Estimates for Periodic and Antiperiodic Eigenvalues of the Schrödinger operator with the Kronig-Penney Model

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Analytic and Algebraic Methods in Physics XXI
August 27-August 30, 2024, Czech Technical University, Prague

OUTLINE

The present talk deals with the operator $H_t(q)$, for $t = 0, 1$, generated in $L_2[0, \pi]$ by the differential expression

$$-y''(x) + q(x)y(x) \tag{1}$$

and the boundary conditions

$$y(\pi) = e^{i\pi t}y(0), \qquad y'(\pi) = e^{i\pi t}y'(0), \tag{2}$$

where q is a real potential of the form

$$q(x) = \begin{cases} a & \text{if } x \in [0, c], \\ b & \text{if } x \in (c, \pi], \end{cases} \tag{3}$$

$q(x + \pi) = q(x)$, and $c \in (0, \pi)$. Without loss of generality, we assume that $a < b$, and

$$q_0 = \frac{1}{\pi}\int_0^\pi q(x)dx = 0.$$

Therefore, we have

$$ac + b(\pi - c) = 0, \qquad a < 0 < b, \tag{4}$$

and $(b - a)c = b\pi$.

The Kronig-Penney model is a simplified model of the electron in a one-dimensional periodic potential and has been studied in many works (see, for example, [1, Kronig, R.D.L., Penney, W.G.: Quantum mechanics in cristal lattices. Proc. R. Soc. 130, 499–513 (1931)], [2, Chap.3, Brown, B.M., Eastham, M.S.P., Schmidt, K.M.: Periodic differential operators, Operator Theory: Advances and Applications. 230, Birkhuser/Springer: Basel AG, Basel (2013)], [3, Chap.21, E. C. Titchmarsh, Eigenfunction Expansion (Part II). Oxford University Press, London (1958)], [4, Veliev, O. (2024), From One-Dimensional to Multidimensional. In: Multidimensional Periodic Schrödinger Operator. Springer Tracts in Modern Physics, vol 291. Springer, Cham. https://doi.org/10.1007/978-3-031-49035-4_2.], [5, O. A. Veliev, On Exact Estimates of Instability Zones of the Hill's Equation with Locally Integrable Potential, arxiv.org/abs/2311.11568v2, 2023] and references therein).

In the case of the Kronig-Penney model, the potential $q(x)$ has the form

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

and $q(x + d) = q(x)$, where $c \in (0, d)$. In the present work, without loss of generality, we assume that $d = \pi$. Veliev [4, 5, Veliev, O. (2024), From One-Dimensional to Multidimensional. In: Multidimensional Periodic Schrödinger Operator. Springer Tracts in Modern Physics, vol 291. Springer, Cham. https://doi.org/10.1007/978-3-031-49035-4_2; O. A. Veliev, On Exact Estimates of Instability Zones of the Hill's Equation with Locally Integrable Potential, arxiv.org/abs/2311.11568v2, 2023] studied the bands and gaps in the spectrum of the Schrödinger operator, generated in $L_2[0,1]$ by the differential expression (1) with potential (5), for $d = 1$, and obtained asymptotic formulas for the length of the gaps in the spectrum.

The eigenvalues of $H_0(q)$ and $H_1(q)$ are called the periodic and antiperiodic eigenvalues of the Hill operator $H(q)$, generated in $L_2[0, \pi]$ by the differential expression (1) with potential (3), and they are denoted by $\lambda_{n,j}$ and $\mu_{n,j}$, respectively, for $n \in \mathbb{Z}^+$, $j = 1, 2$, where $\mathbb{Z}^+$ is the set of positive integers. The first periodic eigenvalue is denoted by λ_0 and without loss of generality, it is assumed that $\lambda_{n,1} \leq \lambda_{n,2}$ and $\mu_{n,1} \leq \mu_{n,2}$, for $n \in \mathbb{Z}^+$. It is known that (see [6, M. S. P. Eastham, The Spectral Theory of Periodic Differential Equations.Scottish Academic Press, Edinburgh, UK (1973)]),
the spectrum of the Schrödinger operator $H(q)$ consists of the real intervals

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

The bands $\Gamma_1, \Gamma_2, \ldots$ of the spectrum $\sigma(H(q))$ of $H(q)$ are separated by the gaps

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

For this reason, the investigation of the periodic and antiperiodic eigenvalues is of great importance. In [4, 5, Veliev, O. (2024), From One-Dimensional to Multidimensional. In: Multidimensional Periodic Schrödinger Operator. Springer Tracts in Modern Physics, vol 291. Springer, Cham. https://doi.org/10.1007/978-3-031-49035-4_2; O. A. Veliev, On Exact Estimates of Instability Zones of the Hill's Equation with Locally Integrable Potential, arxiv.org/abs/2311.11568v2, 2023], Veliev investigated the asymptotic behavior of large periodic and antiperiodic eigenvalues to obtain asymptotic formulas for the length of the gaps in the spectrum.

In this work, we provide estimates for small periodic and antiperiodic eigenvalues of the Schrödinger operator $H(q)$. We obtain some useful equations for calculating the periodic and antiperiodic eigenvalues using Rouche's theorem. These equations are derived from some iterations formulas by the methods used in [7, 8, 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); Shkalikov, A.A., Veliev, A.A.: On the Riesz basis property of the eigen- and associated functions of periodic and antiperiodic Sturm-Liouville Problems. Math. Notes 85(5), 647–660 (2009)].

It is important to note that in [7, 8, 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); Shkalikov, A.A., Veliev, A.A.: On the Riesz basis property of the eigen- and associated functions of periodic and antiperiodic Sturm-Liouville Problems. Math. Notes 85(5), 647–660 (2009)],
the authors used asymptotic formulas for large eigenvalues, which cannot be used for small eigenvalues. In our work, we consider small eigenvalues by numerical methods. We also note that, it is not easy to find conditions on the potential for which the small eigenvalues satisfy the equations derived from the iterations formulas, the calculations are very long and technical.

We shall focus on the periodic eigenvalues. The investigation of the antiperiodic eigenvalues is similar. To give estimates for small periodic eigenvalues, first, we prove (see Theorem 3) that the periodic eigenvalue $\lambda_{n,j}$ is either the root of the equation

$$\lambda = (2n)^2 + \sum_{k=1}^{\infty} A_{k,n}(\lambda) + e^{i2nc}\left(q_{2n} + \sum_{k=1}^{\infty} B_{k,n}(\lambda)\right), \tag{6}$$

or the root of the equation

$$\lambda = (2n)^2 + \sum_{k=1}^{\infty} A_{k,n}(\lambda) - e^{i2nc}\left(q_{2n} + \sum_{k=1}^{\infty} B_{k,n}(\lambda)\right), \tag{7}$$

in the set $D_n := \left[(2n)^2 - M_n, (2n)^2 + M_n\right]$, if $M_n \leq \dfrac{4(2n-1)}{3}$, for $n = 1, 2, \ldots$, where $M_n = \max\{|a|, b\}$, $q_k = (q, e^{i2kx}) = \dfrac{1}{\pi}\displaystyle\int_0^{\pi} q(x)e^{-i2kx}dx$ and the infinite series $A_{k,n}$ and $B_{k,n}$ are defined in (13).

We also prove (see Theorem 4) that the first periodic eigenvalue λ_0 satisfies the equation

$$\lambda = \sum_{k=1}^{\infty} A_{k,0}(\lambda), \tag{8}$$

if $M_0 = \max\{|a|, b\} \leq 4/3$. Then, to use numerical methods we take finite sums instead of the infinite series in the equations obtained. To approximate the roots of the equations (6), (7), and (8), we use the fixed point iteration. It can also be used the Newton-Raphson method but in this case it is necessary to compute the derivatives of the functions $K_{n,j}(\lambda)$ and $K_0(\lambda)$ defined by (20) and (21). Then, using the Banach fixed point theorem, we prove that each of these equations containing the finite sums has a unique solution in the appropriate set $D_n = [(2n)^2 - M_n, (2n)^2 + M_n]$, (see Theorem 5 and Theorem 6). Moreover, we give error analysis (see Theorem 7 and Theorem 8) and present a numerical example.

Now, we state some preliminary facts. It is well known that the spectra of the operators $H_0(q)$ and $H_1(q)$ are discrete and for large enough n, there are two periodic (if n is even) or antiperiodic (if n is odd) eigenvalues (counting multiplicities) in the neighborhood of n^2. See the basic and detailed classical results in [2, 9, 10, 11, Brown, B.M., Eastham, M.S.P., Schmidt, K.M.: Periodic differential operators, Operator Theory: Advances and Applications. 230, Birkhuser/Springer: Basel AG, Basel (2013); Levy, M., Keller, B.: Instability intervals of Hill's equation. Comm. on Pure and Appl. Math. 16, 469-476 (1963); Magnus, W., Winkler, S.: Hill's Equation. Interscience Publishers, New York (1966); Marchenko, V.: Sturm-Liouville Operators and Applications. Basel, Birkhauser Verlag (1986)] and references therein.
The eigenvalues of the operators $H_0(0)$ and $H_1(0)$ are $(2n)^2$ and $(2n+1)^2$, for $n \in \mathbb{Z}$, respectively and all the eigenvalues of $H_0(0)$ and $H_1(0)$, except 0, are double.

It is also known that [12, J. Pöschel and E. Trubowitz, Inverse Spectral Theory (Academic Press: Boston,Mass, USA, 1987)]

$$|\lambda_{n,j} - (2n)^2| \leq M_n,$$

for $n \geq 1$, where $M_n = \max\{|a|, b\}$. Therefore, we have

$$(2n)^2 - M_n \leq \lambda_{n,j} \leq (2n)^2 + M_n,$$

for $n \geq 1$. Here, we choose the number M_n depending on the index n. Besides,

$$|\lambda_0| \leq M_0,$$

where $M_0 = \max\{|a|, b\}$ and we assume $M_0 \leq 4/3$.

If $k \neq \pm n$, then

$$|\lambda_{n,j} - (2k)^2| \geq |(2n)^2 - (2k)^2| - M_n = 4|n-k||n+k| - M_n \\ \geq 4(2n-1) - M_n, \tag{9}$$

for $n \geq 1$ and under the assumption $M_n \leq \dfrac{4(2n-1)}{3}$. If $n = 1$, we have $|\lambda_{1,j}| \leq 4 + M_1$ and

$$|\lambda_{1,j} - (2k)^2| \geq ||\lambda_{1,j}| - (2k)^2| \geq 16 - |\lambda_{1,j}| \geq 12 - M_1,$$

for $|k| \geq 2$. Besides, if $n \geq 2$, we have $|\lambda_{n,j}| \geq |\lambda_{2,j}| \geq 16 - M_2$ and

$$|\lambda_{n,j} - (2k-1)^2| \geq ||\lambda_{2,j}| - (2k)^2| \geq |\lambda_{2,j}| - 4 \geq 12 - M_2,$$

for $k \neq \pm n$.

The analogous inequalities can be written for the antiperiodic eigenvalues, from the inequalities

$$(2n-1)^2 - m_n \leq \mu_{n,j} \leq (2n-1)^2 + m_n,$$

for $n \geq 2$. If $k \neq \pm n$, then

$$\begin{aligned} |\mu_{n,j} - (2k-1)^2| &\geq |(2n-1)^2 - (2k-1)^2| - m_n \\ &= 4|n-k||n+k-1| - m_n \geq 4(2n-2) - m_n, \end{aligned} \tag{10}$$

for $n \geq 2$, under the assumption $m_n \leq \dfrac{8(n-1)}{3}$. If $n = 1$, we have $|\mu_{1,j}| \leq 1 + m_1$ and

$$|\mu_{1,j} - (2k-1)^2| \geq ||\mu_{1,j}| - (2k-1)^2| \geq 9 - |\mu_{1,j}| \geq 8 - m_1,$$

for $|k| \geq 2$, and we assume $m_1 \leq 8/3$.

To obtain iteration formulas, we use the equations

$$(\lambda_{N,j} - (2n)^2)(\Psi_{N,j}, e^{i2nx}) = (q\Psi_{N,j}, e^{i2nx}), \tag{11}$$

$$(\lambda_{N,j} - (2n)^2)(\Psi_{N,j}, e^{-i2nx}) = (q\Psi_{N,j}, e^{-i2nx}) \tag{12}$$

which are obtained from

$$-\Psi''_{N,j}(x) + q(x)\Psi_{N,j}(x) = \lambda_{N,j}\Psi_{N,j}(x),$$

by multiplying both sides of the equality by e^{i2nx} and e^{-i2nx}, respectively, where $\Psi_{N,j}(x)$ is an eigenfunction corresponding to the eigenvalue $\lambda_{N,j}$.

Iterating equation (11) m times for $N = n$, the way it was done in the paper [7, N. Dernek, O. A. Veliev, On the Riesz basisness of the root functions of the non-selfadjoint Sturm-Liouville operator. Isr. J. Math. (2005)], we obtain

$$\left(\lambda_{n,j} - (2n)^2 - \sum_{k=1}^{m} A_{k,n}(\lambda_{n,j})\right)(\Psi_{n,j}, e^{i2nx}) - \left(q_{2n} + \sum_{k=1}^{m} B_{k,n}(\lambda_{n,j})\right)(\Psi_{n,j}, e^{-i2nx}) = R_{m,n}(\lambda_{n,j}), \tag{13}$$

where

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

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

$$R_{m,n}(\lambda) = \sum_{n_1,n_2,\ldots,n_{m+1}} \frac{q_{n_1} q_{n_2} \cdots q_{n_m} q_{n_{m+1}} (q\Psi_{n,j}, e^{i2(n-n_1-\cdots-n_{m+1})x})}{[\lambda - (2(n-n_1))^2] \cdots [\lambda - (2(n-n_1-\cdots-n_{m+1}))^2]}$$

Here, the sums are taken under the conditions $n_s = \pm 1$, $\sum\limits_{j=1}^{s} n_j \neq 0, 2n$, for $s = 1, 2, ..., m+1$.

Similarly, iterating equation (12) m times, we obtain

$$\left(\lambda_{n,j} - (2n)^2 - \sum_{k=1}^{m} A_{k,n}^{*}(\lambda_{n,j})\right)(\Psi_{n,j}, e^{-i2nx}) - \left(q_{-2n} + \sum_{k=1}^{m} B_{k,n}^{*}(\lambda_{n,j})\right)(\Psi_{n,j}, e^{i2nx}) = R_{m,n}^{*}(\lambda_{n,j}), \tag{14}$$

where

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

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

$$R_{m,n}^{*}(\lambda) = \sum_{n_1,n_2,\ldots,n_{m+1}} \frac{q_{n_1} q_{n_2} \cdots q_{n_m} q_{n_{m+1}} (q\Psi_{n,j}, e^{-i2(n+n_1+\cdots+n_{m+1})x})}{[\lambda - (2(n+n_1))^2] \cdots [\lambda - (2(n+n_1+\cdots+n_{m+1}))^2}$$

Here, the sums are taken under the conditions $n_s = \pm 1$, $\sum_{j=1}^{s} n_j \neq 0, -2n$, for $s = 1, 2, \ldots, m+1$.

We note that, the iteration formulas (13) and (14) were used in [7, 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)]
for large eigenvalues to obtain asymptotic formulas. In this work, we find conditions on potential (3) for which the iteration formulas (13) and (14) are also valid for the small eigenvalues, as m tends to infinity. We also note that, it is not easy to give such conditions, there are many technical calculations. Since the potential q is of the form (3), we have the followings, after some calculations:

$$q_k = \frac{a-b}{i2\pi k}(1-e^{-i2kc}), \qquad q_{-k} = e^{i2kc}q_k, \qquad |q_{-k}| = |q_k|,$$
$$A^*_{k,n}(\lambda) = A_{k,n}(\lambda), \qquad B^*_{k,n}(\lambda) = e^{i4nc}B_{k,n}(\lambda),$$

for $k = 1, 2, \ldots$.

In order to give the main results, we state the following lemmas. Without loss of generality, we assume that $\Psi_{n,j}(x)$ is a normalized eigenfunction corresponding to the eigenvalue $\lambda_{n,j}$. First, we consider the case $n \geq 1$.

Lemma

If $M_n \leq \dfrac{4(2n-1)}{3}$, *for* $n = 1, 2, \ldots$, *where* $M_n = \max\{|a|, b\}$, *then the statements*

(a) $\lim_{m\to\infty} R_{m,n}(\lambda) = 0, \qquad \lim_{m\to\infty} R^*_{m,n}(\lambda) = 0,$

(b) $|u_{n,j}|^2 + |v_{n,j}|^2 > 0$, *where* $u_{n,j} = (\Psi_{n,j}, e^{i2nx})$ *and* $v_{n,j} = (\Psi_{n,j}, e^{-i2nx})$

are valid.

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

Lemma

If $M_0 = \max\{|a|, b\} \leq 4/3$, *then the statements*

(a) $\lim_{m\to\infty} R_{m,0}(\lambda) = 0, \qquad$ **(b)** $|(\Psi_0, 1)| > 0$

are valid.

Before stating the main results, we introduce the following notations and relations which were used in the works [4, 5, 8, Veliev, O. (2024), From One-Dimensional to Multidimensional. In: Multidimensional Periodic Schrödinger Operator. Springer Tracts in Modern Physics, vol 291. Springer, Cham. https://doi.org/10.1007/978-3-031-49035-4_2; O. A. Veliev, On Exact Estimates of Instability Zones of the Hill's Equation with Locally Integrable Potential, arxiv.org/abs/2311.11568v2, 2023; Shkalikov, A.A., Veliev, A.A.: On the Riesz basis property of the eigen- and associated functions of periodic and antiperiodic Sturm-Liouville Problems. Math. Notes 85(5), 647–660 (2009)]
to obtain subtle asymptotic formulas for large eigenvalues and the length of the gaps in the spectrum:

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

Obviously,

$$Q'(x) = q(x), \qquad S'(x) = 2Q(x)q(x),$$

and

$$Q(0) = Q(\pi) = 0, \qquad S(0) = S(\pi) = 0.$$

By (3), we have

$$Q(x) = \begin{cases} ax & \text{if } x \in [0, c], \\ bx - b\pi & \text{if } x \in (c, \pi] \end{cases}$$

and

$$S(x) = \begin{cases} a^2x^2 & \text{if } x \in [0, c], \\ (bx - b\pi)^2 & \text{if } x \in (c, \pi]. \end{cases}$$

The Fourier coefficients of $Q(x)$ and $S(x)$ are

$$Q_k = (Q, e^{i2kx}) = \frac{1}{\pi}\int_0^{\pi} Q(x)e^{-i2kx}dx = \frac{q_k}{i2k} = \frac{b-a}{4\pi k^2}(1-e^{-i2kc})$$

and

$$\begin{aligned} S_k &= (S, e^{i2kx}) = \frac{1}{\pi}\int_0^{\pi} S(x)e^{-i2kx}dx \\ &= \frac{1}{\pi}\int_0^{c} a^2x^2e^{-i2kx}dx + \frac{1}{\pi}\int_c^{\pi}(bx-b\pi)^2e^{-i2kx}dx \\ &= \frac{(a^2-b^2)(e^{-i2kc}-1)}{i4\pi k^3} + \frac{(a^2-b^2)ce^{-i2kc}}{2\pi k^2} + \frac{b^2e^{-i2kc}}{2k^2}. \end{aligned}$$

In particular,

$$Q_0 = \frac{1}{\pi}\int_0^{\pi} Q(x)dx = \frac{b}{2}(c-\pi) = \frac{ac}{2}, \qquad Q_{2n} = \frac{(b-a)(1-e^{-i4nc})}{16\pi n^2}$$

and

$$S_{2n} = \frac{(a^2-b^2)(e^{-i4nc}-1)}{i32\pi n^3} + \frac{(a^2-b^2)ce^{-i4nc}}{8\pi n^2} + \frac{b^2 e^{-i4nc}}{8n^2}.$$

Using the Fourier decomposition $Q(x) = \sum_{k=-\infty}^{\infty} Q_k e^{i2kx}$ of $Q(x)$ and the integration by parts, we obtain

$$B_{1,n}((2n)^2) = \sum_{\substack{k=-\infty \\ k\neq 0,2n}}^{\infty} \frac{q_k q_{2n-k}}{(2n)^2 - (2(n-k))^2} = \frac{1}{4} \sum_{\substack{k=-\infty \\ k\neq 0,2n}}^{\infty} \frac{q_k q_{2n-k}}{k(2n-k)}$$

$$= -\sum_{\substack{k=-\infty \\ k\neq 0,2n}}^{\infty} Q_k Q_{2n-k} = 2Q_0 Q_{2n} - \frac{1}{\pi} \int_0^{\pi} \left(\sum_{k=-\infty}^{\infty} Q_k e^{i2kx} \right)^2 e^{-i4nx} dx$$

$$= 2Q_0 Q_{2n} - \frac{1}{\pi} \int_0^{\pi} Q^2(x) e^{-i4nx} dx = 2Q_0 Q_{2n} - S_{2n}.$$

Now we introduce the integral (see [4, 5, 8, Veliev, O. (2024), From One-Dimensional to Multidimensional. In: Multidimensional Periodic Schrödinger Operator. Springer Tracts in Modern Physics, vol 291. Springer, Cham. https://doi.org/10.1007/978-3-031-49035-4_2; O. A. Veliev, On Exact Estimates of Instability Zones of the Hill's Equation with Locally Integrable Potential, arxiv.org/abs/2311.11568v2, 2023; Shkalikov, A.A., Veliev, A.A.: On the Riesz basis property of the eigen- and associated functions of periodic and antiperiodic Sturm-Liouville Problems. Math. Notes 85(5), 647–660 (2009)])

$$I = \int_0^{\pi} (P(x,n) - P_0(n))^2 e^{-i8nx} dx,$$

where

$$P(x,n) = \int_0^x q(t) e^{i4nt} dt - q_{-2n} x.$$

It is obvious that

$$P(0,n) = P(\pi,n) = 0, \qquad P'(x,n) = q(x)e^{i4nx} - q_{-2n},$$

and

$$P(x,n) = \begin{cases} \dfrac{a}{i4n}(e^{i4nx} - 1) - q_{-2n}x & \text{if } x \in [0,c], \\ \dfrac{b}{i4n}(e^{i4nx} - 1) - q_{-2n}x - q_{-2n}\pi & \text{if } x \in (c,\pi]. \end{cases}$$

The Fourier coefficients of $P(x,n)$ are

$$P_k(n) = \frac{1}{\pi}\int_0^{\pi} P(x,n)e^{-i2kx}dx, \qquad P_0(n) = \frac{1}{\pi}\int_0^{\pi} P(x,n)dx.$$

The integration by parts gives

$$P_{2n+k}(n) = (P(x,n), e^{i2(2n+k)x}) = \frac{q_k}{i2(2n+k)}$$

for the Fourier coefficients $P_{2n+k}(n)$ of $P(x,n)$, for $2n+k \neq 0$. Using the Fourier decomposition

$$P(x,n) - P_0(n) = \sum_{\substack{k=-\infty \\ k\neq 0,-2n}}^{\infty} \frac{q_k e^{i2(2n+k)x}}{i2(2n+k)}$$

of $P(x,n) - P_0(n)$ in the integral I, we obtain

$$A_{1,n}((2n)^2) = \sum_{\substack{k=-\infty \\ k\neq 0,2n}}^{\infty} \frac{|q_k|^2}{(2n)^2 - (2(n-k))^2}$$

$$= \sum_{\substack{k=1 \\ k\neq 2n}}^{\infty} \left(\frac{|q_k|^2}{(2n)^2 - (2(n-k))^2} + \frac{|q_{-k}|^2}{(2n)^2 - (2(n+k))^2} \right)$$

$$= \frac{1}{2} \sum_{\substack{k=1 \\ k\neq 2n}}^{\infty} \frac{|q_k|^2}{(2n-k)(2n+k)} = -\frac{1}{\pi} I.$$

$P_0(n)$ can be calculated as

$$P_0(n) = \frac{1}{\pi} \int_0^{\pi} P(x,n)dx = \frac{(b-a)(e^{i4nc}-1)}{16\pi n^2} + q_{-2n}(\frac{\pi}{2} - c)$$

$$= \frac{(b-a)(e^{i4nc}-1)}{16\pi n^2} + \frac{a(e^{i4nc}-1)}{i4n}$$

Now, the integration by parts in the integral I, gives

$$I = \frac{1}{i4n} \int_0^{\pi} (P(x,n) - P_0(n))(q(x)e^{i4nx} - q_{-2n})e^{-i8nx} dx$$
$$= \frac{1}{i4n} I_1 - \frac{q_{-2n}}{i4n} I_2 - \frac{\pi q_{2n} P_0(n)}{i4n},$$

where

$$I_1 = \int_0^{\pi} P(x,n) q(x) e^{-i4nx} dx, \qquad I_2 = \int_0^{\pi} P(x,n) e^{-i8nx} dx.$$

By direct calculations, we obtain

$$I_1 = \int_0^{\pi} P(x,n)q(x)e^{-i4nx}dx = \frac{(b-a)(a+b+q_{-2n})(e^{-i4nc}-1)}{16n^2} - \frac{ab\pi}{i4n},$$
$$I_2 = \int_0^{\pi} P(x,n)e^{-i8nx}dx = \frac{(b-a)(1-e^{-i4nc})}{32n^2},$$

and

$$I = \frac{ab\pi}{16n^2} + \frac{(a^2-b^2)\sin(4nc)}{64n^3} + \frac{(b-a)^2(1-\cos(4nc))}{64n^4} + \frac{(b-a)^2(1-\cos(4nc))}{2^8\pi n^4}.$$

Therefore, we have

$$-A_{1,n}((2n)^2) = \frac{1}{\pi} I = \frac{ab}{16n^2} + \frac{(a^2-b^2)\sin(4nc)}{64\pi n^3} + \frac{(b-a)^2(1-\cos(4nc))}{64\pi n^4} + \frac{(b-a)^2(1-\cos(4nc))}{2^8\pi^2 n^4}, \tag{15}$$

and

$$e^{i2nc}\left(q_{2n} + B_{1,n}((2n)^2)\right) = e^{i2nc}\left(q_{2n} + 2Q_0 Q_{2n} - S_{2n}\right) = \frac{(a-b)\sin(2nc)}{2\pi n} + \frac{ab\cos(2nc)}{8n^2} + \frac{(a^2-b^2)\sin(2nc)}{16\pi n^3}. \tag{16}$$

Letting m tend to infinity in the equations (13) and (14), we obtain the following main results. First, we consider the case $n \geq 1$:

Theorem

(a) *If* $M_n \leq \frac{4(2n-1)}{3}$, *for* $n = 1, 2, \ldots$, *where* $M_n = \max\{|a|, b\}$, *then* $\lambda_{n,j}$ *is an eigenvalue of* $H_0(q)$ *if and only if it is either the root of the equation*

$$\lambda - (2n)^2 - \sum_{k=1}^{\infty} A_{k,n}(\lambda) - e^{i2nc}\left(q_{2n} + \sum_{k=1}^{\infty} B_{k,n}(\lambda)\right) = 0 \qquad (17)$$

or the root of

$$\lambda - (2n)^2 - \sum_{k=1}^{\infty} A_{k,n}(\lambda) + e^{i2nc}\left(q_{2n} + \sum_{k=1}^{\infty} B_{k,n}(\lambda)\right) = 0 \qquad (18)$$

in the set $D_n := [(2n)^2 - M_n, (2n)^2 + M_n]$. *Moreover, the roots of* (17) *and* (18) *in* D_n, *coincide with the* $(2n)$*th and* $(2n+1)$*st periodic eigenvalues* $\lambda_{n,1}$ *and* $\lambda_{n,2}$ *of* H_0.

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

Theorem

If $M_0 = \max\{|a|, b\} \leq 4/3$, then the first periodic eigenvalue λ_0 is the root of the equation

$$\lambda - \sum_{k=1}^{\infty} A_{k,0}(\lambda) = 0, \tag{19}$$

in the set $D_0 = [-M_0, M_0]$. Moreover, (19) *has exactly one root (counting multiplicity) in the set D_0 and this root coincides with the first eigenvalue λ_0 of H_0.*

We can use numerical methods by taking finite sums instead of the infinite series in (17), (18) and (19), and obtain

$$\lambda-(2n)^2-\sum_{k=1}^{r}A_{s,k,n}(\lambda)+(-1)^j e^{i2nc}\left(q_{2n}+\sum_{k=1}^{r}B_{s,k,n}(\lambda)\right)=0,$$

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

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

respectively, where

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

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

Define the functions

$$K_{n,j}(\lambda) := \lambda - (2n)^2 - g_{n,j}(\lambda) \tag{20}$$

and

$$K_0(\lambda) := \lambda - g_0(\lambda), \tag{21}$$

where

$$g_{n,j}(\lambda) = \sum_{k=1}^{r} A_{s,k,n}(\lambda) - (-1)^j e^{i2nc}\left(q_{2n} + \sum_{k=1}^{r} B_{s,k,n}(\lambda)\right) \tag{22}$$

and

$$g_0(\lambda) = \sum_{k=1}^{r} A_{s,k,0}(\lambda). \tag{23}$$

Then,

$$\lambda = (2n)^2 + g_{n,j}(\lambda), \tag{24}$$

for $j = 1$ and $j = 2$, and $n \geq 1$.

Now we state another main result.

Theorem

Suppose that $M_n \leq \dfrac{4(2n-1)}{3}$, *for* $n = 1, 2, \ldots$, *where* $M_n = \max\{|a|, b\}$. *Then for all* x *and* y *from the interval* $D_n = [(2n)^2 - M_n, (2n)^2 + M_n]$, *the relations*

$$|g_{n,j}(x) - g_{n,j}(y)| \leq C_n |x - y|, \tag{25}$$

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

hold for $j = 1, 2$, *and equation* (24) *has a unique solution* $\rho_{n,j}$ *in* D_n, *for each* j. *Moreover*

$$|\lambda_{n,j} - \rho_{n,j}| < \frac{6(b-a)^2}{\pi^2(s+1)^2[4(s+1)|s+1-2n| - M_n](1 - C_n)} + \frac{3(b-a)^{r+2}}{2\pi^{r+1}(4(2n-1) - M_n)^r[\pi(4(2n-1) - M_n) - (b-a)](1 - C_n)}, \tag{26}$$

for $j = 1, 2$

We give an analogous theorem to Theorem 5 for the case $n = 0$.

Theorem

Suppose that $M_0 \leq 4/3$, *where* $M_0 = \max\{|a|, b\}$. *Then for all* x *and* y *from the interval* $D_0 = [-M_0, M_0]$ *the relations*

$$|g_0(x) - g_0(y)| \leq C_0|x - y|,$$
$$C_0 = \frac{3(b-a)^2}{4\pi(2-M_0)[\pi(4-M_0)-(b-a)]} \leq \frac{3}{\pi(\pi-1)} < 1,$$

hold and the equation

$$\lambda = g_0(\lambda)$$

has a unique solution ρ_0 *in* D_0, *for each* j, *where* $g_0(\lambda) = \sum\limits_{k=1}^{r} A_{s,k,0}(\lambda)$.

Moreover

$$|\lambda_0 - \rho_0| < \frac{3(b-a)^2}{\pi^2(s+1)^2[4(s+1)^2 - M_0](1-C_0)} + \frac{9(b-a)^{r+2}}{16\pi^{r+1}(4-M_0)^{r-1}(2-M_0)[\pi(4-M_0)-(b-a)](1-C_0)}. \tag{27}$$

Let us approximate $\rho_{n,j}$ by the fixed point iterations:

$$x_{n,i+1} = (2n)^2 + g_{n,1}(x_{n,i}), \tag{28}$$

and

$$y_{n,i+1} = (2n)^2 + g_{n,2}(y_{n,i}), \tag{29}$$

where

$$g_{n,j}(\lambda) = \sum_{k=1}^{r} A_{s,k,n}(\lambda) - (-1)^j e^{i2nc}\left(q_{2n} + \sum_{k=1}^{r} B_{s,k,n}(\lambda)\right)$$

for $j = 1, 2$.

Now we state the following result.

Theorem

If $M_n \leq \dfrac{4(2n-1)}{3}$, *for* $n = 1, 2, \ldots$, *where* $M_n = \max\{|a|, b\}$, *then the following estimations hold for the sequences* $\{x_{n,i}\}$ *and* $\{y_{n,i}\}$ *defined by* (28) *and* (29)*:*

$$|x_{n,i} - \rho_{n,1}| < (C_n)^i \left(\frac{(b-a)}{2\pi n(1-C_n)} + \frac{3(b-a)^2}{2\pi[4\pi(2n-1)-(b-a)](1-C_n)} \right), \tag{30}$$

$$|y_{n,i} - \rho_{n,2}| < (C_n)^i \left(\frac{(b-a)}{2\pi n(1-C_n)} + \frac{3(b-a)^2}{2\pi[4\pi(2n-1)-(b-a)](1-C_n)} \right), \tag{31}$$

for $i = 1, 2, 3, \ldots$, *where*

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

An analogous theorem to Theorem 7 can be stated for the case $n = 0$.

Theorem

If $M_0 \leq 4/3$, where $M_0 = \max\{|a|, b\}$, then the following estimation holds for the sequence $\{x_{0,i}\}$ defined by $x_{0,i} = g_0(x_{0,i})$, where $g_0(\lambda) = \sum_{k=1}^{r} A_{s,k,0}(\lambda)$:

$$|x_{0,i} - \rho_0| \leq (C_0)^i \frac{b-a}{2\pi[2\pi - (b-a)](1 - C_0)}, \tag{32}$$

where

$$C_0 = \frac{3(b-a)^2}{4\pi(2 - M_0)[\pi(4 - M_0) - (b-a)]} \leq \frac{3}{\pi(\pi - 1)} < 1$$

is defined in Theorem 6.

Thus by (26), (27), (30)-(32), we have the approximations $x_{0,i}$, $x_{n,i}$, and $y_{n,i}$ for λ_0, $\lambda_{n,1}$, and $\lambda_{n,2}$, respectively, with the errors

$$
\begin{aligned}
|\lambda_0 - x_{0,i}| < &\frac{3(b-a)^2}{\pi^2(s+1)^2[4(s+1)^2 - M_0](1-C_0)} \\
&+ \frac{9(b-a)^{r+2}}{16\pi^{r+1}(4-M_0)^{r-1}(2-M_0)[\pi(4-M_0)-(b-a)](1-C_0)} \\
&+ (C_0)^i \frac{b-a}{2\pi[2\pi-(b-a)](1-C_0)},
\end{aligned}
$$

$$
\begin{aligned}
|\lambda_{n,1} - x_{n,i}| < &\frac{6(b-a)^2}{\pi^2(s+1)^2[4(s+1)|s+1-2n| - M_n](1-C_n)} \\
&+ \frac{3(b-a)^{r+2}}{2\pi^{r+1}(4(2n-1)-M_n)^r[\pi(4(2n-1)-M_n)-(b-a)](1-C_n)} \\
&+ (C_n)^i \left(\frac{(b-a)}{2\pi n(1-C_n)} + \frac{3(b-a)^2}{2\pi[4\pi(2n-1)-(b-a)](1-C_n)} \right),
\end{aligned}
$$

and

$$|\lambda_{n,2} - y_{n,i}| < \frac{6(b-a)^2}{\pi^2(s+1)^2[4(s+1)|s+1-2n| - M_n](1-C_n)}$$
$$+ \frac{3(b-a)^{r+2}}{2\pi^{r+1}(4(2n-1)-M_n)^r[\pi(4(2n-1)-M_n)-(b-a)](1-C_n)}$$
$$+ (C_n)^i\left(\frac{(b-a)}{2\pi n(1-C_n)} + \frac{3(b-a)^2}{2\pi[4\pi(2n-1)-(b-a)](1-C_n)}\right),$$

By these error formulas it is clear that the error gets smaller as r and s grow.

Now, we present a numerical example. From the numerical results, we conclude that, we can impose the conditions $M_0 < 2$ and $M_n < 2(2n-1)$, for $n = 1, 2, \ldots$, where $M_n = \max\{|a|, b\}$, for the periodic eigenvalues, instead of the conditions $M_0 \leq \frac{4}{3}$ and $M_n \leq \frac{4(2n-1)}{3}$, for $n = 1, 2, \ldots$, for some specific values of $c \in (0, \pi)$. Similarly, we can impose the conditions $m_1 < 4$ and $m_n < 4(n-1)$, for $n = 2, 3, \ldots$, where $m_n = \max\{|a|, b\}$, for the antiperiodic eigenvalues, instead of the conditions $m_1 \leq \frac{8}{3}$ and $m_n \leq \frac{8(n-1)}{3}$, for $n = 2, 3, \ldots$, for some specific values of $c \in (0, \pi)$.

Example

For $a = -1$, $b = 1$, and $c = \pi/2$, we have the following approximations for the first periodic eigenvalues λ_0, $\lambda_{1,1}$, $\lambda_{1,2}$ and antiperiodic eigenvalues $\mu_{1,1}$, $\mu_{1,2}$. In our calculations, we take $r = s = 5$.

$$\begin{aligned}
\lambda_0 &= -0.100720167503 \\
\lambda_{1,1} &= 3.953707280198 \\
\lambda_{1,2} &= 3.976894161836 \\
\mu_{1,1} &= 0.317539742073 \\
\mu_{1,2} &= 1.578063115969.
\end{aligned}$$

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.

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Thank you...

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