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## Refined asymptotics of the spectral gap for the Mathieu operator

Berkay Anahtarci, Plamen Djakov\*

Sabanci University, Orhanli, 34956 Tuzla, Istanbul, Turkey

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### ABSTRACT

The Mathieu operator

$$L(y) = -y'' + 2a \cos(2x)y, \quad a \in \mathbb{C}, \quad a \neq 0,$$

considered with periodic or anti-periodic boundary conditions has, close to  $n^2$  for large enough  $n$ , two periodic (if  $n$  is even) or anti-periodic (if  $n$  is odd) eigenvalues  $\lambda_n^-, \lambda_n^+$ . For fixed  $a$ , we show that

$$\lambda_n^+ - \lambda_n^- = \pm \frac{8(a/4)^n}{[(n-1)!]^2} \left[ 1 - \frac{a^2}{4n^3} + O\left(\frac{1}{n^4}\right) \right], \quad n \rightarrow \infty.$$

This result extends the asymptotic formula of Harrell–Avron–Simon by providing more asymptotic terms.

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### 1. Introduction

The one-dimensional Schrödinger operator

$$L(y) = -y'' + v(x)y, \tag{1.1}$$

considered on  $\mathbb{R}$  with  $\pi$ -periodic real-valued potential  $v \in L_{loc}^2(\mathbb{R})$ , is self-adjoint, and its spectrum has a gap-band structure (see Thm 2.3.1 in [1], or Thm 2.1 in [2]); namely, there are points

$$\lambda_0^+ < \lambda_1^- \leq \lambda_1^+ < \lambda_2^- \leq \lambda_2^+ < \lambda_3^- \leq \lambda_3^+ < \lambda_4^- \leq \lambda_4^+ < \dots$$

such that

$$Sp(L) = \bigcup_{n=1}^{\infty} [\lambda_{n-1}^+, \lambda_n^-]$$

and the intervals of the spectrum are separated by the spectral gaps

$$(-\infty, \lambda_0^+), (\lambda_1^-, \lambda_1^+), \dots, (\lambda_n^-, \lambda_n^+), \dots$$

The points  $\lambda_n^-, \lambda_n^+$  could be determined as eigenvalues of the Hill equation

$$-y'' + v(x)y = \lambda y, \tag{1.2}$$

considered on  $[0, \pi]$ , respectively, with periodic boundary conditions

$$y(0) = y(\pi), \quad y'(0) = y'(\pi), \tag{1.3}$$

\* Corresponding author.

E-mail addresses: [berkaya@sabanciuniv.edu](mailto:berkaya@sabanciuniv.edu) (B. Anahtarci), [djakov@sabanciuniv.edu](mailto:djakov@sabanciuniv.edu) (P. Djakov).

for even  $n$ , and with anti-periodic boundary conditions

$$y(0) = -y(\pi), \quad y'(0) = -y'(\pi), \tag{1.4}$$

for odd  $n$ . See basics and details in [1–3].

Hochstadt [4,5] discovered a direct connection between the smoothness of  $v$  and the rate of decay of the lengths of spectral gaps  $\gamma_n = \lambda_n^+ - \lambda_n^-$ : If

(A)  $v \in C^\infty$ , i.e.,  $v$  is infinitely differentiable, then

(B)  $\gamma_n$  decreases more rapidly than any power of  $1/n$ .

If a continuous function  $v$  is a finite-zone potential, i.e.,  $\gamma_n = 0$  for large enough  $n$ , then  $v \in C^\infty$ .

In the mid-70s (see [6,7]) the latter statement was extended, namely, it was shown, for real  $L^2([0, \pi])$ -potentials  $v$ , that (B)  $\Rightarrow$  (A). Moreover, Trubowitz [8] proved that an  $L^2([0, \pi])$ -potential  $v$  is analytic if and only if  $(\gamma_n)$  decays exponentially.

If  $v$  is a complex-valued potential then the operator (1.1) is non-self-adjoint, so one cannot talk about spectral gaps. Moreover, the periodic and anti-periodic eigenvalues  $\lambda_n^\pm$  are well-defined for large  $n$  (see Lemma 1 below) but the asymptotics of  $|\lambda_n^+ - \lambda_n^-|$  does not determine the smoothness of  $v$ . In [9] Tkachenko brought into this discussion the Dirichlet b.v.p.  $y(\pi) = y(0) = 0$ . For large enough  $n$ , close to  $n^2$  there is exactly one Dirichlet eigenvalue  $\mu_n$ , so the deviation

$$\delta_n = \left| \mu_n - \frac{1}{2}(\lambda_n^+ + \lambda_n^-) \right| \tag{1.5}$$

is well defined. Using an adequate parametrization of potentials in spectral terms similar to Marchenko–Ostrovskii’s ones [3,6] for self-adjoint operators, Tkachenko [9,10] (see also [11]) characterized  $C^\infty$ -smoothness and analyticity in terms of  $\delta_n$  and differences between critical values of Lyapunov functions and  $(-1)^n$ . See further references and later results in [12–15].

In the case of specific potentials, like the Mathieu potential

$$v(x) = 2a \cos 2x, \quad a \neq 0, \text{ real}, \tag{1.6}$$

or more general trigonometric polynomials

$$v(x) = \sum_{-N}^N c_k \exp(2ikx), \quad c_k = \overline{c_{-k}}, \quad 0 \leq k \leq N < \infty, \tag{1.7}$$

one comes to two classes of questions:

(i) Is the  $n$ th spectral gap closed, i.e.,

$$\gamma_n = \lambda_n^+ - \lambda_n^- = 0, \tag{1.8}$$

or, equivalently, is the multiplicity of  $\lambda_n^+$  equal to 2?

(ii) If  $\gamma_n \neq 0$ , could we tell more about the size of this gap, or, for large enough  $n$ , what is the asymptotic behavior of  $\gamma_n = \gamma_n(v)$ ?

Ince [16] proved that the Mathieu–Hill operator has only simple eigenvalues both for periodic and anti-periodic boundary conditions, i.e.,  $\gamma_n \neq 0$  for every  $n \in \mathbb{N}$ . His proof is presented in [1]; see other proofs of this fact in [17–19], and further references in [1,20].

For fixed  $n$  and  $a \rightarrow 0$ , Levy and Keller [21] gave an asymptotics of the spectral gap  $\gamma_n = \gamma_n(a)$ ,  $v \in (1.6)$ ; namely

$$\gamma_n = \lambda_n^+ - \lambda_n^- = \frac{8(|a|/4)^n}{[(n-1)!]^2} (1 + O(a)), \quad a \rightarrow 0. \tag{1.9}$$

Almost 20 years later, Harrell [22] found, up to a constant factor, the asymptotics of the spectral gaps of the Mathieu operator for fixed  $a$  as  $n \rightarrow \infty$ . Avron and Simon [23] gave an alternative proof of E. Harrell’s asymptotics and found the exact value of the constant factor, which led to the formula

$$\gamma_n = \lambda_n^+ - \lambda_n^- = \frac{8(|a|/4)^n}{[(n-1)!]^2} \left( 1 + o\left(\frac{1}{n^2}\right) \right) \quad n \rightarrow \infty. \tag{1.10}$$

Later, another proof of (1.10) was given by Hochstadt [24]. For general trigonometric polynomial potentials, Grigis [25] obtained a generic form of the main term in the gap asymptotics.

In this paper, we extend the result of Harrell–Avron–Simon and give the following more precise asymptotics of the size of spectral gap for the Mathieu operator (even in the case when the parameter  $a$  is a complex number):

$$\lambda_n^+ - \lambda_n^- = \pm \frac{8(a/4)^n}{[(n-1)!]^2} \left[ 1 - \frac{a^2}{4n^3} + O\left(\frac{1}{n^4}\right) \right], \quad n \rightarrow \infty. \tag{1.11}$$

Our approach is based on the methods developed in [26,27], where the gap asymptotics of the Hill operator with two term potential of the form

$$v(x) = A \cos 2x + B \cos 4x, \quad A \neq 0, B \neq 0$$

was found. The same methods play a crucial role in the study of Riesz basis property of the root system of Hill operators with trigonometric polynomial potentials (see [28,29]).

Our approach could be applied (with slight modifications) in order to find the asymptotics of  $\lambda_n^+ - \lambda_n^-$  in the case of potentials of the form

$$v(x) = ce^{-2ix} + de^{2ix}, \quad c, d \in \mathbb{C}. \tag{1.12}$$

But as Veliev [30] observed, the operators (1.1) generated by potentials (1.12) with  $cd = \text{const}$  are isospectral if considered with periodic or antiperiodic boundary conditions. Therefore, from (1.11) with  $a = \sqrt{cd}$  it follows that

$$\lambda_n^+ - \lambda_n^- = \pm \frac{8(\sqrt{cd}/4)^n}{[(n-1)!]^2} \left[ 1 - \frac{cd}{4n^3} + O\left(\frac{1}{n^4}\right) \right], \quad n \rightarrow \infty \tag{1.13}$$

in the case of potentials (1.12).

Let us mention that the paper [31] claims to provide “the formula which states the isolated terms of arbitrary number in the asymptotics of the sequence  $\gamma_n$ ”. However, this claim is false due to an unavoidable technical mistake (in [31], formula (5) does not imply (4) for  $m = k + 1$  since, by Stirling’s formula, the remainder in (5) is much larger than the main term in (4)).

To the best of our knowledge, (1.11) is the first formula that gives more asymptotic terms than the formula of Harrell–Avron–Simon.

## 2. Preliminaries

Let  $L_{Per^+}(v)$  and  $L_{Per^-}(v)$  denote, respectively, the operator (1.1) considered with periodic ( $Per^+$ ) or antiperiodic ( $Per^-$ ) boundary conditions. Further we assume that  $v \in L^2([0, \pi])$  is a complex-valued potential such that

$$V(0) = \int_0^\pi v(x)dx = 0. \tag{2.1}$$

The following assertion is well-known (e.g., [27, Proposition 1]).

**Lemma 1.** *The spectra of  $L_{Per^\pm}(v)$  are discrete. There is an  $N_0 = N_0(v)$  such that the union  $\cup_{n>N_0} D_n$  of the discs  $D_n = \{z : |z - n^2| < 1\}$  contains all but finitely many of the eigenvalues of  $L_{Per^\pm}$ .*

*Moreover, for  $n > N_0$  the disc  $D_n$  contains exactly two (counted with algebraic multiplicity) periodic (if  $n$  is even) or antiperiodic (if  $n$  is odd) eigenvalues  $\lambda_n^-, \lambda_n^+$  (where  $\text{Re } \lambda_n^- < \text{Re } \lambda_n^+$  or  $\text{Re } \lambda_n^- = \text{Re } \lambda_n^+$  and  $\text{Im } \lambda_n^- \leq \text{Im } \lambda_n^+$ ).*

**Remark.** In the following we assume that  $N_0 > 1$  and consider only integers  $n > N_0$ .

In view of Lemma 1,

$$|\lambda_n^\pm - n^2| < 1, \quad \text{for } n \geq N_0. \tag{2.2}$$

Moreover, Lemma 1 allows us to apply the Lyapunov–Schmidt projection method and reduce the eigenvalue equation  $Ly = \lambda y$  for  $\lambda \in D_n$  to an eigenvalue equation in the two-dimensional space  $E_n^0 = \{L^0 y = n^2 y\}$  (see [14, Section 2.2] for more comments).

This leads to the following (see the formulas (2.24)–(2.30) in [14]).

**Lemma 2.** *In the above notations,  $\lambda_n^\pm = n^2 + z$ , for  $|z| < 1$ , is an eigenvalue of  $L_{Per^\pm}(v)$  if and only if  $z$  is a root of the equation*

$$\begin{vmatrix} z - S^{11} & S^{12} \\ S^{21} & z - S^{22} \end{vmatrix} = 0, \tag{2.3}$$

where  $S^{11}, S^{12}, S^{21}, S^{22}$  can be represented as

$$S^{ij}(n, z) = \sum_{k=0}^\infty S_k^{ij}(n, z), \quad i, j = 1, 2, \tag{2.4}$$

with

$$S_0^{11} = S_0^{22} = 0, \quad S_0^{12} = V(-2n), \quad S_0^{21} = V(2n), \tag{2.5}$$

and for each  $k = 1, 2, \dots$ ,

$$S_k^{11}(n, z) = \sum_{j_1, \dots, j_k \neq \pm n} \frac{V(-n + j_1)V(j_2 - j_1) \cdots V(j_k - j_{k-1})V(n - j_k)}{(n^2 - j_1^2 + z) \cdots (n^2 - j_k^2 + z)}, \tag{2.6}$$

$$S_k^{22}(n, z) = \sum_{j_1, \dots, j_k \neq \pm n} \frac{V(n + j_1)V(j_2 - j_1) \cdots V(j_k - j_{k-1})V(-n - j_k)}{(n^2 - j_1^2 + z) \cdots (n^2 - j_k^2 + z)}, \tag{2.7}$$

$$S_k^{12}(n, z) = \sum_{j_1, \dots, j_k \neq \pm n} \frac{V(-n + j_1)V(j_2 - j_1) \cdots V(j_k - j_{k-1})V(-n - j_k)}{(n^2 - j_1^2 + z) \cdots (n^2 - j_k^2 + z)}, \tag{2.8}$$

$$S_k^{21}(n, z) = \sum_{j_1, \dots, j_k \neq \pm n} \frac{V(n + j_1)V(j_2 - j_1) \cdots V(j_k - j_{k-1})V(n - j_k)}{(n^2 - j_1^2 + z) \cdots (n^2 - j_k^2 + z)}. \tag{2.9}$$

The above series converge absolutely and uniformly for  $|z| \leq 1$ .

Moreover, (2.4)–(2.9) imply the following (see Lemma 23 in [14]).

**Lemma 3.** For any (complex-valued) potential  $v$

$$S^{11}(n, z) = S^{22}(n, z). \tag{2.10}$$

Moreover, if  $V(-m) = \overline{V(m)} \forall m$ , then

$$S^{12}(n, z) = \overline{S^{21}(n, \bar{z})}, \tag{2.11}$$

and if  $V(-m) = V(m) \forall m$ , then

$$S^{12}(n, z) = S^{21}(n, z). \tag{2.12}$$

**Proof.** For each  $k \in \mathbb{N}$ , the change of summation indices  $i_s = -j_{k+1-s}$ ,  $s = 1, \dots, k$  proves that  $S_k^{11}(n, z) = S_k^{22}(n, z)$ . In view of (2.4) and (2.5), (2.10) follows.

In a similar way, we obtain that (2.11) and (2.12) hold by using for each  $k \in \mathbb{N}$  the change of indices  $i_s = j_{k+1-s}$ ,  $s = 1, 2, \dots, k$ .  $\square$

In the sequel we consider only the Mathieu potential, i.e.,

$$v(x) = 2a \cos 2x = ae^{-2ix} + ae^{2ix}, \quad V(\pm 2) = a, \quad V(k) = 0 \quad \text{if } k \neq \pm 2. \tag{2.13}$$

For convenience, we set

$$\alpha_n(z) := S^{11}(n, z) = S^{22}(n, z), \quad \beta_n(z) := S^{21}(n, z) = S^{12}(n, z). \tag{2.14}$$

In these notations the basic equation (2.3) becomes

$$(z - \alpha_n(z))^2 = (\beta_n(z))^2. \tag{2.15}$$

By Lemmas 1 and 2, for large enough  $n \in \mathbb{N}$ , this equation has in the unit disc exactly the following two roots (counted with multiplicity):

$$z_n^- = \lambda_n^- - n^2, \quad z_n^+ = \lambda_n^+ - n^2. \tag{2.16}$$

### 3. Asymptotic estimates for $z_n^\pm$ and $\alpha_n(z)$

In this section, we use the basic equation (2.15) to derive asymptotic estimates for  $z_n^\pm = \lambda_n^\pm - n^2$ . It turns out that  $|\beta_n(z)|$ ,  $|z| \leq 1$ , is much smaller than  $|\alpha_n(z)|$ , so it is enough to analyze the asymptotics of  $\alpha_n(z_n^\pm)$  in order to find asymptotic estimates for  $z_n^\pm$ .

The following inequality is well known (e.g., see Lemma 78 in [14]):

$$\sum_{j \neq \pm n} \frac{1}{|n^2 - j^2|} < \frac{2 \log 6n}{n}, \quad \text{for } n \in \mathbb{N}. \tag{3.1}$$

**Lemma 4.** If  $|z| \leq 1$ , then

$$\sum_{j_1, \dots, j_\nu \neq \pm n} \frac{1}{|n^2 - j_1^2 + z| \cdots |n^2 - j_\nu^2 + z|} < \left( \frac{4 \log 6n}{n} \right)^\nu. \tag{3.2}$$

**Proof.** If  $|z| \leq 1$  and  $j \neq \pm n$ , then

$$|n^2 - j^2 + z| \geq |n^2 - j^2| - 1 \geq \frac{1}{2}|n^2 - j^2|.$$

Therefore,

$$\sum_{j_1, \dots, j_\nu \neq \pm n} \frac{1}{|n^2 - j_1^2 + z| \cdots |n^2 - j_\nu^2 + z|} \leq 2^\nu \left( \sum_{j \neq \pm n} \frac{1}{|n^2 - j^2|} \right)^\nu,$$

so (3.2) follows from (3.1).  $\square$

The next lemma gives a rough estimate for  $\beta_n(z)$ ; we improve this estimate in the next section.

**Lemma 5.** For  $|z| \leq 1$  we have

$$\beta_n(z) = O\left(\left(\frac{C \log n}{n}\right)^n\right), \tag{3.3}$$

where  $C$  depends only on  $a$ .

**Proof.** If  $\nu < n - 1$ , then all terms of the sum  $S_\nu^{21}(n, z)$  in (2.9) vanish. Indeed, each term of the sum  $S_\nu^{21}(n, z)$  is a fraction in which numerator has the form  $V(x_1)V(x_2) \cdots V(x_{\nu+1})$  with  $x_1 = n + j_1, x_2 = j_2 - j_1, \dots, x_{\nu+1} = n - j_\nu$ . Therefore, if  $\nu < n - 1$  then there are no  $x_1, x_2, \dots, x_{\nu+1} \in \{-2, 2\}$  satisfying  $x_1 + x_2 + \cdots + x_{\nu+1} = 2n$ , so every term of the sum  $S_\nu^{21}(n, z)$  vanishes due to (2.13). Hence, by (2.13) we have

$$|\beta_n(z)| \leq \sum_{\nu=n-1}^\infty \sum_{j_1, \dots, j_\nu \neq \pm n} \frac{|a|^{\nu+1}}{|n^2 - j_1^2 + z| \cdots |n^2 - j_\nu^2 + z|},$$

so (3.3) follows from (3.2).  $\square$

**Lemma 6.** In the above notations,

$$z_n^\pm = \frac{a^2}{2n^2} + O\left(\frac{1}{n^4}\right), \quad \alpha_n(z_n^\pm) = \frac{a^2}{2n^2} + O\left(\frac{1}{n^4}\right), \quad n \rightarrow \infty. \tag{3.4}$$

**Proof.** In view of (2.4), (2.6) and (2.14), we have

$$\alpha_n(z) = \sum_{p=1}^\infty A_p(n, z), \tag{3.5}$$

where

$$A_p(n, z) = \sum_{j_1, \dots, j_p \neq \pm n} \frac{V(-n + j_1)V(j_2 - j_1) \cdots V(j_p - j_{p-1})V(n - j_p)}{(n^2 - j_1^2 + z) \cdots (n^2 - j_p^2 + z)}. \tag{3.6}$$

First we show that

$$A_{2k}(n, z) \equiv 0 \quad \forall k \in \mathbb{N}. \tag{3.7}$$

Indeed, for  $p = 2k$  each term of the sum in (3.6) is a fraction in which numerator has the form  $V(x_1)V(x_2) \cdots V(x_{2k+1})$  with

$$x_1 = -n + j_1, \quad x_2 = j_2 - j_1, \dots, x_{2k+1} = n - j_{2k}.$$

Since  $x_1 + x_2 + \cdots + x_{2k+1} = 0$ , it follows that there is  $i_0$  such that  $x_{i_0} \neq \pm 2$ , so  $V(x_{i_0}) = 0$  due to (2.13). Therefore, every term of the sum  $A_{2k}(n, z)$  vanishes; hence (3.7) holds.

Next we estimate iteratively, in two steps,  $\alpha_n(z)$  and  $z_n^\pm$ . The first step provides rough estimates which we improve in the second step.

*Step 1.* By (3.6), we have

$$A_1(n, z) = \sum_{j_1 \neq \pm n} \frac{V(-n + j_1)V(n - j_1)}{n^2 - j_1^2 + z}.$$

In view of (2.13), we get a non-zero term in the above sum if and only if  $j_1 = n + 2$ , or  $j_1 = n - 2$ . Therefore,

$$A_1(n, z) = \frac{a^2}{n^2 - (n - 2)^2 + z} + \frac{a^2}{n^2 - (n + 2)^2 + z} = a^2 \frac{8 - 2z}{(4n)^2 - (4 - z)^2}, \tag{3.8}$$

which implies that

$$A_1(n, z) = O\left(\frac{1}{n^2}\right) \quad \text{for } |z| \leq 1. \quad (3.9)$$

On the other hand, from (2.13), (3.2) and (3.6) it follows that

$$|A_{2k-1}(n, z)| \leq |a|^{2k} \left(\frac{4 \log 6n}{n}\right)^{2k-1}, \quad k = 2, 3, \dots, \quad (3.10)$$

which implies

$$\sum_{k=2}^{\infty} |A_{2k-1}(n, z)| \leq \sum_{k=2}^{\infty} |a|^{2k} \left(\frac{4 \log 6n}{n}\right)^{2k-1} = o(1/n^2). \quad (3.11)$$

Hence, by (3.9) and (3.11) we obtain

$$\alpha_n(z) = O\left(\frac{1}{n^2}\right) \quad \text{for } |z| \leq 1. \quad (3.12)$$

Furthermore, from (2.15), (2.16) and (3.3) it follows immediately that

$$z_n^{\pm} - \alpha_n(z_n^{\pm}) = O\left(\frac{1}{n^k}\right), \quad \forall k \in \mathbb{N}. \quad (3.13)$$

Therefore, (3.12) implies that

$$z_n^{\pm} = O\left(\frac{1}{n^2}\right). \quad (3.14)$$

Step 2. By (3.8) we have

$$A_1(n, z) = \frac{a^2}{2n^2} + O\left(\frac{1}{n^4}\right) \quad \text{if } z = O(1/n^2). \quad (3.15)$$

Let us consider

$$A_3(n, z) = \sum_{j_1, j_2, j_3 \neq \pm n} \frac{V(-n+j_1)V(j_2-j_1)V(j_3-j_2)V(n-j_3)}{(n^2-j_1^2+z)(n^2-j_2^2+z)(n^2-j_3^2+z)}.$$

In view of (2.13), we get a non-zero term in the above sum if and only if

$$j_1 = n+2; \quad j_2 = n+4; \quad j_3 = n+2,$$

or

$$j_1 = n-2; \quad j_2 = n-4; \quad j_3 = n-2.$$

Hence,

$$A_3(n, z) = \frac{a^4}{[n^2 - (n+2)^2 + z][n^2 - (n+4)^2 + z][n^2 - (n+2)^2 + z]} + \frac{a^4}{[n^2 - (n-2)^2 + z][n^2 - (n-4)^2 + z][n^2 - (n-2)^2 + z]},$$

so it is easy to see that

$$A_3(n, z) = O\left(\frac{1}{n^4}\right) \quad \text{if } |z| \leq 1. \quad (3.16)$$

On the other hand, by (3.10) we have

$$\sum_{k=3}^{\infty} |A_{2k-1}(n, z)| \leq \sum_{k=3}^{\infty} |a|^{2k} \left(\frac{4 \log 6n}{n}\right)^{2k-1} = o(1/n^4). \quad (3.17)$$

Therefore, by (3.15), (3.16) and (3.17) imply that

$$\alpha_n(z) = \frac{a^2}{2n^2} + O\left(\frac{1}{n^4}\right) \quad \text{if } z = O(1/n^2). \tag{3.18}$$

Hence, from (3.13) it follows that

$$z_n^\pm = \frac{a^2}{2n^2} + O\left(\frac{1}{n^4}\right). \quad \square \tag{3.19}$$

**Remark.** From (3.8) and (3.19) it follows that

$$A_1(n, z_n^\pm) = \frac{a^2}{2n^2} + \frac{a^2}{2n^4} - \frac{a^4}{16n^4} + O\left(\frac{1}{n^6}\right). \tag{3.20}$$

Similarly, it is easily seen that

$$A_3(n, z_n^\pm) = \frac{a^4}{16n^4} + O\left(\frac{1}{n^6}\right). \tag{3.21}$$

On the other hand, analyzing  $A_5(n, z)$  one can show that

$$A_5(n, z) = O\left(\frac{1}{n^6}\right) \quad \text{if } |z| \leq 1. \tag{3.22}$$

Moreover, by (3.10) we have

$$\sum_{k=4}^{\infty} |A_{2k-1}(n, z)| = o\left(\frac{1}{n^6}\right) \quad \text{if } |z| \leq 1. \tag{3.23}$$

Hence, in view of (3.13), the estimates (3.20)–(3.23) lead to

$$z_n^\pm = \frac{a^2}{2n^2} + \frac{a^2}{2n^4} + O\left(\frac{1}{n^6}\right). \tag{3.24}$$

This analysis could be extended in order to obtain more asymptotic terms of  $z_n^\pm$ , and even to explain that the corresponding asymptotic series along the powers of  $1/n$  contains only even nontrivial terms. However, in this paper we need only the estimate (3.19).

The following assertion plays an essential role later.

**Lemma 7.** With  $\gamma_n = \lambda_n^+ - \lambda_n^- = z_n^+ - z_n^-$ ,

$$\alpha_n(z_n^+) - \alpha_n(z_n^-) = \gamma_n \left[ -\frac{a^2}{8n^2} + O\left(\frac{1}{n^4}\right) \right]. \tag{3.25}$$

**Proof.** By (3.5) and (3.7) we obtain

$$\alpha_n(z_n^+) - \alpha_n(z_n^-) = A_1(n, z_n^+) - A_1(n, z_n^-) + \int_{z_n^-}^{z_n^+} \frac{d}{dz} \tilde{\alpha}_n(z) dz, \tag{3.26}$$

where we integrate along the segment between  $z_n^-$  and  $z_n^+$ , and

$$\tilde{\alpha}_n(z) = \alpha_n(z) - A_1(n, z) = A_3(n, z) + A_5(n, z) + \dots$$

In view of (3.16) and (3.17),

$$\tilde{\alpha}_n(z) = O(1/n^4) \quad \text{for } |z| \leq 1.$$

By the Cauchy formula for derivatives, this estimate implies that

$$\frac{d\tilde{\alpha}_n}{dz}(z) = O(1/n^4) \quad \text{for } |z| \leq 1/2.$$

Hence, we obtain

$$\int_{z_n^-}^{z_n^+} \frac{d\tilde{\alpha}_n}{dz}(z) dz = \gamma_n O\left(\frac{1}{n^4}\right). \tag{3.27}$$

On the other hand, by (3.8)

$$\begin{aligned} A_1(n, z_n^+) - A_1(n, z_n^-) &= \left[ \frac{8 - 2z_n^+}{(4n)^2 - (4 - z_n^+)^2} - \frac{8 - 2z_n^-}{(4n)^2 - (4 - z_n^-)^2} \right] a^2 \\ &= \gamma_n \left[ \frac{-32n^2 - 32 + 8(z_n^+ + z_n^-) - 2z_n^+ z_n^-}{[(4n)^2 - (4 - z_n^+)^2][(4n)^2 - (4 - z_n^-)^2]} \right] a^2. \end{aligned}$$

Therefore, taking into account (3.4), we obtain

$$A_1(n, z_n^+) - A_1(n, z_n^-) = \gamma_n \left[ \frac{-a^2}{8n^2} + O\left(\frac{1}{n^4}\right) \right]. \tag{3.28}$$

In view of (3.26), the estimates (3.27) and (3.28) lead to (3.25).  $\square$

**4. Asymptotic formulas for  $\beta_n(z_n^\pm)$  and  $\gamma_n$ .**

In this section, we find more precise asymptotics of  $\beta_n(z_n^\pm)$ . These asymptotics, combined with the results of the previous section, lead to an asymptotics for  $\gamma_n$ .

In view of (2.13), each nonzero term in (2.9) corresponds to a  $k$ -tuple of indices  $(j_1, \dots, j_k)$  with  $j_1, \dots, j_k \neq \pm n$  such that

$$(n + j_1) + (j_2 - j_1) + \dots + (j_k - j_{k-1}) + (n - j_k) = 2n \tag{4.1}$$

and

$$n + j_1, j_2 - j_1, \dots, j_k - j_{k-1}, n - j_k \in \{-2, 2\}. \tag{4.2}$$

By (4.1) and (4.2), there is one-to-one correspondence between the nonzero terms in (2.9) and the *admissible* walks  $x = (x(t))_{t=1}^{k+1}$  on  $\mathbb{Z}$  from  $-n$  to  $n$  with steps  $x(t) = \pm 2$  and vertices  $j_0 = -n, j_{k+1} = n$ ,

$$j_s = -n + \sum_{t=1}^s x(t) \neq \pm n, \quad s = 1, \dots, k. \tag{4.3}$$

Let  $X_n(p), p = 0, 1, 2, \dots$  denote the set of all such walks with  $p$  negative steps. It is easy to see that every walk  $x \in X_n(p)$  has totally  $n + 2p$  steps because  $\sum x(t) = 2n$ . Therefore, every admissible walk has at least  $n$  steps.

In view of (2.4), (2.9), (2.13) and (2.14), we have

$$\beta_n(z) = \sum_{p=0}^{\infty} \sigma_p(n, z) \quad \text{with} \quad \sigma_p(n, z) = \sum_{x \in X_n(p)} h(x, z), \tag{4.4}$$

where, for  $x = (x(t))_{t=1}^{k+1}$ ,

$$h(x, z) = \frac{a^{k+1}}{(n^2 - j_1^2 + z)(n^2 - j_2^2 + z) \cdots (n^2 - j_k^2 + z)} \tag{4.5}$$

with  $j_1, \dots, j_k$  given by (4.3).

The set  $X_n(0)$  has only one element, namely the walk

$$\xi = (\xi(t))_{t=1}^n, \quad \xi(t) = 2 \quad \forall t. \tag{4.6}$$

Therefore,

$$\sigma_0(n, z) = h(\xi, z) = \frac{a^n}{(n^2 - j_1^2 + z) \cdots (n^2 - j_{n-1}^2 + z)} \tag{4.7}$$

with  $j_k = -n + 2k, k = 1, \dots, n - 1$ . Moreover, since

$$\prod_{k=1}^{n-1} (n^2 - (-n + 2k)^2) = 4^{n-1} [(n - 1)!]^2,$$

the following holds.



**Lemma 8.** In the above notations,

$$\sigma_0(n, 0) = h(\xi, 0) = \frac{4(a/4)^n}{[(n-1)!]^2}. \tag{4.8}$$

It is well known (as a partial case of the Euler–Maclaurin sum formula, see [32, Sect. 3.6]) that

$$\sum_{k=1}^n \frac{1}{k} = \log n + g + \frac{1}{2n} - \frac{1}{12n^2} + O\left(\frac{1}{n^4}\right), \quad n \in \mathbb{N}, \tag{4.9}$$

where  $g = \lim_{n \rightarrow \infty} \left(\sum_{k=1}^n \frac{1}{k} - \log n\right)$  is the Euler constant.

**Lemma 9.** In the above notations,

$$\sigma_0(n, z_n^\pm) = \sigma_0(n, 0) \left[ 1 - \frac{a^2 \log n}{4n^3} - \frac{a^2 g}{4n^3} + O\left(\frac{1}{n^4}\right) \right]. \tag{4.10}$$

**Proof.** By (4.7), we have

$$\sigma_0(n, z_n^\pm) = \sigma_0(n, 0) \prod_{k=1}^{n-1} \left( 1 + \frac{z_n^\pm}{n^2 - (-n + 2k)^2} \right)^{-1}. \tag{4.11}$$

For simplicity, we set  $b_k = \frac{z_n^\pm}{n^2 - (-n + 2k)^2} = \frac{z_n^\pm}{4k(n-k)}$ . Then,

$$\log \left( \prod_{k=1}^{n-1} (1 + b_k)^{-1} \right) = - \sum_{k=1}^{n-1} \log(1 + b_k) = - \sum_{k=1}^{n-1} b_k + O\left(\sum_{k=1}^{n-1} |b_k|^2\right).$$

Using (3.4), we obtain

$$\begin{aligned} \sum_{k=1}^{n-1} b_k &= \left( \sum_{k=1}^{n-1} \frac{1}{4k(n-k)} \right) \left[ \frac{a^2}{2n^2} + O\left(\frac{1}{n^4}\right) \right] \\ &= \frac{1}{2n} \left( \sum_{k=1}^{n-1} \frac{1}{k} \right) \left[ \frac{a^2}{2n^2} + O\left(\frac{1}{n^4}\right) \right]. \end{aligned}$$

By (4.9), it follows that

$$\sum_{k=1}^{n-1} b_k = \frac{a^2 \log n}{4n^3} + \frac{a^2 g}{4n^3} + O\left(\frac{1}{n^4}\right).$$

On the other hand, by (3.4),

$$\sum_{k=1}^{n-1} |b_k|^2 = \left( \sum_{k=1}^{n-1} \frac{1}{[4k(n-k)]^2} \right) O\left(\frac{1}{n^4}\right) = O\left(\frac{1}{n^4}\right).$$

Hence,

$$\log \left( \prod_{k=1}^{n-1} (1 + b_k)^{-1} \right) = - \frac{a^2 \log n}{4n^3} - \frac{a^2 g}{4n^3} + O\left(\frac{1}{n^4}\right),$$

which implies (4.10).  $\square$

Next we study the ratio  $\sigma_1(n, z)/\sigma_0(n, z)$ .

**Lemma 10.** We have

$$\sigma_1(n, z) = \sigma_0(n, z) \cdot \Phi(n, z), \tag{4.12}$$

where

$$\Phi(n, z) = \sum_{k=2}^{n-1} \varphi_k(n, z) \tag{4.13}$$

with

$$\varphi_k(n, z) = \frac{a^2}{[n^2 - (-n + 2k)^2 + z][n^2 - (-n + 2k - 2)^2 + z]}. \tag{4.14}$$

**Proof.** From the definition of  $X_n(1)$  and (4.4) it follows that

$$\sigma_1(n, z) = \sum_{x \in X_n(1)} h(x, z) = \sum_{k=2}^{n-1} h(x_k, z), \tag{4.15}$$

where  $x_k$  denotes the walk with  $(k + 1)$ 'th step equal to  $-2$ , i.e.,

$$x_k(t) = \begin{cases} 2 & \text{if } t \neq k + 1 \\ -2 & \text{if } t = k + 1 \end{cases}, \quad 1 \leq t \leq n + 2.$$

Now, we figure out the connection between vertices of  $\xi$  and  $x_k$  as follows:

$$j_\alpha(x_k) = \begin{cases} j_\alpha(\xi), & 1 \leq \alpha \leq k, \\ j_{k-1}(\xi) & \alpha = k + 1, \\ j_{\alpha-2}(\xi) & k + 2 \leq \alpha \leq n + 2. \end{cases}$$

Therefore, by (4.5)

$$h(x_k, z) = h(\xi, z) \frac{a^2}{(n^2 - [j_{k-1}(\xi)]^2 + z)(n^2 - [j_k(\xi)]^2 + z)}. \tag{4.16}$$

Since  $j_k(\xi) = -n + 2k$ ,  $k = 2, \dots, n - 1$ , (4.15) and (4.16) imply (4.12).  $\square$

**Lemma 11.** *In the above notations, if  $z = O(1/n^2)$  then*

$$\Phi(n, z) = \Phi(n, 0) + O(1/n^4) \tag{4.17}$$

and

$$\Phi^*(n, z) := \sum_{k=2}^{n-1} |\varphi_k(n, z)| = \Phi(n, 0) + O(1/n^4). \tag{4.18}$$

Moreover,

$$\Phi(n, 0) = \frac{a^2}{8n^2} + \frac{a^2 \log n}{4n^3} + \frac{a^2(g - 1)}{4n^3} + O(1/n^4). \tag{4.19}$$

**Proof.** Since

$$\frac{\varphi_k(n, z)}{\varphi_k(n, 0)} = \left[ 1 + \frac{z}{n^2 - (-n + 2k)^2} \right]^{-1} \left[ 1 + \frac{z}{n^2 - (-n + 2k - 2)^2} \right]^{-1},$$

it is easily seen that

$$\varphi_k(n, z)/\varphi_k(n, 0) = 1 + O(1/n^3) \quad \text{if } z = O(1/n^2).$$

On the other hand,  $\varphi_k(n, 0) = O(1/n^2)$ , so it follows that

$$\varphi_k(n, z) - \varphi_k(n, 0) = \varphi_k(n, 0) O(1/n^3) = O(1/n^5) \quad \text{if } z = O(1/n^2).$$

Therefore, we obtain that

$$\sum_{k=2}^{n-1} |\varphi_k(n, z) - \varphi_k(n, 0)| = O(1/n^4) \quad \text{if } z = O(1/n^2).$$

The latter sum dominates both  $|\Phi(n, z) - \Phi(n, 0)|$  and  $|\Phi^*(n, z) - \Phi(n, 0)|$ . Hence, (4.17) and (4.18) hold.

Next we prove (4.19). Since

$$\Phi(n, 0) = \sum_{k=2}^{n-1} \frac{a^2}{16(k - 1)k(n - k)(n + 1 - k)},$$

by using the identities

$$\frac{1}{k(n-k)} = \frac{1}{n} \left( \frac{1}{k} + \frac{1}{n-k} \right), \quad \frac{1}{(k-1)(n+1-k)} = \frac{1}{n} \left( \frac{1}{k-1} + \frac{1}{n+1-k} \right)$$

we obtain

$$\Phi(n, 0) = \frac{a^2}{16n^2} \sum_{i=1}^4 D_i(n), \tag{4.20}$$

where

$$D_1(n) = \sum_{k=2}^{n-1} \frac{1}{k(k-1)}, \quad D_2(n) = \sum_{k=2}^{n-1} \frac{1}{(n-k)(n+1-k)},$$

$$D_3(n) = \sum_{k=2}^{n-1} \frac{1}{k(n+1-k)}, \quad D_4(n) = \sum_{k=2}^{n-1} \frac{1}{(k-1)(n-k)}.$$

The change of summation index  $m = n + 1 - k$  shows that  $D_2(n) = D_1(n)$ , and we have

$$D_1(n) = \sum_{k=2}^{n-1} \left( \frac{1}{k-1} - \frac{1}{k} \right) = 1 - \frac{1}{n-1} = 1 - \frac{1}{n} + O\left(\frac{1}{n^2}\right). \tag{4.21}$$

Moreover, since

$$D_3(n) = \frac{1}{n+1} \left( \sum_{k=2}^{n-1} \frac{1}{k} + \sum_{k=2}^{n-1} \frac{1}{n+1-k} \right) = \frac{2}{n+1} \sum_{k=2}^{n-1} \frac{1}{k},$$

by (4.9) we obtain that

$$D_3(n) = \frac{2 \log n}{n} + \frac{2(g-1)}{n} - \frac{2 \log n}{n^2} + O\left(\frac{1}{n^2}\right). \tag{4.22}$$

Similarly,

$$D_4(n) = \frac{1}{n-1} \left( \sum_{m=1}^{n-2} \frac{1}{m} + \sum_{m=1}^{n-2} \frac{1}{n-m-1} \right) = \frac{2}{n-1} \sum_{m=1}^{n-2} \frac{1}{m},$$

and (4.9) leads to

$$D_4(n) = \frac{2 \log n}{n} + \frac{2g}{n} + \frac{2 \log n}{n^2} + O\left(\frac{1}{n^2}\right). \tag{4.23}$$

Hence, in view of (4.20)–(4.23), we obtain (4.19).  $\square$

**Proposition 12.** *We have*

$$\beta_n(z_n^\pm) = \sigma_0(n, 0) \left[ 1 + \frac{a^2}{8n^2} - \frac{a^2}{4n^3} + O\left(\frac{1}{n^4}\right) \right]. \tag{4.24}$$

**Proof.** From (4.10), (4.12), (4.17) and (4.19) it follows immediately that

$$\sigma_1(n, z_n^\pm) + \sigma_0(n, z_n^\pm) = \sigma_0(n, 0) \left[ 1 + \frac{a^2}{8n^2} - \frac{a^2}{4n^3} + O\left(\frac{1}{n^4}\right) \right].$$

Since  $\beta_n(z) = \sum_{p=0}^\infty \sigma_p(n, z)$ , in view of (4.10) to complete the proof it is enough to show that

$$\sum_{p=2}^\infty \sigma_p(n, z_n^\pm) = \sigma_0(n, z_n^\pm) O\left(\frac{1}{n^4}\right). \tag{4.25}$$

Next we prove (4.25). Recall that  $\sigma_p(n, z) = \sum_{x \in X_n(p)} h(x, z)$ . Now we set

$$\sigma_p^*(n, z) = \sum_{x \in X_n(p)} |h(x, z)|.$$

We are going to show that there is an absolute constant  $C > 0$  such that

$$\sigma_p^*(n, z_n^\pm) \leq \sigma_{p-1}^*(n, z_n^\pm) \cdot \frac{C}{n^2}, \quad p \in \mathbb{N}, \quad n \geq N_0. \tag{4.26}$$

Since  $\sigma_0(n, z)$  has one term only, we have  $\sigma_0^*(n, z) = |\sigma_0(n, z)|$ .

Let  $p \in \mathbb{N}$ . To every walk  $x \in X_n(p)$  we assign a pair  $(\tilde{x}, j)$ , where  $\tilde{x} \in X_n(p - 1)$  is the walk that we obtain after dropping the first cycle  $\{+2, -2\}$  from  $x$ , and  $j$  is the vertex of  $x$  where the first negative step of  $x$  is performed. In other words, we consider the map

$$\varphi : X_n(p) \longrightarrow X_n(p - 1) \times I, \quad I = \{-n + 4, -n + 6, \dots, n - 2\},$$

defined by  $\varphi(x) = (\tilde{x}, j)$ , where

$$\tilde{x}(t) = \begin{cases} x(t) & \text{if } 1 \leq t \leq k - 1 \\ x(t + 2) & \text{if } k \leq t \leq n + 2p - 2 \end{cases},$$

where  $k = \min\{t : x(t) = 2, x(t + 1) = -2\}$  and  $j = -n + 2k$ .

The map  $\varphi$  is clearly injective, and moreover, we have

$$h(x, z) = h(\tilde{x}, z) \frac{a^2}{(n^2 - j^2 + z)(n^2 - (j - 2)^2 + z)}. \tag{4.27}$$

Since the mapping  $\varphi$  is injective, from (4.14), (4.18) and (4.27) it follows that

$$\sigma_p^*(n, z) \leq \sigma_{p-1}^*(n, z) \cdot \Phi^*(n, z). \tag{4.28}$$

Hence, by (4.18) and (4.19), we obtain that (4.26) holds.

From (4.26) it follows (since  $\sigma_0^*(n, z_n^\pm) = |\sigma_0(n, z_n^\pm)|$ ) that

$$\sigma_p^*(n, z_n^\pm) \leq |\sigma_0(n, z_n^\pm)| \cdot \left(\frac{C}{n^2}\right)^p.$$

Hence, (4.25) holds, which completes the proof.  $\square$

**Theorem 13.** *The Mathieu operator*

$$L(y) = -y'' + 2a \cos(2x)y, \quad a \in \mathbb{C}, \quad a \neq 0,$$

considered with periodic or anti-periodic boundary conditions has, close to  $n^2$  for large enough  $n$ , two periodic (if  $n$  is even) or anti-periodic (if  $n$  is odd) eigenvalues  $\lambda_n^-, \lambda_n^+$ . For fixed nonzero  $a \in \mathbb{C}$ ,

$$\lambda_n^+ - \lambda_n^- = \pm \frac{8(a/4)^n}{[(n - 1)!]^2} \left[ 1 - \frac{a^2}{4n^3} + O\left(\frac{1}{n^4}\right) \right], \quad n \rightarrow \infty. \tag{4.29}$$

**Proof.** The basic equation (2.15) splits into two equations

$$z - \alpha_n(z) - \beta_n(z) = 0, \tag{4.30}$$

$$z - \alpha_n(z) + \beta_n(z) = 0. \tag{4.31}$$

In view of (3.3) and (3.12), it follows that for large enough  $n$

$$|z - \alpha_n(z) \pm \beta_n(z)| < |z| \quad \text{if } |z| = 1.$$

Hence, for large enough  $n$ , each of the equations (4.30) and (4.31) has only one root in the unit disc due to Rouché's theorem.

On the other hand, by Lemmas 1 and 2, for large enough  $n$  the basic equation has exactly two roots  $z_n^-, z_n^+$  in the unit disc, so either  $z_n^-$  is the root of (4.30) and  $z_n^+$  is the root of (4.31), or  $z_n^+$  is the root of (4.30) and  $z_n^-$  is the root of (4.31). Therefore, we obtain

$$z_n^+ - z_n^- - [\alpha_n(z_n^+) - \alpha_n(z_n^-)] = \pm[\beta_n(z_n^+) + \beta_n(z_n^-)].$$

Now, (3.25) and (4.24) imply, with  $\gamma_n = \lambda_n^+ - \lambda_n^-$ ,

$$\gamma_n \left[ 1 + \frac{a^2}{8n^2} + O\left(\frac{1}{n^4}\right) \right] = \pm 2\sigma_0(n, 0) \left[ 1 + \frac{a^2}{8n^2} - \frac{a^2}{4n^3} + O\left(\frac{1}{n^4}\right) \right].$$

Therefore,

$$\begin{aligned}\gamma_n &= \pm 2\sigma_0(n, 0) \left[ 1 + \frac{a^2}{8n^2} - \frac{a^2}{4n^3} + O\left(\frac{1}{n^4}\right) \right] \left[ 1 - \frac{a^2}{8n^2} + O\left(\frac{1}{n^4}\right) \right] \\ &= \pm 2\sigma_0(n, 0) \left[ 1 - \frac{a^2}{4n^3} + O\left(\frac{1}{n^4}\right) \right].\end{aligned}$$

Hence, in view of (4.8), (4.29) holds.  $\square$

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