-660, (2009).

- E. C. Titchmarsh, Eigenfunction Expansion (Part II). Oxford University Press, London (1958).
- O. A. Veliev, Toppamuk Duman, The spectral expansion for the non-self-adjoint Hill operators with a locally integrable potential. Journal of Mathematical Analysis and Applications, 265, no. 1, pp. 76-90 (2002).
- O. A. Veliev, Non-self-adjoint Schrödinger Operator with a Periodic Potential, Springer, Switzerland 2021.
- O. A. Veliev, Multidimensional Periodic Schrödinger Operator. Springer Tracts in Modern Physics, vol 291. Springer, Switzerland 2024.
- O. A. Veliev, On the band functions and Bloch functions, Turkish Journal of Mathematics, (2023) Volume 47, No.1 pp. 248-255.

Thank you...

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