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REGULARIZED TRACE OF THE STURM-LIOUVILLE OPERATOR WITH IRREGULAR BOUNDARY CONDITIONS

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Abstract. We consider the spectral problem for the Sturm-Liouville equation with a complex-valued potential $q(x)$ and with irregular boundary conditions on the interval $(0, \pi)$. We establish a formula for the first regularized trace of the this operator.

1. Introduction and main result

This paper deals with the eigenvalue problem for the Sturm-Liouville equation

$$u'' - q(x)u + \lambda u = 0 \tag{1.1}$$

on the interval $(0, \pi)$ with the boundary conditions

$$u'(0) + (-1)^{\theta} u'(\pi) + bu(\pi) = 0, \quad u(0) + (-1)^{\theta+1} u(\pi) = 0, \tag{1.2}$$

where b is a complex number, $b \neq 0$, $\theta = 0, 1$. The goal of this article is to calculate the first-order regularized trace for (1.1)-(1.2).

The theory of regularized traces of ordinary differential operators has a long history. First, the trace formulas for the Sturm-Liouville operator with the Dirichlet boundary conditions and sufficiently smooth potential $q(x)$ were established in [1, 2]. Afterwards these investigations were continued in many directions, for instance, the trace formulas for the Sturm-Liouville operator with periodic or antiperiodic boundary conditions were obtained in [3, 11], and for regular but not strongly regular ones [9] similar formulas were found in [7]. A method for calculating trace formulas for general problems involving ordinary differential equations on a finite interval was proposed in [5]. The bibliography on the subject is very extensive and we refer to the list of the works in [4, 10].

The trace formulas can be used for approximate calculation of the first eigenvalues of an operator [10], and in order to establish necessary and sufficient conditions for a set of complex numbers to be the spectrum of an operator [11].

We will prove the following statement.

Theorem 1.1. *Let $q(x)$ be an arbitrary complex-valued function in $W_1^1(0, \pi)$ and denote by λ_n $(n = 1, 2, \dots)$ the eigenvalues of* (1.1)-(1.2). *Then we have the trace*

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formula

$$\sum_{n=1}^{\infty}\Big\{\lambda_n - n^2 - \langle q\rangle - \frac{(-1)^\theta(q(\pi)-q(0)-\int_0^\pi q'(t)\cos(2nt)dt)}{\pi b}\Big\}
- \frac{\langle q\rangle}{2} + \frac{(q(\pi)-q(0))^2}{2b^2} + \frac{q(\pi)+q(0)}{4} = 0, \tag{1.3}$$

where $\langle q\rangle = \pi^{-1}\int_0^\pi q(t)dt$.

This article is organized as follows. Section 2 is devoted to the analysis of the characteristic determinant. In section 3, we obtain a formula of the regularized trace in explicit form.

2. Analysis of the characteristic determinant

Denote by $c(x,\mu), s(x,\mu)$ $(\mu^2=\lambda)$ the fundamental system of solutions to (1.1) with the initial conditions $c(0,\mu)=s'(0,\mu)=1$, $c'(0,\mu)=s(0,\mu)=0$. Simple calculations show that the characteristic equation of (1.1)-(1.2) can be reduced to the form $\Delta(\mu)=0$, where

$$\Delta(\mu) = c(\pi,\mu) - s'(\pi,\mu) - (-1)^\theta b s(\pi,\mu). \tag{2.1}$$

Denote by $\varphi(x,\mu), \psi(x,\mu)$ the system of solutions to (1.1) with the initial conditions $\varphi(0,\mu)=\psi(0,\mu)=1$, $\varphi'_x(0,\mu)=i\mu$, $\psi'_x(0,\mu)=-i\mu$. It is readily seen that

$$\begin{gathered}\varphi(x,\mu)=\psi(x,-\mu), \quad c(x,\mu)=(\varphi(x,\mu)+\psi(x,\mu))/2,\\ s(x,\mu)=(\varphi(x,\mu)-\psi(x,\mu))/(2i\mu),\\ s'(x,\mu)=(\varphi'(x,\mu)-\psi'(x,\mu))/(2i\mu).\end{gathered} \tag{2.2}$$

For convenience, we introduce $I(x)=\int_0^x q(t)dt$. Asymptotic formulas for the functions $\varphi(x,\mu)$ and $\varphi'(x,\mu)$ were established in [7]:

$$\begin{aligned}\varphi(x,\mu) &= e^{i\mu x}[1+\frac{1}{2i\mu}I(x)-\frac{1}{8\mu^2}I^2(x)]\\ &\quad - \frac{e^{-i\mu x}}{2i\mu}\int_0^x e^{2i\mu t}q(t)dt + A(x,\mu) + R_1(x,\mu),\end{aligned} \tag{2.3}$$

and

$$\begin{aligned}\varphi'_x(x,\mu) &= i\mu e^{i\mu x}[1+\frac{1}{2i\mu}I(x)-(8\mu^2)^{-1}I^2(x)]\\ &\quad + \frac{e^{-i\mu x}}{2}\int_0^x e^{2i\mu t}q(t)dt + B(x,\mu) + R_3(x,\mu) + R_4(x,\mu) + R_5(x,\mu),\end{aligned} \tag{2.4}$$

where

$$\begin{aligned}A(x,\mu) &= (4\mu^2)^{-1}(e^{-i\mu x}\int_0^x e^{2i\mu t}q(t)dt\int_0^t q(s)ds\\ &\quad + e^{i\mu x}\int_0^x e^{-2i\mu t}q(t)dt\int_0^t e^{2i\mu s}q(s)ds - e^{-i\mu x}\int_0^x q(t)dt\int_0^t e^{2i\mu s}q(s)ds),\end{aligned}$$

$$
\begin{aligned}
R_1(x,\mu) &= -(4\mu^3)^{-1}\int_0^x (e^{i\mu(x-t)} - e^{-i\mu(x-t)})q(t)dt \\
&\quad\times \int_0^t (e^{i\mu(t-s)} - e^{-i\mu(t-s)})q(s)ds \int_0^s \sin\mu(s-y)q(y)\varphi(y,\mu)dy,
\end{aligned} \tag{2.5}
$$

$$
\begin{aligned}
B(x,\mu) &= -(4i\mu)^{-1}[e^{i\mu x}\int_0^x e^{-2i\mu t}q(t)dt\int_0^t e^{2i\mu s}q(s)ds \\
&\quad - e^{-i\mu x}\int_0^x e^{2i\mu t}q(t)dt\int_0^t q(s)ds + e^{-i\mu x}\int_0^x q(t)dt\int_0^t e^{2i\mu s}q(s)ds],
\end{aligned}
$$

$$
R_2(x,\mu) = -\frac{1}{16\mu^2}e^{i\mu x}\int_0^x (1+e^{2i\mu(t-x)})q(t)I^2(t)dt, \tag{2.6}
$$

$$
R_3(x,\mu) = \frac{1}{2}\int_0^x (e^{i\mu(x-t)} + e^{-i\mu(x-t)})q(t)R_2(t,\mu)dt, \tag{2.7}
$$

$$
R_4(x,\mu) = \frac{1}{2}\int_0^x (e^{i\mu(x-t)} + e^{-i\mu(x-t)})q(t)A(t,\mu)dt. \tag{2.8}
$$

We need more precise asymptotic formulas for the functions $\varphi(x,\mu)$ and $\varphi'(x,\mu)$. Substituting known the expression [8] for the function $\varphi(y,\mu) = e^{i\mu y}+O(1/\mu)e^{|Im\mu|y}$ into (2.5), we obtain

$$
\begin{aligned}
R_1(x,\mu) &= -(8i\mu^3)^{-1}\int_0^x (e^{i\mu(x-t)} - e^{-i\mu(x-t)})q(t)dt \\
&\quad\times \int_0^t (e^{i\mu(t-s)} - e^{-i\mu(t-s)})q(s)ds \int_0^s (e^{i\mu(s-y)} - e^{-i\mu(s-y)})q(y) \\
&\quad\times [e^{i\mu y} + O(1/\mu)e^{|Im\mu|y}]dy \\
&= -\frac{e^{i\mu x}}{8i\mu^3}\int_0^x (1-e^{-2i\mu(x-t)})q(t)dt\int_0^t (1-e^{-2i\mu(t-s)})q(s)ds \\
&\quad\times \int_0^s (1-e^{-2i\mu(s-y)})q(y)dy + O(1/\mu^4)e^{|Im\mu|x} \\
&= -\frac{e^{i\mu x}}{8i\mu^3}\int_0^x q(t)dt\int_0^t q(s)ds\int_0^s q(y) \\
&\quad\times [1 - e^{-2i\mu(x-t)} - e^{-2i\mu(t-s)} - e^{-2i\mu(s-y)} + e^{-2i\mu(x-s)} \\
&\quad + e^{-2i\mu(x-t+s-y)} + e^{-2i\mu(t-y)} - e^{-2i\mu(x-y)}]dy + O(1/\mu^4)e^{|Im\mu|x} \\
&= -\frac{e^{i\mu x}}{8i\mu^3}\int_0^x q(t)dt\int_0^t q(s)ds\int_0^s q(y)dy - \frac{1}{8i\mu^3}K(x,\mu) + O(1/\mu^4)e^{|Im\mu|x},
\end{aligned}
$$

where

$$
\begin{aligned}
K(x,\mu) &= e^{i\mu x}\int_0^x q(t)dt\int_0^t q(s)ds\int_0^s q(y) \\
&\quad\times [-e^{-2i\mu(x-t)} - e^{-2i\mu(t-s)} - e^{-2i\mu(s-y)} + e^{-2i\mu(x-s)} \\
&\quad + e^{-2i\mu(x-t+s-y)} + e^{-2i\mu(t-y)} - e^{-2i\mu(x-y)}]dy.
\end{aligned}
$$

Arguing as in [6], we see that

$$\int_0^x q(t)dt\int_0^t q(s)ds\int_0^s q(y)dy=\frac{1}{6}I^3(x).$$

The obvious inequality $0\le y\le s\le t\le x$, together with the inequality $|x-2z|\le x$ valid for $0\le z\le x$ and the Riemann lemma [8], implies

$$K(x,\mu)=o(1)e^{|Im\mu|x},\quad R_1(x,\mu)=-\frac{1}{48i\mu^3}I^3(x)+o(1/\mu^3)e^{|Im\mu|x}. \tag{2.9}$$

Continuing this line of reasoning, we reduce (2.6) and (2.8) to the form

$$R_2(x,\mu)=-\frac{1}{48\mu^2}e^{i\mu x}I^3(x)+o(1/\mu^2)e^{|Im\mu|x},\quad R_4(x,\mu)=o(1/\mu^2)e^{|Im\mu|x}. \tag{2.10}$$

It follows from (2.7) and (2.9) that

$$R_3(x,\mu)=O(1/\mu^3)e^{|Im\mu|x}. \tag{2.11}$$

Combining (2.3) and (2.9), we obtain

$$\begin{aligned}\varphi(x,\mu)&=e^{i\mu x}[1+\frac{1}{2i\mu}I(x)-\frac{1}{8\mu^2}I^2(x)]\\&\quad-\frac{e^{-i\mu x}}{2i\mu}\int_0^x e^{2i\mu t}q(t)dt+A(x,\mu)-\frac{e^{i\mu x}}{48i\mu^3}I^3(x)+o(1/\mu^3)e^{|Im\mu|x},\end{aligned} \tag{2.12}$$

It follows from (2.4), (2.10) and (2.11) that

$$\begin{aligned}\varphi'_x(x,\mu)&=i\mu e^{i\mu x}[1+\frac{1}{2i\mu}I(x)-(8\mu^2)^{-1}I^2(x)]\\&\quad+\frac{e^{-i\mu x}}{2}\int_0^x e^{2i\mu t}q(t)dt+B(x,\mu)-\frac{1}{48\mu^2}e^{i\mu x}I^3(x)+o(1/\mu^2)e^{|Im\mu|x}.\end{aligned} \tag{2.13}$$

Substituting into (2.1) the expressions for $c(\pi,\mu)$, $s(\pi,\mu)$, $s'(\pi,\mu)$ of (2.2), (2.12), (2.13), respectively, we obtain

$$\begin{aligned}&\Delta(\mu)\\&=\frac{1}{2}\Big\{e^{i\mu\pi}[1+\frac{1}{2i\mu}I(\pi)-\frac{1}{8\mu^2}I^2(\pi)]\\&\quad-\frac{e^{-i\mu\pi}}{2i\mu}\int_0^\pi e^{2i\mu t}q(t)dt+A(\pi,\mu)-\frac{e^{i\pi\mu}}{48i\mu^3}I^3(\pi)+o(1/\mu^3)e^{|Im\mu|\pi}\\&\quad+e^{-i\mu\pi}[1-\frac{1}{2i\mu}I(\pi)-\frac{1}{8\mu^2}I^2(\pi)]\\&\quad+\frac{e^{i\mu\pi}}{2i\mu}\int_0^\pi e^{-2i\mu t}q(t)dt+A(\pi,-\mu)+\frac{e^{-i\pi\mu}}{48i\mu^3}I^3(\pi)+o(1/\mu^3)e^{|Im\mu|\pi}\Big\}\\&\quad-\frac{1}{2i\mu}\Big\{i\mu e^{i\mu\pi}[1+\frac{1}{2i\mu}I(\pi)-(8\mu^2)^{-1}I^2(\pi)]\\&\quad+\frac{e^{-i\mu\pi}}{2}\int_0^\pi e^{2i\mu t}q(t)dt+B(\pi,\mu)-\frac{1}{48\mu^2}e^{i\mu\pi}I^3(\pi)+o(1/\mu^2)e^{|Im\mu|\pi}\\&\quad-[-i\mu e^{-i\mu\pi}[1-\frac{1}{2i\mu}I(\pi)-(8\mu^2)^{-1}I^2(\pi)]\end{aligned}$$

$$
\begin{aligned}
&+ \frac{e^{i\mu\pi}}{2}\int_0^\pi e^{-2i\mu t}q(t)dt + B(\pi,-\mu) - \frac{1}{48\mu^2}e^{-i\mu\pi}I^3(\pi) + o(1/\mu^2)e^{|Im\mu|\pi}]\Big\} \\
&- (-1)^\theta \frac{b}{2i\mu}\Big\{e^{i\mu\pi}[1+\frac{1}{2i\mu}I(\pi) - \frac{1}{8\mu^2}I^2(\pi)] \\
&- \frac{e^{-i\mu\pi}}{2i\mu}\int_0^\pi e^{2i\mu t}q(t)dt + o(1/\mu^2)e^{|Im\mu|\pi} \\
&- [e^{-i\mu\pi}[1-\frac{1}{2i\mu}I(\pi) - \frac{1}{8\mu^2}I^2(\pi)] - \frac{e^{i\mu\pi}}{2i\mu}\int_0^\pi e^{-2i\mu t}q(t)dt + o(1/\mu^2)e^{|Im\mu|\pi}]\Big\}.
\end{aligned}
$$

Define $\Delta_0(\mu) = \frac{-(-1)^\theta b}{2i\mu}(e^{i\pi\mu} - e^{-i\pi\mu})$. Combining like terms in the above expression, gives

$$
\begin{aligned}
\Delta(\mu) = \Delta_0(\mu) &- \frac{1}{2i\mu}[e^{-i\pi\mu}\int_0^\pi e^{2i\mu t}q(t)dt - e^{i\pi\mu}\int_0^\pi e^{-2i\mu t}q(t)dt] \\
&+ \frac{1}{4\mu^2}[e^{i\pi\mu}\int_0^\pi e^{-2i\mu t}q(t)dt\int_0^t q(s)\,ds + e^{-i\pi\mu}\int_0^\pi e^{2i\mu t}q(t)dt\int_0^t q(s)\,ds \\
&- e^{i\pi\mu}\int_0^\pi q(t)dt\int_0^t e^{-2i\mu s}q(s)ds - e^{-i\pi\mu}\int_0^\pi q(t)dt\int_0^t e^{2i\mu s}q(s)ds] \\
&- (-1)^\theta\frac{b}{2i\mu}\{\frac{e^{i\pi\mu}+e^{-i\pi\mu}}{2i\mu}I(\pi) - \frac{e^{i\pi\mu}-e^{-i\pi\mu}}{8\mu^2}I^2(\pi) \\
&- \frac{1}{2i\mu}(e^{-i\pi\mu}\int_0^\pi e^{2i\mu t}q(t)dt + e^{i\pi\mu}\int_0^\pi e^{-2i\mu t}q(t)dt)\} + o(1/\mu^3)e^{|Im\mu|\pi}.
\end{aligned} \tag{2.14}
$$

3. Calculation of the regularized trace

First, consider the case $\langle q\rangle = 0$. Formula (2.14) is then noticeably simplified:

$$
\Delta(\mu) = \Delta_0(\mu)(1+r(\mu)), \tag{3.1}
$$

where

$$
\begin{aligned}
&r(\mu) \\
&= \frac{1}{\Delta_0(\mu)}\Big\{-\frac{1}{2i\mu}[e^{-i\pi\mu}\int_0^\pi e^{2i\mu t}q(t)dt - e^{i\pi\mu}\int_0^\pi e^{-2i\mu t}q(t)dt] \\
&+ \frac{1}{4\mu^2}[e^{i\pi\mu}\int_0^\pi e^{-2i\mu t}q(t)dt\int_0^t q(s)\,ds + e^{-i\pi\mu}\int_0^\pi e^{2i\mu t}q(t)dt\int_0^t q(s)\,ds \\
&- e^{i\pi\mu}\int_0^\pi q(t)dt\int_0^t e^{-2i\mu s}q(s)ds - e^{-i\pi\mu}\int_0^\pi q(t)dt\int_0^t e^{2i\mu s}q(s)ds] \\
&+ (-1)^{\theta+1}\frac{b}{4\mu^2}(e^{-i\pi\mu}\int_0^\pi e^{2i\mu t}q(t)dt + e^{i\pi\mu}\int_0^\pi e^{-2i\mu t}q(t)dt) + o(1/\mu^3)e^{|Im\mu|\pi}\Big\}.
\end{aligned} \tag{3.2}
$$

Integrating by parts the terms on the right-hand side of (3.2), we have

$$
\begin{aligned}
r(\mu) = \frac{(-1)^{\theta+1}}{4b\mu\sin\pi\mu}&\{(e^{i\pi\mu}+e^{-i\pi\mu})(q(\pi)-q(0)) \\
&- [e^{i\pi\mu}\int_0^\pi e^{-2i\mu t}q'(t)dt + e^{-i\pi\mu}\int_0^\pi e^{2i\mu t}q'(t)dt]\} + \frac{q(\pi)+q(0)}{4\mu^2} + o(1/\mu^2).
\end{aligned} \tag{3.3}
$$

Denote by Γ_N the circle of radius $N+1/2$ centered at the origin. It is well known [8] that the eigenvalues of (1.1)-(1.2) form a sequence $\lambda_n = \mu_n^2$, where $\mu_n = n + o(1)$, $n = 1, 2, \dots$. This asymptotic relation for the eigenvalues implies that, for all sufficiently large N, the numbers μ_n with $n \le N$ are inside Γ_N, and the numbers μ_n with $n > N$ are outside Γ_N. It follows that

$$2\sum_{n=1}^{N}\mu_n^2 = \frac{1}{2\pi i}\oint_{\Gamma_N}\mu^2\frac{\Delta'(\mu)}{\Delta(\mu)}d\mu;$$

see [8]. Obviously, if $\mu \in \Gamma_N$, then $|\Delta_0(\mu)| \ge c_1 e^{|Im\mu|\pi}/|\mu|$ ($c_1 > 0$). This inequality and the Riemann lemma [8] imply that $\max_{\mu\in\Gamma_N}|r(\mu)| \to 0$ as $N \to \infty$. Combining this with (3.1) yields

$$\begin{aligned}\frac{1}{2\pi i}\oint_{\Gamma_N}\mu^2\frac{\Delta'(\mu)}{\Delta(\mu)}d\mu &= \frac{1}{2\pi i}\oint_{\Gamma_N}\mu^2\big(\frac{\Delta_0'(\mu)}{\Delta_0(\mu)} + \frac{r'(\mu)}{1+r((\mu)}\big)d\mu \\ &= 2\sum_{n=1}^{N}n^2 + \frac{1}{2\pi i}\oint_{\Gamma_N}\mu^2 d\ln(1+r(\mu)) \\ &= 2\sum_{n=1}^{N}n^2 - \frac{1}{2\pi i}\oint_{\Gamma_N}2\mu\ln(1+r(\mu))d\mu.\end{aligned}\tag{3.4}$$

Expanding $\ln(1+r(\mu))$ by the Maclaurin formula and applying (3.3) and the Riemann lemma [8], we find that

$$\ln(1+r(\mu)) = r(\mu) - \frac{(q(\pi)-q(0))^2}{2b^2\mu^2}\cot^2\pi\mu + \frac{o(1)}{\mu^2}\tag{3.5}$$

on Γ_N. Evidently,

$$\lim_{|Im\mu|\to\infty}(\cot^2\pi\mu + 1) = 0.\tag{3.6}$$

It follows from (3.5) and (3.6) that

$$\begin{aligned}&\frac{1}{2\pi i}\oint_{\Gamma_N}2\mu\ln(1+r(\mu))d\mu \\ &= \frac{1}{2\pi i}\oint_{\Gamma_N}\big[\frac{(-1)^{\theta+1}}{2b\sin\pi\mu}\{(e^{i\pi\mu}+e^{-i\pi\mu})(q(\pi)-q(0)) \\ &\quad - (e^{i\pi\mu}\int_0^\pi e^{-2i\mu t}q'(t)dt + e^{-i\pi\mu}\int_0^\pi e^{2i\mu t}q'(t)dt)\} \\ &\quad - \frac{(q(\pi)-q(0))^2}{b^2\mu}cot^2\pi\mu + \frac{q(\pi)+q(0)}{2\mu} + \frac{o(1)}{\mu}\big]d\mu \\ &= \sum_{n=-N}^{N}\Big[(-1)^{\theta+1}\big[(e^{i\pi n}+e^{-i\pi n})(q(\pi)-q(0)) - (e^{i\pi n}\int_0^\pi e^{-2int}q'(t)dt \\ &\quad + e^{-int}\int_0^\pi\int e^{2int}q'(t)dt)\big]\Big]/(2b\pi\cos\pi n) \\ &\quad + \frac{1}{2\pi i}\oint_{\Gamma_N}\big[\frac{(q(\pi)-q(0))^2}{b^2\mu} + \frac{q(\pi)+q(0)}{2\mu}\big]d\mu + o(1) \\ &= \frac{2(-1)^{\theta+1}}{\pi b}\sum_{n=1}^{N}(q(\pi)-q(0)\end{aligned}$$

$$
- \int_0^\pi q'(t)\cos(2nt)dt) + \frac{(q(\pi)-q(0))^2}{b^2} + \frac{q(\pi)+q(0)}{2} + o(1).
$$

Combining this and (3.4), we obtain

$$
\begin{aligned}
2\sum_{n=1}^N \mu_n^2 = 2\sum_{n=1}^N n^2 + \frac{2(-1)^\theta}{\pi b}\sum_{n=1}^N (q(\pi)-q(0) - \int_0^\pi q'(t)\cos(2nt)dt) \\
- \frac{(q(\pi)-q(0))^2}{b^2} - \frac{q(\pi)+q(0)}{2} + o(1).
\end{aligned} \tag{3.7}
$$

Passing to the limit as $N\to\infty$ in (3.7), we have

$$
\begin{aligned}
\sum_{n=1}^\infty \{\lambda_n - n^2 - \frac{(-1)^\theta (q(\pi)-q(0) - \int_0^\pi q'(t)\cos(2nt)dt)}{\pi b}\} \\
+ \frac{(q(\pi)-q(0))^2}{2b^2} + \frac{q(\pi)+q(0)}{4} = 0.
\end{aligned} \tag{3.8}
$$

Now consider the case $\langle q\rangle \neq 0$. Let $\tilde q(x) = q(x) - \langle q\rangle$. Then $\langle \tilde q\rangle = 0$. Suppose that (1.1)-(1.2) with potential $\tilde q$ has eigenvalues $\tilde\lambda_n$. Then $\tilde\lambda_n = \lambda_n - \langle q\rangle$. According to (3.8), we have

$$
\begin{aligned}
\sum_{n=1}^\infty \{\tilde\lambda_n - n^2 - \frac{(-1)^\theta (\tilde q(\pi)-\tilde q(0) - \int_0^\pi \tilde q'(t)\cos(2nt)dt)}{\pi b}\} \\
+ \frac{(\tilde q(\pi)-\tilde q(0))^2}{2b^2} + \frac{\tilde q(\pi)+\tilde q(0)}{4} = 0.
\end{aligned}
$$

Substituting the expressions for $\tilde\lambda_n$ and $\tilde q(x)$ into this equality, we obtain formula (1.3).

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