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Analysis on the derivative of the discriminant polynomial for the critical almost Mathieu operator

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Abstract. This article first introduces the discriminant polynomial and the central spectral band of the critical almost Mathieu operator. The Hardy–Littlewood method and the symbolic coding of continued fractions are introduced and applied to estimate the first-order and the second-order derivatives of the discriminant polynomial. Finally, these results are applied to obtain a lower bound for the measure of the central spectral band.

1. Introduction

Given $\alpha, \lambda, \theta \in \mathbb{R}$, the *almost Mathieu operator* is a discrete Schrödinger operator on $\ell^2(\mathbb{Z})$ which is defined by

$$(H\phi)(n) = \phi(n+1) + \phi(n-1) + \lambda \cos(2\pi\alpha n + \theta)\phi(n).$$

The condition $\lambda = 2$ is critical and the critical almost Mathieu operator is also known as *Harper's equation* or the *Azbel–Hofstadter model* in modern physics. The spectrum of the almost Mathieu operator $\sigma(\alpha, \lambda, \theta)$ is an important mathematical object with abundant spectral properties, which are related to number theory and fractal geometry. Moreover, the almost Mathieu operator describes the motion of an electron in a one-dimensional lattice under the potential, and it has deep connections with various fields of modern physics, such as quasi-crystals and the quantum Hall effect.

The almost Mathieu operator has been a subject of mathematical research. J. Bellissard and B. Simon applied the integrated density of states and the Baire category theorem to construct a dense G_δ set of $(\alpha, \lambda) \in \mathbb{R}^2$ (see [3]). For any (α, λ) in this set, they proved that the spectrum $\sigma(\alpha, \lambda, \theta)$ is a Cantor set. A. Avila and S. Jitomirskaya solved the Ten-Martini problem [1]. They demonstrated that the spectrum $\sigma(\alpha, \lambda, \theta)$ is a Cantor set for $\lambda \neq 0, \alpha \in \mathbb{Q}^c$ and $\theta \in \mathbb{R}$. The measure of the spectrum has also been studied. Y. Last demonstrated that $|\sigma(\alpha, \lambda, \theta)| = |4 - 2|\lambda||$, when

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$\lambda, \theta \in \mathbb{R}$, and $\alpha \in (0,1) \cap \mathbb{Q}^c$ can be approximated by a sequence of rationals p_n/q_n $(n \geq 1)$ with $q_n^2|\alpha - p_n/q_n| \to 0$ $(n \to \infty)$, see [8]. Jitomirskaya and I. Krasovsky proved that $|\sigma(\alpha, \lambda, \theta)| = |4 - 2|\lambda||$ for $\lambda \neq \pm 2, \theta \in \mathbb{R}$ and $\alpha \in (0,1) \cap \mathbb{Q}^c$, see [5]. Avila and R. Krikorian solved the critical condition $|\sigma(\alpha, \pm 2, \theta)| = 0$, when $\theta \in \mathbb{R}$ and α has the constant type [2]. The works [2, 5, 8] completed the Aubry–André conjecture. The Hausdorff dimension of the spectrum has also been studied under the critical condition. Last and M. Shamis applied the Green function to construct a refining family of covering intervals over the spectrum, which implies $\dim_H(\sigma(\alpha, 2, \theta)) = 0$ for a dense G_δ set of $\alpha \in \mathbb{R}$ (see [9]). Jitomirskaya and Krasovsky proved that $\dim_H(\sigma(\alpha, 2, \theta)) \leq 1/2$ for $\alpha \in (0,1) \cap \mathbb{Q}^c$ and $\theta \in \mathbb{R}$ (see [6]). B. Helffer, Q. Liu, Y. Qu, and Q. Zhou constructed a dense subset $\mathcal{F} \subseteq (0,1) \cap \mathbb{Q}^c$ with positive Hausdorff dimension, and they demonstrated that $\dim_H(\sigma(\alpha, 2, \theta)) > 0$ for any $\theta \in \mathbb{R}$ and $\alpha \in \mathcal{F}$ (see [4]).

The discriminant polynomial is an essential notion in the analysis of the critical almost Mathieu operator, which has a close connection to the spectrum. Krasovsky applied the Hardy–Littlewood method to derive a bound for the first-order derivative of the discriminant polynomial when the angular velocity is of the form $\alpha = [o, e, e, \ldots, e]$ (see [7]). This article generalizes the method of Krasovsky to obtain a bound for the first-order and the second-order derivatives under the general condition. A lower bound for the measure of the central spectral band is also obtained. We introduce the discriminant polynomial and the central spectral band for the critical almost Mathieu operator in Section 2. We also derive explicit expressions for the derivatives of the discriminant polynomial (Proposition 2.1). The complete Hardy–Littlewood method is introduced in Section 3 and Section 4. We introduce the symbolic encoding of continued fractions in Section 5, which is applied to derive a bound for the first-order and the second-order derivatives of the discriminant polynomial (Theorem 5.1). Finally, this result is applied to obtain a lower bound for the measure of the central spectral band in Section 6 (Corollary 6.4).

2. Derivative of the discriminant polynomial

We first introduce the spectrum and the discriminant polynomial of the critical almost Mathieu operator. For $\alpha, \theta \in \mathbb{R}$, the critical almost Mathieu operator is

$$H: \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z}), \quad \phi \mapsto H\phi,$$

where

$$(H\phi)(n) = \phi(n+1) + \phi(n-1) + 2\cos(2\pi\alpha n + \theta)\phi(n).$$

The critical almost Mathieu operator is bounded and self-adjoint. The spectrum of the operator is denoted by $\sigma(\alpha, \theta) \subseteq \mathbb{R}$, which is nonempty and compact. For $m, n \in \mathbb{N}$, we denote by (m,n) their greatest common divisor. Given $\alpha = p/q \leq 1$ and $(p,q)=1$, we can define the discriminant polynomial

$$D_\alpha(x,\theta) = \mathrm{Tr}(M_{\alpha,\theta}(x,q)M_{\alpha,\theta}(x,q-1)\cdots M_{\alpha,\theta}(x,1)),$$

where the transition matrix is

$$M_{\alpha,\theta}(x,n) = \begin{pmatrix} x - 2\cos(2\pi\alpha n + \theta) & -1 \\ 1 & 0 \end{pmatrix}.$$

Chambers described the dependence of the discriminant polynomial on θ (see [3]), and we only need to study the special discriminant polynomial $\sigma_\alpha(x) = D_\alpha(x,\pi/2q)$. The spectrum can be described by the discriminant polynomial. The union of the spectrum $\sigma(\alpha,\theta)$ over $\theta \in \mathbb{R}$ is defined to be $S(\alpha)$ and we have $S(\alpha) = \sigma_\alpha^{-1}([-4,4])$. The discriminant polynomial $\sigma_\alpha(x)$ has q distinct real roots. Around each root, the preimage of $[-4,4]$ is a closed band. The discriminant polynomial $\sigma_\alpha(x)$ is an odd function when q is odd, and it is an even function when q is even. This implies that these closed bands are symmetric about the origin. When q is odd, the central spectral band is the closed band containing the origin. When q is even, the origin is a common endpoint of the left band and the right band. Under this condition, we define the central spectral band to be the union of the left band and the right band. As we will see, the measure of the central spectral band can be described by the derivatives $\sigma'_\alpha(0)$ and $\sigma''_\alpha(0)$.

We now calculate the expression for the derivative of the discriminant polynomial. When $p = q = 1$, the discriminant polynomial is $\sigma_\alpha(x) = x$. We consider the condition $p < q$ and $(p,q) = 1$. Given $\varphi = \alpha\pi$, we suppose that A is a q-order matrix with $A(n,n+1) = A(n+1,n) = 2\sin(n\varphi)$ (for $1 \leq n \leq q-1$) and the other elements are zero. By the chiral gauge transformation [6], we have $\sigma_\alpha(x) = \det(xI - A)$. By the parity of the discriminant polynomial, we have $\sigma'_\alpha(0) = 0$ when q is even and $\sigma''_\alpha(0) = 0$ when q is odd. The following proposition completes the expression of the first-order and the second-order derivatives. Proposition 2.1 (1) summarizes relevant results in [7], and Proposition 2.1 (2) deals with the second-order condition.

Proposition 2.1. *The following statements hold true.*

(1) *Suppose $\alpha = p/q$ with $p < q$ and $(p,q) = 1$. Denote $\varphi = \alpha\pi$ and let $\sigma_\alpha(x)$ be the discriminant polynomial of the critical almost Mathieu operator. When q is odd, we denote $r = (q-1)/2$ and we have*

$$|\sigma'_\alpha(0)| = \sum_{\gamma=0}^{r} e^{L_\gamma} \tag{1}$$

where $L_\gamma = \sum_{n=1}^{r} 2\ln|2\sin(2(n+\gamma)\varphi)|$.

(2) *Suppose* $\alpha = p/q$ *with* $p < q$ *and* $(p, q) = 1$. *Denote* $\varphi = \alpha\pi$ *and let* $\sigma_\alpha(x)$ *be the discriminant polynomial of the critical almost Mathieu operator. When* q *is even, we have*

$$|\sigma''_\alpha(0)| = \sum_{2\nmid\mu, 2|\nu, 1\le\mu<\nu\le q} 2e^{L_{\mu\nu}} \tag{2}$$

where $L_{\mu\nu} = \sum_n^{(\mu,\nu)} 2\ln|2\sin(n\varphi)|$ *and the summation is defined by*

$$\sum_n^{(\mu,\nu)} = \sum_{2\nmid n, 1\le n\le\mu-2} + \sum_{2|n, \mu+1\le n\le\nu-2} + \sum_{2\nmid n, \nu+1\le n\le q-1}.$$

Proof. We suppose P is an $(m+1)$-order matrix with $P(n, n+1) = P(n+1, n) = a_n$ (for $1 \le n \le m$) and that the other elements are zero. By Laplace's expansion of the determinant, we demonstrate $\det(P) = 0$ when m is even and

$$\det(P) = \prod_{2\nmid n, 1\le n\le m} (-a_n^2)$$

when m is odd. This observation enables us to calculate the derivative of the discriminant polynomial.

(1) Suppose q is odd and denote $r = (q-1)/2$. For the determinant $\det(xI - A)$, we calculate the derivative of the m-th column and take $x = 0$ (for $1 \le m \le q$). We thus obtain two submatrices and the determinants of them are nonzero only when m is odd. We have

$$\sigma'_\alpha(0) = (-1)^r \sum_{\gamma=0}^{r} \Big(\prod_{n=1}^{\gamma} 2\sin((2n-1)\varphi) \prod_{n=\gamma+1}^{r} 2\sin(2n\varphi) \Big)^2$$

and $|\sigma'_\alpha(0)| = \sum_{\gamma=0}^{r} e^{L_\gamma}$, where

$$\begin{aligned} L_\gamma &= \sum_{n=1}^{\gamma} 2\ln|2\sin((2n-1)\varphi)| + \sum_{n=\gamma+1}^{r} 2\ln|2\sin(2n\varphi)| \\ &= \sum_{n=1}^{\gamma} 2\ln|2\sin((2n-1)\varphi)| + \sum_{n=\gamma-r+1}^{0} 2\ln|2\sin((2n-1)\varphi)| \\ &= \sum_{n=1}^{r} 2\ln|2\sin(2(n+\gamma)\varphi)|. \end{aligned}$$

The proof of equation (1) is completed.

(2) Suppose that q is even. The proof is similar to that of (1). By calculating the derivative of the determinant, we have

$$\sigma_\alpha''(0) = 2 \sum_{1\le\mu<\nu\le q}^{2\nmid\mu,2|\nu} \prod_n^{(\mu,\nu)} (-(2\sin(n\varphi))^2)$$

where

$$\prod_n^{(\mu,\nu)} = \prod_{1\le n\le\mu-2}^{2\nmid n} \cdot \prod_{\mu+1\le n\le\nu-2}^{2|n} \cdot \prod_{\nu+1\le n\le q-1}^{2\nmid n} .$$

We further have

$$|\sigma_\alpha''(0)| = \sum_{2\nmid\mu,2|\nu,1\le\mu<\nu\le q} 2e^{L_{\mu\nu}}$$

where $L_{\mu\nu} = \sum_n^{(\mu,\nu)} 2\ln|2\sin(n\varphi)|$. ∎

To obtain an upper bound of the derivatives $|\sigma_\alpha'(0)|$ and $|\sigma_\alpha''(0)|$, we need to estimate the terms L_γ and $L_{\mu\nu}$ given in Proposition 2.1. I. Krasovsky derived an upper bound of L_γ in [7]. We review the method of I. Krasovsky and generalize it to estimate the term $L_{\mu\nu}$. For $x \in (0,\pi)$, we define $f(x) = \ln(2\sin(x))$ and we have $f \in L^2((0,\pi))$. We first calculate the Fourier transformation of $f(x)$, which is given in the following proposition.

Proposition 2.2. *For $x \in (0,\pi)$, we define the function $f(x) = \ln(2\sin(x))$. We have $f \in L^2((0,\pi))$ and its Fourier transformation is*

$$f(x) = -\sum_{n=1}^{\infty} \frac{\cos(2nx)}{n}.$$

Proof. The set $(e^{2inx})_{n\in\mathbb{Z}}$ is an orthogonal basis of the Hilbert space $L^2((0,\pi))$. We denote the Fourier transformation by $f(x) = \sum_{n\in\mathbb{Z}} a(n)e^{2inx}$, where

$$a(n) = \frac{1}{\pi}\int_0^\pi f(x)e^{-2inx}\,\mathrm{d}x = \frac{1}{\pi}\int_0^\pi \ln(2\sin(x))\cos(2nx)\,\mathrm{d}x.$$

The Fourier transformation is convergent everywhere since $f(x)$ is smooth on $(0,\pi)$. To calculate the coefficient $a(0)$, we introduce the integral

$$I = \int_0^{\frac{\pi}{2}} \ln(\sin(x))\,\mathrm{d}x = \int_0^{\frac{\pi}{2}} \ln(\cos(x))\,\mathrm{d}x$$

and we have

$$a(0) = \frac{1}{\pi}\int_0^\pi \ln(2\sin(x))\,\mathrm{d}x = \ln(2) + \frac{1}{\pi}\int_0^\pi \ln(\sin(x))\,\mathrm{d}x = \ln(2) + \frac{2I}{\pi}.$$

We consider the integral

$$\int_0^{\frac{\pi}{2}} \ln(\sin(2x))\,\mathrm{d}x = \int_0^{\frac{\pi}{2}} \ln(2) + \ln(\sin(x)) + \ln(\cos(x))\,\mathrm{d}x = 2I + \frac{\pi\ln(2)}{2}, \quad (3)$$

which is also equal to

$$\int_0^{\frac{\pi}{2}} \ln(\sin(2x))\,\mathrm{d}x = \frac{1}{2}\int_0^{\pi} \ln(\sin(x))\,\mathrm{d}x = \int_0^{\frac{\pi}{2}} \ln(\sin(x))\,\mathrm{d}x = I. \quad (4)$$

Combining equations (3) and (4), we obtain $I = -\pi\ln(2)/2$ and $a(0) = 0$. We continue to calculate other coefficients. Given $n \geq 1$, we have

$$\begin{aligned} a(\pm n) &= -\frac{1}{2n\pi}\int_0^\pi \frac{\sin(2nx)\cos(x)}{\sin(x)}\,\mathrm{d}x \\ &= -\frac{1}{2n\pi}\int_0^\pi \frac{\sin((2n+1)x) + \sin((2n-1)x)}{2\sin(x)}\,\mathrm{d}x \\ &= -\frac{1}{4n\pi}\left(2\pi + \sum_{m=1}^{n}\int_0^\pi 2\cos(2mx)\,\mathrm{d}x + \sum_{m=1}^{n-1}\int_0^\pi 2\cos(2mx)\,\mathrm{d}x\right) \\ &= -\frac{1}{2n} \end{aligned}$$

where we use the identities

$$\begin{aligned} \sum_{m=1}^{n} 2\sin(x)\cos(2mx) &= \sum_{m=1}^{n} \sin((2m+1)x) - \sin((2m-1)x) \\ &= \sin((2n+1)x) - \sin(x). \end{aligned}$$

Combining the results above, we obtain the Fourier transformation of $f(x)$. ■

By the Fourier transformation of $f(x)$, we can transform the terms L_γ and $L_{\mu\nu}$ in Proposition 2.1 to another form. Suppose $\alpha = p/q$ with $p < q$ and $(p, q) = 1$.

We denote $\varphi = \alpha\pi$ and we first consider the condition when q is odd. Combining Proposition 2.1 and Proposition 2.2, we obtain

$$L_\gamma = -\sum_{n=1}^{r}\sum_{m=1}^{\infty}\frac{2\cos(4m(n+\gamma)\varphi)}{m}$$

where $r = (q-1)/2$ and $0 \le \gamma \le r$. For $0 \le \gamma \le r$ and $1 \le m \le q-1$, we define

$$F_\gamma(m) = -\sum_{n=1}^{r} 2\cos(4(n+\gamma)m\varphi),\ S_\gamma = \sum_{m=1}^{q-1}\frac{F_\gamma(m)}{m}. \tag{5}$$

We represent $m \in \mathbb{N}$ in the form $m = aq + t$, where $1 \le t \le q-1$ for $a = 0$ and $0 \le t \le q-1$ for $a \ge 1$. We thus obtain the expression

$$\begin{aligned} L_\gamma = \sum_{m=1}^{\infty}\frac{F_\gamma(m)}{m} &= S_\gamma + \sum_{a=1}^{\infty}\sum_{t=0}^{q-1}\frac{F_\gamma(aq+t)}{aq+t} \\ &= S_\gamma - \sum_{a=1}^{\infty}\Big(\frac{q-1}{qa} - \frac{1}{q}\sum_{t=1}^{q-1}\frac{F_\gamma(t)}{a+t/q}\Big). \end{aligned} \tag{6}$$

The following proposition is summarized from [7] which studies properties of the term $F_\gamma(m)$.

Proposition 2.3. *Denote $\alpha = p/q$ and $\varphi = \alpha\pi$, where $p < q, (p,q) = 1$ and q is odd. For $0 \le \gamma \le r$ and $1 \le m \le q-1$, define $F_\gamma(m)$ by equation (5). We have*

$$F_\gamma(m) = \frac{\cos((4\gamma+1)m\varphi)}{\cos(m\varphi)}$$

and

$$\sum_{m=1}^{q-1} F_\gamma(m) = q-1.$$

Proof. (1) Given $0 \le \gamma \le r$ and $1 \le m \le q-1$, denote $\phi = m\varphi$. We have $1 - e^{4i\phi} \ne 0$. By direct calculation, we have

$$\begin{aligned} F_\gamma(m) &= -\sum_{n=1}^{r}\mathrm{Re}(2e^{4i(n+\gamma)\phi}) \\ &= \mathrm{Re}\Big(2e^{4i\gamma\phi}\frac{e^{2i\phi} - e^{4i\phi}}{1-e^{4i\phi}}\Big) \\ &= \mathrm{Re}\Big(\frac{e^{4i(1+\gamma)\phi} - e^{4i(1/2+\gamma)\phi} - e^{4i\gamma\phi} + e^{4i(\gamma-1/2)\phi}}{\cos(4\phi)-1}\Big). \end{aligned}$$

By the trigonometric identities, we also obtain

$$F_\gamma(m) = \frac{\cos((4\gamma+4)\phi) - \cos((4\gamma+2)\phi) - \cos(4\gamma\phi) + \cos((4\gamma-2)\phi)}{\cos(4\phi)-1}$$
$$= \frac{2\sin(\phi)\sin((4\gamma-1)\phi) - 2\sin(\phi)\sin((4\gamma+3)\phi)}{\cos(4\phi)-1}$$
$$= \frac{2\sin(\phi)\sin(2\phi)\cos((4\gamma+1)\phi)}{\sin^2(2\phi)} = \frac{\cos((4\gamma+1)\phi)}{\cos(\phi)}.$$

(2) Given $0 \le \gamma \le r$, we have

$$\sum_{m=1}^{q-1} F_\gamma(m) = -\mathrm{Re}\Big(\sum_{n=1}^{r}\sum_{m=1}^{q-1} 2e^{4i(n+\gamma)\phi}\Big)$$
$$= -\mathrm{Re}\Big(\sum_{n=1}^{r} \frac{2(e^{4i(n+\gamma)\varphi} - e^{4i(n+\gamma)q\varphi})}{1-e^{4i(n+\gamma)\varphi}}\Big) = q-1,$$

and the proof is completed. ■

Suppose $\alpha = p/q$ with $p<q$ and $(p,q)=1$. We now consider the condition when q is even. Combining Proposition 2.1 and Proposition 2.2, we obtain

$$L_{\mu\nu} = -2\sum_{n}^{(\mu,\nu)}\sum_{m=1}^{\infty}\frac{\cos(2nm\varphi)}{m}.$$

Given $1 \le m \le q-1$ and $1 \le \mu < \nu \le q$, we assume μ is odd and ν is even. We define

$$F_{\mu\nu}(m) = -\sum_{n}^{(\mu,\nu)} 2\cos(2nm\varphi),\ S_{\mu\nu} = \sum_{m=1}^{q-1}\frac{F_{\mu\nu}(m)}{m}. \tag{7}$$

Similarly, we represent $m \in \mathbb{N}$ in the form $m = aq+t$ where $1 \le t \le q-1$ for $a=0$ and $0 \le t \le q-1$ for $a \ge 1$. We obtain the expression

$$L_{\mu\nu} = \sum_{m=1}^{\infty}\frac{F_{\mu\nu}(m)}{m} = S_{\mu\nu} + \sum_{a=1}^{\infty}\sum_{t=0}^{q-1}\frac{F_{\mu\nu}(aq+t)}{aq+t}$$
$$= S_{\mu\nu} - \sum_{a=1}^{\infty}\Big(\frac{2N_{\mu\nu}}{qa} - \frac{1}{q}\sum_{t=1}^{q-1}\frac{F_{\mu\nu}(t)}{a+t/q}\Big), \tag{8}$$

where $N_{\mu\nu} = \sum_{n}^{(\mu,\nu)} 1$. The following proposition shows the properties of the term $F_{\mu\nu}(m)$.

Proposition 2.4. *Denote $\alpha = p/q, \varphi = \alpha\pi$, where $p < q, (p, q) = 1$ and q is even. Given $1 \le m \le q-1$ and $1 \le \mu < \nu \le q$, we assume μ is odd and ν is even. We define $F_{\mu\nu}(m)$ by equation (7). We have $F_{\mu\nu}(q/2) = 2\mu - 2\nu + q$ and $F_{\mu\nu}(m) = (\cos((2\mu-1)m\varphi) + \cos((2\nu-1)m\varphi))/\cos(m\varphi)$ when $m \ne q/2$. Moreover, we have*

$$\sum_{m=1}^{q-1} F_{\mu\nu}(m) = 2N_{\mu\nu}.$$

Proof. (1) The calculation is similar to that in Proposition 2.3. Since $(p, q) = 1$ and q is even, we demonstrate that p is odd and we have

$$\begin{aligned}F_{\mu\nu}(q/2) &= -\sum_{n}^{(\mu,\nu)} 2\cos(\pi n p)\\ &= 2\Big(\frac{\mu-3}{2}+1\Big) - 2\Big(\frac{\nu-\mu-3}{2}+1\Big) + 2\Big(\frac{q-\nu-2}{2}+1\Big)\\ &= 2\mu - 2\nu + q.\end{aligned}$$

We now consider the condition $m \ne q/2$. Denote $\phi = m\varphi$. We have $1 - e^{4i\phi} \ne 0$. We define

$$G_{\mu\nu}(m) = \sum_{n}^{(\mu,\nu)} e^{2in\phi},$$

and we have $F_{\mu\nu}(m) = -\mathrm{Re}(2G_{\mu\nu}(m))$. By direct calculation, we have

$$\begin{aligned}(1-e^{4i\phi})G_{\mu\nu}(m) &= e^{2i\phi} - e^{2i\mu\phi} + e^{2i(\mu+1)\phi} - e^{2i\nu\phi} + e^{2i(\nu+1)\phi} - e^{2i(q+1)\phi}\\ &= (e^{2i\phi}-1)(e^{2i\mu\phi} + e^{2i\nu\phi})\end{aligned}$$

and

$$G_{\mu\nu}(m) = G_\mu(m) + G_\nu(m),$$

where

$$G_\mu(m) = \frac{e^{2i\mu\phi}(e^{2i\phi}-1)(1-e^{-4i\phi})}{2-2\cos(4\phi)},$$

$$G_\nu(m) = \frac{e^{2i\nu\phi}(e^{2i\phi}-1)(1-e^{-4i\phi})}{2-2\cos(4\phi)}.$$

We first consider the term $G_\mu(m)$. By the trigonometric identities, we have

$$\begin{aligned}&\mathrm{Re}(e^{2i\mu\phi}(e^{2i\phi}-1)(1-e^{-4i\phi}))\\ &= \cos(2(\mu+1)\phi) - \cos(2(\mu-1)\phi) - \cos(2\mu\phi) + \cos(2(\mu-2)\phi)\\ &= 2\sin(2\phi)(\sin(2(\mu-1)\phi) - \sin(2\mu\phi))\end{aligned}$$

and we thus obtain

$$\mathrm{Re}(G_\mu(m)) = \frac{\sin(2(\mu-1)\phi) - \sin(2\mu\phi)}{2\sin(2\phi)} = -\frac{\cos((2\mu-1)\phi)}{2\cos(\phi)}.$$

Similarly, we have $\mathrm{Re}(G_\nu(m)) = -\cos((2\nu-1)\phi)/(2\cos(\phi))$. Combining the results above, we have $F_{\mu\nu}(m) = (\cos((2\mu-1)\phi) + \cos((2\nu-1)\phi))/\cos(\phi)$.

(2) By direct calculation, we have

$$\begin{aligned}\sum_{m=1}^{q-1} F_{\mu\nu}(m) &= -\mathrm{Re}\Big(\sum_{m=1}^{q-1}\sum_{n}^{(\mu,\nu)} 2e^{2in\phi}\Big)\\ &= -\mathrm{Re}\Big(\sum_{n}^{(\mu,\nu)}\sum_{m=1}^{q-1} 2e^{2in\phi}\Big) = 2N_{\mu\nu},\end{aligned}$$

and the proof is completed. ■

Before we obtain an upper bound of the terms L_γ and $L_{\mu\nu}$, we first review the definition and the properties of the ψ-function. Euler's constant is denoted by

$$\gamma_0 = \lim_{m\to\infty}\sum_{n=1}^{m}\frac{1}{n} - \ln(m)$$

and we have $\gamma_0 \in (1/2, 1)$. For $x > 0$, we define the Gamma function and the ψ-function

$$\Gamma(x) = \int_0^{+\infty} t^{x-1}e^{-t}\,\mathrm{d}t, \quad \psi(x) = \Gamma'(x)/\Gamma(x).$$

The ψ-function has the following properties:

(1) for $x > 0$, we have $\psi(x+1) = \psi(x) + 1/x$;

(2) for $x \geq 0$, we have $\psi(x+1) = \sum_{n=1}^{\infty}(1/n - 1/(n+x)) - \gamma_0$;

(3) for $x \in [1,2]$, we have $\psi'(x) \geq 0$ and the function is non-decreasing. Since $\psi(1) = -\gamma_0$ and $\psi(2) = \psi(1) + 1 = 1 - \gamma_0$, we also have $|\psi(x)| \leq \gamma_0$.

Now, we are able to obtain an upper bound of the terms L_γ and $L_{\mu\nu}$ in the following theorem.

Theorem 2.5. *The following statements hold true.*

(1) *Given $(p,q) = 1$, with $q > p$ and q odd, we denote $r = (q-1)/2$. For $0 \leq \gamma \leq r$, the definitions of L_γ and S_γ are given by equations (1) and (5). We have*

$$L_\gamma \leq \gamma_0(\ln(q) + 2) + |S_\gamma|.$$

(2) *Suppose* $(p,q)=1$, *with* $q>p$ *and* q *even. Given* $1\le\mu<\nu\le q$, *we assume* μ *is odd and* ν *is even. The definitions of* $L_{\mu\nu}$ *and* $S_{\mu\nu}$ *are given by equations* (2) *and* (7). *We have*

$$L_{\mu\nu}\le 2\gamma_0(\ln(q)+3)+|S_{\mu\nu}|.$$

Proof. (1) We first assume q is odd and we take $0\le\gamma\le r$. The proof is an application of the ψ-function and equation (6). For $x\ge 0$, the properties of the ψ-function show that

$$\begin{aligned}\lim_{m\to\infty}\sum_{n=1}^{m}\frac{1}{n+x}-\ln(m)&=\lim_{m\to\infty}\sum_{n=1}^{m}\Big(\frac{1}{n+x}-\frac{1}{n}\Big)+\lim_{m\to\infty}\sum_{n=1}^{m}\frac{1}{n}-\ln(m)\\&=-\psi(x+1).\end{aligned}\tag{9}$$

Combining equations (6) and (9), we obtain

$$\begin{aligned}&L_\gamma-S_\gamma\\&=-\lim_{m\to\infty}\Big(\frac{q-1}{q}\Big(\sum_{n=1}^{m}\frac{1}{n}-\ln(m)\Big)-\frac{1}{q}\sum_{t=1}^{q-1}F_\gamma(t)\Big(\sum_{n=1}^{m}\frac{1}{n+\frac{t}{q}}-\ln(m)\Big)\Big)\\&=-\frac{\gamma_0(q-1)}{q}-\frac{1}{q}\sum_{t=1}^{q-1}F_\gamma(t)\psi\Big(1+\frac{t}{q}\Big),\end{aligned}\tag{10}$$

where Proposition 2.3 is applied. We need to estimate the summation in equation (10). Since we have $|\psi(x)|\le\gamma_0(x\in[1,2])$, we obtain the inequality

$$\Big|\frac{1}{q}\sum_{t=1}^{q-1}F_\gamma(t)\psi\Big(1+\frac{t}{q}\Big)\Big|\le\frac{\gamma_0}{q}\sum_{t=1}^{q-1}|F_\gamma(t)|\le\frac{\gamma_0}{q}\sum_{t=1}^{q-1}\frac{1}{|\cos(\frac{\pi tp}{q})|}.$$

Note that $|\cos(\pi tp/q)|=|\cos(\pi(tp\pmod q)/q)|$. By the condition $(p,q)=1$, we also obtain

$$\begin{aligned}\frac{\gamma_0}{q}\sum_{t=1}^{q-1}\frac{1}{|\cos(\frac{\pi tp}{q})|}&=\frac{\gamma_0}{q}\sum_{t=1}^{q-1}\frac{1}{|\cos(\frac{\pi t}{q})|}=\frac{2\gamma_0}{q}\sum_{t=1}^{r}\frac{1}{|\cos(\frac{\pi t}{q})|}\\&=\frac{2\gamma_0}{q}\sum_{t=0}^{r-1}\frac{1}{|\cos(\frac{\pi(r-t)}{q})|}=\frac{2\gamma_0}{q}\sum_{t=0}^{r-1}\frac{1}{|\sin(\frac{\pi(2t+1)}{2q})|}\\&=\frac{4\gamma_0}{q}\sum_{t=0}^{r-1}\frac{1}{|1-e^{i\pi(2t+1)/q}|}.\end{aligned}$$

By the inequality $2x\le|1-e^{i\pi x}|(x\in[0,1])$, we have

$$\begin{aligned}\frac{4\gamma_0}{q}\sum_{t=0}^{r-1}\frac{1}{|1-e^{i\pi(2t+1)/q}|}&\le\gamma_0\sum_{t=0}^{r-1}\frac{1}{t+\frac{1}{2}}\le\gamma_0\Big(2+\int_0^{r-1}\frac{1}{x+\frac{1}{2}}\,dx\Big)\\&\le\gamma_0(\ln(q)+2).\end{aligned}$$

Combining the results above, we have

$$L_\gamma \le S_\gamma - \sum_{t=1}^{q-1} \frac{F_\gamma(t)\psi\left(1+\frac{t}{q}\right)}{q} \le \gamma_0(\ln(q)+2) + |S_\gamma|.$$

(2) We now assume q is even and the proof is similar to that in (1). Given $1 \le \mu < \nu \le q$, we assume μ is odd and ν is even. Combining equations (8) and (9), we have

$$\begin{aligned} &L_{\mu\nu} - S_{\mu\nu} \\ &\quad = -\lim_{m\to\infty}\Big(\frac{2N_{\mu\nu}}{q}\Big(\sum_{n=1}^{m}\frac{1}{n} - \ln(m)\Big) - \frac{1}{q}\sum_{t=1}^{q-1} F_{\mu\nu}(t)\Big(\sum_{n=1}^{m}\frac{1}{n+\frac{t}{q}} - \ln(m)\Big)\Big) \\ &\quad = -\frac{2N_{\mu\nu}\gamma_0}{q} - \frac{1}{q}\sum_{t=1}^{q-1} F_{\mu\nu}(t)\psi\left(1+\frac{t}{q}\right). \end{aligned}$$

By Proposition 2.4, we also have the inequality

$$\begin{aligned} \Big|\frac{1}{q}\sum_{t=1}^{q-1} F_{\mu\nu}(t)\psi\left(1+\frac{t}{q}\right)\Big| &\le \frac{\gamma_0}{q}\sum_{t=1}^{q-1}|F_{\mu\nu}(t)| \\ &\le \frac{\gamma_0}{q}\Big(|2\mu - 2\nu + q| + \sum_{t=1, t\neq q/2}^{q-1}\frac{2}{\left|\cos\left(\frac{\pi t p}{q}\right)\right|}\Big) \\ &\le \frac{\gamma_0}{q}\Big(3q + \sum_{t=1, t\neq q/2}^{q-1}\frac{2}{\left|\cos\left(\frac{\pi t p}{q}\right)\right|}\Big). \end{aligned}$$

Similar to the method in (1), we obtain

$$\begin{aligned} \frac{\gamma_0}{q}\sum_{t=1, t\neq q/2}^{q-1}\frac{1}{\left|\cos\left(\frac{\pi t}{q}\right)\right|} &= \frac{2\gamma_0}{q}\sum_{t=1}^{q/2-1}\frac{1}{\left|\sin\left(\frac{\pi t}{q}\right)\right|} = \frac{4\gamma_0}{q}\sum_{t=1}^{q/2-1}\frac{1}{|1-e^{2i\pi t/q}|} \\ &\le \gamma_0\sum_{t=0}^{q/2-2}\frac{1}{t+1} \le \gamma_0\Big(1 + \int_0^{q/2-2}\frac{1}{x+1}\,\mathrm{d}x\Big) \\ &\le \gamma_0(1+\ln(q)). \end{aligned}$$

Combining the results above, we have $L_{\mu\nu} \le S_{\mu\nu} - \sum_{t=1}^{q-1} F_{\mu\nu}(t)\psi(1+t/q)/q \le 2\gamma_0(\ln(q)+3) + |S_{\mu\nu}|$ and the proof is completed. ■

3. Hardy–Littlewood method (I)

To obtain an upper bound of the derivatives $|\sigma'_\alpha(0)|$ and $|\sigma''_\alpha(0)|$, Theorem 2.5 shows that we need to estimate the terms $|S_\gamma|$ and $|S_{\mu\nu}|$. I. Krasovsky applied the Hardy–Littlewood method to estimate the term $|S_\gamma|$ (see [7, 10]). In this section, we review and generalize the method of Krasovsky to estimate the term $|S_{\mu\nu}|$, which relies on a recursive computation of contour integrals. We first introduce some fundamental definitions.

(1) Suppose $(p,q)=1$, $q\ge p$, and $2\gamma\in[p/q,2+p/q]$. The contour

$$\Gamma(q)=\Gamma_1(q)\cup\Gamma_2(q)$$

consists of an upper line and a lower line which are given by

$$\Gamma_1(q)=2\pi i\Big(q-\frac{1}{4}\Big)+\mathbb{R},\quad \Gamma_2(q)=\frac{\pi i}{2}+\mathbb{R}.$$

The upper line $\Gamma_1(q)$ is oriented from $+\infty$ to $-\infty$ and the lower line $\Gamma_2(q)$ is oriented from $-\infty$ to $+\infty$. We define the integral

$$I(p,q,\gamma)=-2\int_{\Gamma(q)}\frac{e^{(1+p/q)z}}{(1+e^{pz/q})(1-e^z)}\frac{e^{-\gamma z}}{z}\,\mathrm{d}z. \tag{11}$$

Note that $(1+e^{pz/q})(1-e^z)\ne 0$ when $z\in\Gamma(q)$. Let $x>0$ and suppose $z_+=2\pi i(q-1/4)+x\in\Gamma_1(q)$ or $z_+=(1/2)\pi i+x\in\Gamma_2(q)$. When x is large enough, we have

$$\Big|\frac{e^{(1+p/q)z_+}}{(1+e^{pz_+/q})(1-e^{z_+})}\frac{e^{-\gamma z_+}}{z_+}\Big|\lesssim\frac{e^{-\gamma x}}{x}. \tag{12}$$

We also suppose $z_-=2\pi i(q-1/4)-x\in\Gamma_1(q)$ or $z_-=(1/2)\pi i-x\in\Gamma_2(q)$. When x is large enough, we have

$$\Big|\frac{e^{(1+p/q)z_-}}{(1+e^{pz_-/q})(1-e^{z_-})}\frac{e^{-\gamma z_-}}{z_-}\Big|\lesssim\frac{e^{-(1+p/q-\gamma)x}}{x}. \tag{13}$$

Inequalities (12) and (13) prove that the integral $I(p,q,\gamma)$ is well defined.

(2) Given $(p,q)=1$, $q\ge p$, $\delta\in\{0,1\}$ and $2\gamma\in[p/q,2+p/q]$, the contour $\Gamma(q)$ and its orientation have been given in (1). We define the integral

$$J(p,q,\gamma,\delta)=2\int_{\Gamma(q)}\frac{(-1)^\delta e^{(1+p/q)z}}{(1-(-1)^\delta e^{pz/q})(1+e^z)}\frac{e^{-\gamma z}}{z}\,\mathrm{d}z. \tag{14}$$

Note that $(1-(-1)^\delta e^{pz/q})(1+e^z)\ne 0$ when $z\in\Gamma(q)$. Similar to inequalities (12) and (13), we show that the integral $J(p,q,\gamma,\delta)$ is well defined.

(3) Suppose $(p,q)=1$, $q \ge p$, and $\gamma \in \mathbb{R}$. When q is odd, we have $\cos(\pi np/q) \neq 0$ (for $1 \le n \le q-1$), and we can define

$$S(p,q,\gamma) = \sum_{n=1}^{q-1} \frac{e^{\pi inp/q - 2\pi in\gamma}}{n\cos(\frac{\pi np}{q})}.$$

When q is even, we define

$$S'(p,q,\gamma) = \sum_{n=1, n\neq q/2}^{q-1} \frac{e^{\pi inp/q - 2\pi in\gamma}}{n\cos(\frac{\pi np}{q})}$$

and the denominator is also nonzero.

(4) Suppose $(p,q)=1$, $q \ge p$, $\gamma \in \mathbb{R}$, and $\delta \in \{0,1\}$. If q is even or $2 \mid (p-1+\delta)$, we can define

$$T(p,q,\gamma,\delta) = \sum_{n=1}^{q} \frac{(-1)^\delta e^{2\pi i(n-1/2)p/q}}{1-(-1)^\delta e^{2\pi i(n-1/2)p/q}} \frac{2e^{-2\pi i(n-1/2)\gamma}}{n-\frac{1}{2}}.$$

Note that the denominator $1-(-1)^\delta e^{2\pi i(n-1/2)p/q}$ is nonzero and $T(p,q,\gamma,\delta)$ is well defined. If q is odd, we can define

$$T'(p,q,\gamma,\delta) = \sum_{n=1, n\neq(q+1)/2}^{q} \frac{(-1)^\delta e^{2\pi i(n-1/2)p/q}}{1-(-1)^\delta e^{2\pi i(n-1/2)p/q}} \frac{2e^{-2\pi i(n-1/2)\gamma}}{n-\frac{1}{2}}$$

and the denominator is also nonzero.

(5) Given $\delta \in \{0,1\}$, we say that $(p,q) \in \mathbb{N}^2$ satisfies the δ-*condition* if (i) p is odd when $\delta = 0$ and (ii) p, q have different parities when $\delta = 1$. We say that $(p,q) \in \mathbb{N}^2$ satisfies the δ'-*condition* if (i) p is even when $\delta = 0$ and (ii) p, q have the same parity when $\delta = 1$.

To utilize the Hardy–Littlewood method, we first derive an upper bound of the integrals $|I(p,q,\gamma)|$ and $|J(p,q,\gamma,\delta)|$. We then calculate the residues of the integrals inside the contour $\Gamma(q)$, which displays the relation between $I(p,q,\gamma)$, $J(p,q,\gamma,\delta)$ and $S(p,q,\gamma)$, $T(p,q,\gamma,\delta)$ (or $S'(p,q,\gamma)$, $T'(p,q,\gamma,\delta)$). We thus obtain an upper bound for $|S(p,q,\gamma)|$, $|T(p,q,\gamma,\delta)|$ and $|S'(p,q,\gamma)|$, $|T'(p,q,\gamma,\delta)|$. In this section, we complete the analysis on the integral $I(p,q,\gamma)$; the analysis on the integral $J(p,q,\gamma,\delta)$ will be given in the next section. We start with the estimate of the integral $|I(p,q,\gamma)|$.

Proposition 3.1 (following [7]). *Given* $(p,q)=1$, $q \ge p$, *and* $2\gamma \in [p/q, 2+p/q]$, *we define the integral* $I(p,q,\gamma)$ *by equation* (11). *We have*

$$|I(p,q,\gamma)| \le 4\ln\Big(\frac{q}{p}\Big) + \frac{6}{\pi p} + \beta,$$

where $\beta = 4(e^{-1} + \operatorname{arcsinh}(4/\pi))$.

Proof. Denote the integral along the lower line by $I_2 = I_+ + I_-$, where I_+ is the integral along the positive half-line and I_- is the integral along the negative half-line. Denote $z = (1/2)\pi i + x$. We have

$$\begin{aligned}
|I_+| &\le 2\int_0^{+\infty} \Big|\frac{e^{(1+p/q)z}}{(1+e^{pz/q})(1-e^z)}\frac{e^{-\gamma z}}{z}\Big|\,\mathrm{d}x \\
&= 2\int_0^{+\infty} \frac{1}{|e^{-pz/q}+1||e^{-z}-1|}\frac{e^{-\gamma x}}{\sqrt{x^2+\frac{\pi^2}{4}}}\,\mathrm{d}x \\
&= 2\int_0^{+\infty} \frac{1}{\sqrt{1+e^{-2xp/q}+2e^{-px/q}\cos(\theta)}\sqrt{1+e^{-2x}}}\frac{e^{-\gamma x}}{\sqrt{x^2+\frac{\pi^2}{4}}}\,\mathrm{d}x \qquad (15)
\end{aligned}$$

where $\theta = p\pi/(2q)$. Denote $z = (1/2)\pi i - x$. We also have

$$\begin{aligned}
|I_-| &\le 2\int_0^{+\infty} \Big|\frac{e^{(1+p/q)z}}{(1+e^{pz/q})(1-e^z)}\frac{e^{-\gamma z}}{z}\Big|\,\mathrm{d}x \\
&= 2\int_0^{+\infty} \frac{1}{|1+e^{pz/q}||1-e^{z}|}\frac{e^{-(1+p/q-\gamma)x}}{\sqrt{x^2+\frac{\pi^2}{4}}}\,\mathrm{d}x \\
&= 2\int_0^{+\infty} \frac{1}{\sqrt{1+e^{-2xp/q}+2e^{-px/q}\cos(\theta)}\sqrt{1+e^{-2x}}}\frac{e^{-(1+p/q-\gamma)x}}{\sqrt{x^2+\frac{\pi^2}{4}}}\,\mathrm{d}x. \qquad (16)
\end{aligned}$$

Note that $\cos(\theta) \ge 0$ and $2\gamma \in [p/q, 2+p/q]$. Combining inequalities (15) and (16), we obtain

$$\begin{aligned}
|I_2| &\le |I_+| + |I_-| \\
&\le 4\int_0^{+\infty} \Big(x^2+\frac{\pi^2}{4}\Big)^{-1/2} e^{-px/(2q)}\,\mathrm{d}x \\
&= 4\int_0^{+\infty} \Big(u^2+\Big(\frac{p\pi}{4q}\Big)^2\Big)^{-1/2} e^{-u}\,\mathrm{d}u \\
&\le 4\Big(\int_0^1 \Big(u^2+\Big(\frac{p\pi}{4q}\Big)^2\Big)^{-1/2}\mathrm{d}u + \Big(1+\Big(\frac{p\pi}{4q}\Big)^2\Big)^{-1/2}\int_1^{+\infty} e^{-u}\,\mathrm{d}u\Big).
\end{aligned}$$

By the transformation $u = p\pi\tan(\theta)/(4q)$, we also obtain

$$\begin{aligned}|I_2| &\le 4\Big(\ln\Big(1+\Big(1+\Big(\frac{p\pi}{4q}\Big)^2\Big)^{1/2}\Big) - \ln\Big(\frac{p\pi}{4q}\Big) + e^{-1}\Big(1+\Big(\frac{p\pi}{4q}\Big)^2\Big)^{-1/2}\Big)\\ &\le 4\Big(\ln\Big(1+\Big(1+\Big(\frac{\pi}{4}\Big)^2\Big)^{1/2}\Big) - \ln\Big(\frac{\pi}{4}\Big) + \ln\Big(\frac{q}{p}\Big) + e^{-1}\Big(1+\Big(\frac{p\pi}{4q}\Big)^2\Big)^{-1/2}\Big)\\ &\le 4\ln\Big(\frac{q}{p}\Big) + \beta.\end{aligned}$$

We use similar methods to estimate the integral along the upper line. We denote $I_1 = I_+ + I_-$ where I_+ is the integral along the positive half-line and I_- is the integral along the negative half-line. Let $z = 2\pi i(q - 1/4) + x$. We have

$$\begin{aligned}|I_+| &\le 2\int_0^{+\infty}\Big|\frac{e^{(1+p/q)z}}{(1+e^{pz/q})(1-e^z)}\frac{e^{-\gamma z}}{z}\Big|\,\mathrm{d}x\\ &\le 2\int_0^{+\infty}\frac{1}{|e^{-pz/q}+1||e^{-z}-1|}\frac{e^{-\gamma x}}{\sqrt{x^2+4\pi^2\big(q-\frac{1}{4}\big)^2}}\,\mathrm{d}x\\ &= 2\int_0^{+\infty}\frac{1}{\sqrt{1+e^{-2xp/q}+2e^{-px/q}\cos(\theta)}\sqrt{1+e^{-2x}}}\frac{e^{-\gamma x}}{\sqrt{x^2+4\pi^2\big(q-\frac{1}{4}\big)^2}}\,\mathrm{d}x.\end{aligned}$$

Let $z = 2\pi i(q - 1/4) - x$. We also have

$$\begin{aligned}|I_-| &\le 2\int_0^{+\infty}\Big|\frac{e^{(1+p/q)z}}{(1+e^{pz/q})(1-e^z)}\frac{e^{-\gamma z}}{z}\Big|\,\mathrm{d}x\\ &\le 2\int_0^{+\infty}\frac{1}{|e^{pz/q}+1||e^{z}-1|}\frac{e^{-(1+p/q-\gamma)x}}{\sqrt{x^2+4\pi^2\big(q-\frac{1}{4}\big)^2}}\,\mathrm{d}x\\ &= 2\int_0^{+\infty}\frac{1}{\sqrt{1+e^{-2xp/q}+2e^{-px/q}\cos(\theta)}\sqrt{1+e^{-2x}}}\frac{e^{-(1+p/q-\gamma)x}}{\sqrt{x^2+4\pi^2\big(q-\frac{1}{4}\big)^2}}\,\mathrm{d}x.\end{aligned}$$

Combining the inequalities above, we obtain

$$\begin{aligned}|I_1| \le |I_+| + |I_-| &\le 4\int_0^{+\infty}\Big(x^2+4\pi^2\Big(q-\frac{1}{4}\Big)^2\Big)^{-1/2}e^{-px/(2q)}\,\mathrm{d}x\\ &= 4\int_0^{+\infty}\Big(u^2+\Big(p\pi\Big(1-\frac{1}{4q}\Big)\Big)^2\Big)^{-1/2}e^{-u}\,\mathrm{d}u \le \frac{6}{\pi p}.\end{aligned}$$

Combining the results above, we have $|I(p,q,\gamma)| \le 4\ln(q/p) + 6/(\pi p) + \beta$, and the proof is completed. ∎

To show the relation between $I(p,q,\gamma)$ and $S(p,q,\gamma)$, we now calculate the residues of the integral $I(p,q,\gamma)$ inside the contour $\Gamma(q)$. The following proposition is essential in the Hardy–Littlewood method.

Proposition 3.2 (following [7]). *Given $(p,q) = 1$, $q > p$, and $2\gamma \in [p/q, 2 + p/q]$, suppose q is odd and*

$$\frac{p}{q} = \frac{1}{a + \frac{p'}{q'}} \tag{17}$$

where $(p',q') = 1, q' \ge p'$ and $a \in \mathbb{N}$. The pair (p',q') satisfies the $(a \pmod 2)$-condition and

$$I(p,q,\gamma) = S(p,q,\gamma) - (-1)^{\varepsilon} T(p',q',\gamma',a \pmod 2)$$

where $\gamma' - \gamma q/p \in \mathbb{Z}$ and $\varepsilon = |\gamma' - \gamma q/p| \pmod 2$.

Proof. By equation (17), we have $p(aq' + p') = qq'$. This shows that $q' \mid p$ and $p \mid q'$, and we thus have $q' = p$. Since $aq' + p' = q$, we prove that p' is odd when a is even, and that p' and q' have different parities when a is odd. Therefore, (p',q') satisfies the $(a \pmod 2)$-condition. Given $\sigma > 0$, we define the path

$$\begin{aligned}
\Gamma_1(\sigma) &= \Big[2\pi i\Big(q - \frac{1}{4}\Big) - \sigma, 2\pi i\Big(q - \frac{1}{4}\Big) + \sigma\Big],\\
\Gamma_2(\sigma) &= \Big[\frac{1}{2}\pi i - \sigma, \frac{1}{2}\pi i + \sigma\Big],\\
\Gamma_3(\sigma) &= \Big[\frac{1}{2}\pi i - \sigma, 2\pi i\Big(q - \frac{1}{4}\Big) - \sigma\Big],\\
\Gamma_4(\sigma) &= \Big[\frac{1}{2}\pi i + \sigma, 2\pi i\Big(q - \frac{1}{4}\Big) + \sigma\Big],
\end{aligned}$$

and the contour is $\Gamma(\sigma) = \bigcup_{i=1}^{4} \Gamma_i(\sigma)$ which has the positive orientation. We define $I(\sigma) = \sum_{i=1}^{4} I_i(\sigma)$, where $I_i(\sigma)$ is the integral along $\Gamma_i(\sigma)$. When σ is large enough, we have

$$|I_3(\sigma)| \lesssim \frac{e^{-(1+p/q-\gamma)\sigma}}{\sigma}, \quad |I_4(\sigma)| \lesssim \frac{e^{-\gamma\sigma}}{\sigma},$$

which shows that $I(p,q,\gamma) = \lim_{\sigma\to+\infty} I(\sigma)$. By the residue theorem, the integral $I(\sigma)$ is determined by the poles inside the contour. By direct calculation, the poles of the integrand are

$$z_m = 2\pi i m, \quad z_n' = 2\pi i\Big(n - \frac{1}{2}\Big)\frac{q}{p},$$

where $1 \leq m \leq q-1$ and $1 \leq n \leq p$. Since $(p,q)=1$ and q is odd, the poles are distinct and we now calculate the residues. For $1 \leq m \leq q-1$, we have

$$\mathrm{Res}(z_m) = \left(\lim_{z\to z_m} \frac{z-z_m}{1-e^z}\right)\frac{e^{2\pi i m(1+p/q-\gamma)}}{2\pi i m(1+e^{2\pi i m p/q})} = -\frac{e^{2\pi i m(p/q-\gamma)}}{2\pi i m(1+e^{2\pi i m p/q})}.$$

We denote by R_1 the contribution of these poles to the integral $I(p,q,\gamma)$. We have

$$R_1 = -\sum_{m=1}^{q-1} 4\pi i \cdot \mathrm{Res}(z_m) = \sum_{m=1}^{q-1} \frac{2e^{\pi i m p/q - 2\pi i m\gamma}}{m(e^{\pi i m p/q}+e^{-\pi i m p/q})} = S(p,q,\gamma). \quad (18)$$

Now, we calculate the residues of $z'_n(1 \leq n \leq p)$. By direct calculation, we have

$$\mathrm{Res}(z'_n) = \left(\lim_{z\to z'_n} \frac{z-z'_n}{1+e^{pz/q}}\right)\frac{e^{(1+p/q-\gamma)z'_n}}{z'_n(1-e^{z'_n})} = \frac{qe^{(1-\gamma)z'_n}}{pz'_n(1-e^{z'_n})}.$$

Denote by R_2 the contribution of these poles to the integral. We have

$$\begin{aligned} R_2 = -\sum_{n=1}^{p} 4\pi i \cdot \mathrm{Res}(z'_n) &= -2\sum_{n=1}^{p} \frac{e^{2\pi i(1-\gamma)(n-1/2)q/p}}{(1-e^{2\pi i(n-1/2)q/p})(n-\frac{1}{2})} \\ &= -2\sum_{n=1}^{p} \frac{e^{2\pi i(n-1/2)(a+p'/q')}}{1-e^{2\pi i(n-1/2)(a+p'/q')}} \frac{e^{-2\pi i(n-1/2)(k+\gamma')}}{n-\frac{1}{2}} \\ &= -(-1)^{\varepsilon} T(p',q',\gamma',a \pmod 2), \end{aligned} \quad (19)$$

where $k=\gamma q/p-\gamma'$. Combining equations (18) and (19), we obtain

$$I(p,q,\gamma) = R_1+R_2 = S(p,q,\gamma) - (-1)^{\varepsilon} T(p',q',\gamma',a \pmod 2)$$

and the proof is completed. ■

Proposition 3.3 is a special condition of Proposition 3.2, which completes the relation between $I(p,q,\gamma)$ and $S(p,q,\gamma)$.

Proposition 3.3. *Suppose that $a \in \mathbb{N}$ is odd and $2\gamma \in [1/a, 2+1/a]$. Then we have*

$$I(1,a,\gamma) = S(1,a,\gamma) + 2e^{-\pi i a\gamma}.$$

Proof. Similar to Proposition 3.2, the integral $I(1,a,\gamma)$ is determined by the poles inside the contour. When $a=1$, the fraction $(1-e^z)^{-1}$ has no pole and we have $S(1,1,\gamma)=0$ by the previous definition. When $a \geq 2$, the poles of the fraction $(1-e^z)^{-1}$ are given by $z_m = 2\pi i m$ (for $1 \leq m \leq a-1$). Similar to the computation in Proposition 3.2, the contribution of these poles to the integral $I(1,a,\gamma)$ is $R_1 = S(1,a,\gamma)$. The only pole of the fraction $(1+e^{z/a})^{-1}$ is $z' = \pi i a$ and we have

$\text{Res}(z') = -e^{-\pi i a\gamma}/(2\pi i)$. Denote by R_2 the contribution of the pole z'. Combining the results above, the integral is

$$I(1,a,\gamma) = R_1 + R_2 = S(1,a,\gamma) - 4\pi i \cdot \text{Res}(z') = S(1,a,\gamma) + 2e^{-\pi i a\gamma}$$

and the proof is completed. ∎

To complete the Hardy–Littlewood method, we also need to consider the relation between $I(p,q,\gamma)$ and $S'(p,q,\gamma)$, which is essential for the estimate of the second-order derivative $|\sigma''_\alpha(0)|$. The calculation is similar to that in Proposition 3.2 and Proposition 3.3, but the central pole inside the contour is second-order under this condition.

Proposition 3.4. *Given $(p,q) = 1, q > p$ and $2\gamma \in [p/q, 2 + p/q]$, suppose q is even and*

$$\frac{p}{q} = \frac{1}{a + \frac{p'}{q'}} \tag{20}$$

where $(p',q') = 1, q' \geq p'$ and $a \in \mathbb{N}$. The pair (p',q') satisfies the $(a \pmod 2)'$-condition and

$$I(p,q,\gamma) = R(p,q,\gamma) + S'(p,q,\gamma) - (-1)^{\varepsilon} T'(p',q',\gamma',a \pmod 2)$$

where $|R(p,q,\gamma)| \leq 12, \gamma' - \gamma q/p \in \mathbb{Z}$ and $\varepsilon = |\gamma' - \gamma q/p| \pmod 2$.

Proof. Equation (20) shows that $q' = p$ and $aq' + p' = q$. Thus q' is odd, since $(p,q) = 1$ and q is even. Similar to Proposition 3.2, we prove that (p',q') satisfies the $(a \pmod 2)'$-condition. The poles of $(1 - e^z)^{-1}$ are $z_m = 2\pi i m$ (for $1 \leq m \leq q-1$) and the poles of $(1 + e^{pz/q})^{-1}$ are $z'_n = 2\pi i (n - 1/2)q/p$ (for $1 \leq n \leq p$). These poles are distinct except $z_m = z'_n$ when $m = q/2$ and $n = (p+1)/2$. The central pole

$$z_0 = z_{q/2} = z'_{(p+1)/2} = \pi i q$$

is second order and the other poles are of first order. To calculate $I(p,q,\gamma)$, we denote by R_1 the contribution of the poles z_m (for $1 \leq m \leq q-1$ and $m \neq q/2$) and by R_2 the contribution of the poles z'_n (for $1 \leq n \leq p$ and $n \neq (p+1)/2$). We also denote by R_3 the contribution of the central pole z_0. By a calculation similar to Proposition 3.2, we obtain

$$R_1 = \sum_{m=1, m \neq q/2}^{q-1} -4\pi i \cdot \text{Res}(z_m) = S'(p,q,\gamma),$$

$$R_2 = \sum_{n=1, n \neq (p+1)/2}^{p} -4\pi i \cdot \text{Res}(z'_n) = -(-1)^{\varepsilon} T'(p',q',\gamma',a \pmod 2).$$

We have $R_3 = -4\pi i \cdot \mathrm{Res}(z_0)$ and we now calculate the residue of z_0. We assume that the expansions around the central pole z_0 are

$$z^{-1}e^{(1+p/q-\gamma)z} = \sum_{n=0}^{\infty} a_n(z-z_0)^n,$$
$$(1+e^{pz/q})^{-1} = \sum_{n=-1}^{\infty} b_n(z-z_0)^n,$$
$$(1-e^{z})^{-1} = \sum_{n=-1}^{\infty} c_n(z-z_0)^n.$$

We calculate the coefficients in the expansions. We have $a_0 = e^{(1+p/q-\gamma)z_0}z_0^{-1}$ and

$$a_1 = (z^{-1}e^{(1+p/q-\gamma)z})'|_{z=z_0} = z_0^{-2}e^{(1+p/q-\gamma)z_0}\Big(\Big(1+\frac{p}{q}-\gamma\Big)z_0 - 1\Big).$$

By direct computation, we obtain

$$b_{-1} = \lim_{z\to z_0}\frac{z-z_0}{1+e^{pz/q}} = -q/p,$$
$$c_{-1} = \lim_{z\to z_0}\frac{z-z_0}{1-e^{z}} = -1,$$

and

$$b_0 = \lim_{z\to z_0}\Big(\frac{z-z_0}{1+e^{pz/q}}\Big)' = \frac{1}{2},$$
$$c_0 = \lim_{z\to z_0}\Big(\frac{z-z_0}{1-e^{z}}\Big)' = \frac{1}{2}.$$

Combining the results above, we obtain

$$\mathrm{Res}(z_0) = a_1b_{-1}c_{-1} + a_0(b_{-1}c_0 + b_0c_{-1}) = a_1\frac{q}{p} - a_0\frac{1+\frac{q}{p}}{2}.$$

We now derive an upper bound of the residue $|\mathrm{Res}(z_0)|$. We have $|a_0| = 1/(\pi q)$ and

$$|a_1| \le \frac{1+\pi q\big|1+\frac{p}{q}-\gamma\big|}{(\pi q)^2} \le \frac{1+\pi q\big(1+\frac{p}{2q}\big)}{(\pi q)^2} \le \frac{2}{\pi q},$$

which implies $|\mathrm{Res}(z_0)| \le 2/(\pi p) + (1/q+1/p)/(2\pi) \le 3/\pi$ and $|R_3| \le 12$. Let $R(p,q,\gamma) = R_3$. We have

$$\begin{aligned} I(p,q,\gamma) &= R_1 + R_2 + R_3 \\ &= R(p,q,\gamma) + S'(p,q,\gamma) - (-1)^{\varepsilon}T'(p',q',\gamma',a \pmod 2). \end{aligned}$$

The proof is completed. ■

Proposition 3.5. *Suppose that $a \in \mathbb{N}$ is even and $2\gamma \in [1/a, 2 + 1/a]$, then*

$$I(1, a, \gamma) = R(1, a, \gamma) + S'(1, a, \gamma),$$

where $|R(1, a, \gamma)| \le 12$.

Similar to Proposition 3.3, we also need to show the relation between $I(p, q, \gamma)$ and $S'(p, q, \gamma)$ under another special condition. This is accomplished in Proposition 3.5 and the proof is omitted. We can obtain the explicit expression of $R(p, q, \gamma)$ in Proposition 3.4 and Proposition 3.5, but this is not necessary.

4. Hardy–Littlewood bethod (II)

In this section, we continue to introduce the Hardy–Littlewood method. We derive an upper bound for $|J(p, q, \gamma, \delta)|$ and calculate the residues inside the contour $\Gamma(q)$. We also consider the relation between $J(p, q, \gamma, \delta)$ and $T(p, q, \gamma, \delta), T'(p, q, \gamma, \delta)$. The method is similar to that in Section 3.

Proposition 4.1 (following [7]). *Given $(p, q) = 1$, $q \ge p$, $2\gamma \in [p/q, 2 + p/q]$, and $\delta \in \{0, 1\}$, the integral $J(p, q, \gamma, \delta)$ is defined by equation (14). We have*

$$|J(p, q, \gamma, \delta)| \le A_\delta \Big(4 \ln \frac{q}{p} + \frac{6}{\pi p} + \beta\Big)$$

where $A_0 = (\sin(\pi p/(2q)))^{-1}$, $A_1 = 1$, and $\beta = 4(e^{-1} + \operatorname{arcsinh}(4/\pi))$.

Proof. Denote the integral along the lower line by $J_2 = J_+ + J_-$, where J_+ is the integral along the positive half-line and J_- is the integral along the negative half-line. Denote $z = \pi i/2 + x$. We have

$$\begin{aligned}
|J_+| &\le 2 \int_0^{+\infty} \left| \frac{(-1)^\delta e^{(1+p/q)z}}{(1 - (-1)^\delta e^{pz/q})(1 + e^z)} \frac{e^{-\gamma z}}{z} \right| \mathrm{d}x \\
&= 2 \int_0^{+\infty} \frac{1}{|e^{-pz/q} - (-1)^\delta||e^{-z} + 1|} \frac{e^{-\gamma x}}{\sqrt{x^2 + \frac{\pi^2}{4}}} \mathrm{d}x \\
&= 2 \int_0^{+\infty} \frac{1}{\sqrt{1 + e^{-2xp/q} - 2(-1)^\delta e^{-px/q} \cos(\theta)} \sqrt{1 + e^{-2x}}} \frac{e^{-\gamma x}}{\sqrt{x^2 + \frac{\pi^2}{4}}} \mathrm{d}x,
\end{aligned}$$

where $\theta = p\pi/(2q)$. Denote $z = \pi i/2 - x$. We have

$$|J_-| \leq 2 \int_0^{+\infty} \left| \frac{(-1)^\delta e^{(1+p/q)z}}{(1-(-1)^\delta e^{pz/q})(1+e^z)} \frac{e^{-\gamma z}}{z} \right| \mathrm{d}x$$
$$\leq 2 \int_0^{+\infty} \frac{1}{|1-(-1)^\delta e^{pz/q}||1+e^z|} \frac{e^{-(1+p/q-\gamma)x}}{\sqrt{x^2+\frac{\pi^2}{4}}} \mathrm{d}x$$
$$= 2 \int_0^{+\infty} \frac{1}{\sqrt{1+e^{-2xp/q}-2(-1)^\delta e^{-px/q}\cos(\theta)}\sqrt{1+e^{-2x}}} \frac{e^{-(1+p/q-\gamma)x}}{\sqrt{x^2+\frac{\pi^2}{4}}} \mathrm{d}x.$$

Note that $2\gamma \in [p/q, 2+p/q]$ and $(1+e^{-2xp/q}-2(-1)^\delta e^{-px/q}\cos(\theta))^{-1/2} \leq A_\delta$. Combining the inequalities above, we obtain

$$|J_2| \leq |J_+| + |J_-|$$
$$\leq 2 \int_0^{+\infty} \frac{e^{-\gamma x}+e^{-(1+p/q-\gamma)x}}{\sqrt{1+e^{-2xp/q}-2(-1)^\delta e^{-px/q}\cos(\theta)}\sqrt{1+e^{-2x}}} \frac{1}{\sqrt{x^2+\frac{\pi^2}{4}}} \mathrm{d}x$$
$$\leq 4A_\delta \int_0^{+\infty} \Big(x^2+\frac{\pi^2}{4}\Big)^{-1/2} e^{-px/(2q)} \mathrm{d}x \leq A_\delta \Big(4\ln\frac{q}{p}+\beta\Big).$$

We now consider the integral along the upper line and denote $J_1 = J_+ + J_-$, where J_+ is the integral along the positive half-line and J_- is the integral along the negative half-line. Denote $z = 2\pi i(q-1/4)+x$. We have

$$|J_+| \leq 2 \int_0^{+\infty} \left| \frac{(-1)^\delta e^{(1+p/q)z}}{(1-(-1)^\delta e^{pz/q})(1+e^z)} \frac{e^{-\gamma z}}{z} \right| \mathrm{d}x$$
$$\leq 2 \int_0^{+\infty} \frac{1}{|e^{-pz/q}-(-1)^\delta||e^{-z}+1|} \frac{e^{-\gamma x}}{\sqrt{x^2+4\pi^2\big(q-\frac{1}{4}\big)^2}} \mathrm{d}x$$
$$= \int_0^{+\infty} \frac{2}{\sqrt{1+e^{-2xp/q}-2(-1)^\delta e^{-px/q}\cos(\theta)}\sqrt{1+e^{-2x}}}$$
$$\times \frac{e^{-\gamma x}}{\sqrt{x^2+4\pi^2\big(q-\frac{1}{4}\big)^2}} \mathrm{d}x.$$

Denote $z = 2\pi i(q - 1/4) - x$. We also have

$$
\begin{aligned}
|J_-| &\le 2 \int_0^{+\infty} \left| \frac{(-1)^\delta e^{(1+p/q)z}}{(1-(-1)^\delta e^{pz/q})(1+e^z)} \frac{e^{-\gamma z}}{z} \right| \mathrm{d}x \\
&\le 2 \int_0^{+\infty} \frac{1}{|1-(-1)^\delta e^{pz/q}||e^z+1|} \frac{e^{-(1+p/q-\gamma)x}}{\sqrt{x^2+4\pi^2\left(q-\frac{1}{4}\right)^2}} \mathrm{d}x \\
&= \int_0^{+\infty} \frac{2}{\sqrt{1+e^{-2xp/q}-2(-1)^\delta e^{-px/q}\cos(\theta)}\sqrt{1+e^{-2x}}} \\
&\quad \times \frac{e^{-(1+p/q-\gamma)x}}{\sqrt{x^2+4\pi^2\left(q-\frac{1}{4}\right)^2}} \mathrm{d}x.
\end{aligned}
$$

Combining the inequalities above, we obtain

$$
|J_1| \le |J_+| + |J_-| \le 4A_\delta \int_0^{+\infty} (x^2+4\pi^2(q-1/4)^2)^{-1/2} e^{-px/(2q)} \mathrm{d}x \le \frac{6A_\delta}{\pi p}
$$

and we have $|J(p,q,\gamma,\delta)| \le |J_1| + |J_2| \le A_\delta(4\ln(q/p) + 6/(\pi p) + \beta)$. ■

To prove the relation between $J(p,q,\gamma,\delta)$ and $T(p,q,\gamma,\delta)$, we now calculate the residues of the integral $J(p,q,\gamma)$ inside the contour $\Gamma(q)$. Proposition 3.2 and Proposition 4.2 enable us to obtain an upper bound of the first-order derivative $|\sigma'_\alpha(0)|$.

Proposition 4.2 (following [7]). *Given $(p,q) = 1, q > p$, $2\gamma \in [p/q, 2 + p/q]$, and $\delta \in \{0,1\}$, we suppose that (p,q) satisfies the δ-condition and that*

$$
\frac{p}{q} = \frac{1}{a + \frac{p'}{q'}}, \tag{21}
$$

where $(p',q') = 1, q' \ge p'$ and $a \in \mathbb{N}$. We claim that q' is odd when $\delta = 0$, and (p',q') satisfies the $(a+1 \pmod 2)$-condition when $\delta = 1$. We also have

$$
J(p,q,\gamma,\delta) = T(p,q,\gamma,\delta) + \begin{cases} -S(p',q',\gamma'), & \delta = 0, \\ (-1)^\varepsilon T(p',q',\gamma',a+1 \pmod 2), & \delta = 1, \end{cases}
$$

where $\gamma' - \gamma q/p \in \mathbb{Z}$ and $\varepsilon = |\gamma' - \gamma q/p| \pmod 2$.

Proof. Equation (21) shows that $q' \mid p$ and $p \mid q'$, and we thus have $q' = p$. We also obtain $aq' + p' = q$. We claim that q' is odd when $\delta = 0$. When $\delta = 1$, we claim that (p',q') satisfies the $(a+1 \pmod 2)$-condition since p and q have different parities.

Similar to Proposition 3.2, the integral $J(p,q,\gamma,\delta)$ is determined by the poles inside the contour. The poles of the fraction $(1+e^z)^{-1}$ are $z_m = 2\pi i(m-1/2)$ (for $1 \le m \le q$). When $\delta = 0$, the poles of the fraction $(1-(-1)^\delta e^{pz/q})^{-1}$ are $z'_n = 2\pi i nq/p$ (for $1 \le n \le p-1$). When $\delta = 1$, the poles of the fraction $(1-(-1)^\delta e^{pz/q})^{-1}$ are $z'_n = 2\pi i(n-1/2)q/p$ (for $1 \le n \le p$). By the δ-condition, these poles are distinct and we now calculate the residues.

(1) For $1 \le m \le q$, we have

$$\operatorname{Res}(z_m) = \Big(\lim_{z\to z_m} \frac{z-z_m}{1+e^z}\Big)\frac{(-1)^\delta e^{(1+p/q-\gamma)z_m}}{z_m(1-(-1)^\delta e^{pz_m/q})} = \frac{(-1)^\delta e^{(p/q-\gamma)z_m}}{z_m(1-(-1)^\delta e^{pz_m/q})}$$

and the contribution of these poles to the integral is

$$\begin{aligned} R_1 &= \sum_{m=1}^{q} 4\pi i \cdot \operatorname{Res}(z_m) = \sum_{m=1}^{q} \frac{(-1)^\delta e^{2\pi i(m-1/2)p/q}}{1-(-1)^\delta e^{2\pi i(m-1/2)p/q}} \frac{2e^{-2\pi i(m-1/2)\gamma}}{m-\frac{1}{2}} \\ &= T(p,q,\gamma,\delta). \end{aligned}$$

(2) We first consider the condition $\delta = 0$. When $p = 1$, we have $q' = 1$ and the fraction $(1-(-1)^\delta e^{pz/q})^{-1}$ has no pole inside the contour. We also have $S(p',1,\gamma') = 0$ by definition. We now assume $p \ge 2$ and calculate the residues. For $1 \le n \le p-1$, we have

$$\operatorname{Res}(z'_n) = \Big(\lim_{z\to z'_n} \frac{z-z'_n}{1-e^{pz/q}}\Big)\frac{e^{(1+p/q-\gamma)z'_n}}{z'_n(1+e^{z'_n})} = -\frac{qe^{(1-\gamma)z'_n}}{pz'_n(1+e^{z'_n})}.$$

The contribution of these poles to the integral $J(p,q,\gamma,\delta)$ is

$$\begin{aligned} R_2 &= \sum_{n=1}^{p-1} 4\pi i \cdot \operatorname{Res}(z'_n) = -2\sum_{n=1}^{p-1} \frac{e^{2\pi i n(1-\gamma)(a+p'/q')}}{n(1+e^{2\pi i n(a+p'/q')})} = -\sum_{n=1}^{p-1} \frac{e^{\pi i n(p'/q'-2\gamma')}}{n\cos(\frac{\pi n p'}{q'})} \\ &= -S(p',q',\gamma'). \end{aligned}$$

(3) We now consider the condition $\delta = 1$. The calculation of residues is similar and we have

$$\begin{aligned} R_2 &= \sum_{n=1}^{p} 4\pi i \cdot \operatorname{Res}(z'_n) = (-1)^{\varepsilon+1}\sum_{n=1}^{p} \frac{e^{2\pi i(n-1/2)(a+p'/q')}}{1+e^{2\pi i(n-1/2)(a+p'/q')}} \frac{2e^{-2\pi i(n-1/2)\gamma'}}{n-\frac{1}{2}} \\ &= (-1)^\varepsilon T(p',q',\gamma',a+1 \pmod 2). \end{aligned}$$

Combining the results in (1)–(3), we have

$$J(p,q,\gamma,\delta) = T(p,q,\gamma,\delta) + \begin{cases} -S(p',q',\gamma'), & \delta = 0, \\ (-1)^\varepsilon T(p',q',\gamma',a+1 \pmod 2)), & \delta = 1, \end{cases}$$

and the proof is completed. ■

Similar to the analysis in Section 3, we also need to study the relation between $J(p,q,\gamma,\delta)$ and $T(p,q,\gamma,\delta)$ under another special condition, which is accomplished in the following proposition.

Proposition 4.3. *Given $a \in \mathbb{N}$ and $2\gamma \in [1/a, 2+1/a]$, suppose that $(1,a)$ satisfies the δ-condition. We have*

$$J(1,a,\gamma,\delta) = T(1,a,\gamma,\delta) - \begin{cases} 0, & \delta = 0, \\ 2e^{-\pi i a\gamma}, & \delta = 1. \end{cases}$$

Proof. The integral $J(1,a,\gamma,\delta)$ is determined by the poles inside the contour. We need to calculate the residues. The poles of the fraction $(1+e^z)^{-1}$ are $z_m = 2\pi i(m-1/2)$ (for $1 \le m \le a$). Similar to the computation in Prorposition 3.2, the contribution of these poles to the integral is $R_1 = T(1,a,\gamma,\delta)$. When $\delta = 0$, then the fraction $(1-(-1)^\delta e^{pz/q})^{-1}$ has no pole inside the contour and the contribution is $R_2 = 0$. When $\delta = 1$, then the only pole of this fraction is $z' = \pi i a$ and the residue is

$$\mathrm{Res}(z') = -\Big(\lim_{z\to\pi i a} \frac{z-\pi i a}{1+e^{z/a}}\Big)\frac{e^{(1+1/a-\gamma)\pi i a}}{\pi i a(1+e^{\pi i a})} = -\frac{e^{-\pi i a\gamma}}{2\pi i}.$$

The contribution of this pole to the integral is $R_2 = -2e^{-\pi i a\gamma}$. Combining the results above, we have

$$J(1,a,\gamma,\delta) = R_1 + R_2 = T(1,a,\gamma,\delta) - \begin{cases} 0, & \delta = 0, \\ 2e^{-\pi i a\gamma}, & \delta = 1, \end{cases}$$

and the proof is completed. ■

To estimate the second-order derivative $|\sigma''_\alpha(0)|$, we also need to consider the relation between $J(p,q,\gamma,\delta)$ and $T'(p,q,\gamma,\delta)$. Different from the proof of Proposition 4.2 and Proposition 4.3, the central pole is of second order under this condition.

Proposition 4.4. *Given $(p,q)=1$, $q>p$, $\delta\in\{0,1\}$, and $2\gamma \in [p/q, 2+p/q]$, we suppose that (p,q) satisfies the δ'-condition and that*

$$\frac{p}{q} = \frac{1}{a+\frac{p'}{q'}} \tag{22}$$

where $(p',q')=1$, $q' \ge p'$, and $a\in\mathbb{N}$. We claim that q' is even when $\delta = 0$, and that (p',q') satisfies the $(a+1 \pmod 2)'$-condition when $\delta = 1$. We also have

$$\begin{aligned} J(p,q,\gamma,\delta) &= Q(p,q,\gamma,\delta) + T'(p,q,\gamma,\delta) \\ &\quad + \begin{cases} -S'(p',q',\gamma'), & \delta = 0, \\ (-1)^\varepsilon T'(p',q',\gamma',a+1 \pmod 2), & \delta = 1, \end{cases} \end{aligned}$$

where $|Q(p,q,\gamma,\delta)| \le 12$, $\gamma' - \gamma q/p \in \mathbb{Z}$, and $\varepsilon = |\gamma' - \gamma q/p| \pmod 2$.

Proof. Similar to the proof of Proposition 4.2, equation (22) shows q' is even when $\delta = 0$, and (p', q') satisfies the $(a+1 \pmod 2)'$-condition when $\delta = 1$. We calculate the poles of the integral $J(p, q, \gamma, \delta)$ inside the contour. The poles of $(1+e^z)^{-1}$ are $z_m = 2\pi i(m - 1/2)$ (for $1 \le m \le q$). We consider the poles of $(1-(-1)^\delta e^{pz/q})^{-1}$ under different conditions. When $\delta = 0$, the poles of $(1-(-1)^\delta e^{pz/q})^{-1}$ are $z'_n = 2\pi i n q/p$ (for $1 \le n \le p-1$) and the central pole is $z_0 = z_{(q+1)/2} = z'_{p/2} = \pi i q$. When $\delta = 1$, then the poles of $(1-(-1)^\delta e^{pz/q})^{-1}$ are $z'_n = 2\pi i(n-1/2)q/p$ (for $1 \le n \le p$) and the central pole is $z_0 = z_{(q+1)/2} = z'_{(p+1)/2} = \pi i q$. Under either condition, the central pole z_0 is second-order and the other poles are first-order. Similar to the calculations in Proposition 4.2, the contribution of the poles z_m (for $1 \le m \le q$ and $m \ne (q+1)/2$) to the integral is

$$R_1 = \sum_{m=1, m\ne(q+1)/2}^{q} 4\pi i \cdot \mathrm{Res}(z_m) = T'(p, q, \gamma, \delta).$$

For the fraction $(1-(-1)^\delta e^{pz/q})^{-1}$, we denote the contribution of its poles by R_2. When $\delta = 0$, we have

$$R_2 = \sum_{n=1, n\ne p/2}^{p-1} 4\pi i \cdot \mathrm{Res}(z'_n) = -S'(p', q', \gamma').$$

When $\delta = 1$, we have

$$R_2 = \sum_{n=1, n\ne(p+1)/2}^{p} 4\pi i \cdot \mathrm{Res}(z'_n) = (-1)^\varepsilon T'(p', q', \gamma', a+1 \pmod 2).$$

We now calculate the residue of the central pole and its contribution to the integral is $R_3 = 4\pi i \cdot \mathrm{Res}(z_0)$. Around the central pole z_0, we have the expansions

$$(-1)^\delta z^{-1} e^{(1+p/q-\gamma)z} = \sum_{n=0}^{\infty} a_n (z-z_0)^n,$$
$$(1-(-1)^\delta e^{pz/q})^{-1} = \sum_{n=-1}^{\infty} b_n (z-z_0)^n,$$
$$(1+e^z)^{-1} = \sum_{n=-1}^{\infty} c_n (z-z_0)^n.$$

We now calculate the coefficients of expansions. We have

$$a_0 = (-1)^\delta z_0^{-1} e^{(1+p/q-\gamma)z_0}$$

and

$$a_1 = (-1)^\delta (z^{-1} e^{(1+p/q-\gamma)z})'|_{z=z_0} = (-1)^\delta z_0^{-2} e^{(1+p/q-\gamma)z_0}\Big(\Big(1+\frac{p}{q}-\gamma\Big)z_0 - 1\Big).$$

By direct calculation, we have

$$b_{-1} = \lim_{z\to z_0} \frac{z-z_0}{1-(-1)^\delta e^{pz/q}} = -\frac{q}{p},$$
$$c_{-1} = \lim_{z\to z_0} \frac{z-z_0}{1+e^z} = -1,$$

and

$$b_0 = \lim_{z\to z_0} \Big(\frac{z-z_0}{1-(-1)^\delta e^{zp/q}}\Big)' = \frac{1}{2},$$
$$c_0 = \lim_{z\to z_0} \Big(\frac{z-z_0}{1+e^z}\Big)' = \frac{1}{2}.$$

Combining the results above, we have

$$\mathrm{Res}(z_0) = a_1 b_{-1} c_{-1} + a_0(b_{-1}c_0 + b_0 c_{-1}) = a_1 \frac{q}{p} - a_0 \frac{1+\frac{q}{p}}{2}.$$

Similarly, we can obtain the bounds $|\,\mathrm{Res}(z_0)| \le 3/\pi$ and $|R_3| \le 12$. Let $Q(p,q,\gamma,\delta) = R_3$. We have

$$J(p,q,\gamma,\delta) = Q(p,q,\gamma,\delta) + T'(p,q,\gamma,\delta) + \begin{cases} -S'(p',q',\gamma'), & \delta = 0, \\ (-1)^\varepsilon T'(p',q',\gamma',a+1 \pmod 2), & \delta = 1. \end{cases}$$

The proof is completed. ■

Proposition 4.5. *Given $a \in \mathbb{N}$ and $2\gamma \in [1/a, 2+1/a]$, suppose that a is odd. We have*

$$J(1,a,\gamma,1) = Q(1,a,\gamma,1) + T'(1,a,\gamma,1)$$

where $|Q(1,a,\gamma,1)| \le 12$.

Proposition 4.5 shows the relation between $J(p,q,\gamma,\delta)$ and $T'(p,q,\gamma,\delta)$ under a special condition. We can also obtain the explicit expression of $Q(p,q,\gamma,\delta)$, but this is not necessary. We have introduced the complete Hardy–Littlewood method and we are able to estimate the derivatives of the discriminant polynomial.

5. Bound for the derivatives of the discriminant polynomial

In this section, the Hardy–Littlewood method is applied to estimate the derivatives $\sigma'_\alpha(0)$ and $\sigma''_\alpha(0)$ of the discriminant polynomial. We will derive an upper bound of the derivatives, which enables us to obtain a lower bound for the measure of the central spectral band. We first introduce the symbolic encoding of continued fractions. The character e represents an even integer and o represents an odd integer. The character a represents an even or odd integer. We define the sequences of characters

(1) $\tau = ea$,

(2) $\varepsilon = oee \cdots e \cdots$,

(3) $\omega_n = oee \cdots eoa (n \geq 0)$,

where there are n continued characters e in the sequence ω_n and there are infinite continued characters e in the sequence ε. Suppose the continued fraction is $\alpha = [a_1, a_2, \ldots, a_n, \ldots]$ where $a_n \geq 1$ (for $n \geq 1$). It is not hard to prove that there is a unique symbolic encoding of α with the sequences τ, ε and ω_n (for $n \geq 0$). There are three possible types of symbolic encodings:

(1) $\alpha = \varepsilon$,

(2) $\alpha = r_1 r_2 \cdots r_m \varepsilon$ where $r_i = \tau$ or $r_i = \omega_n$ for $n \geq 0$ and $1 \leq i \leq m$,

(3) $\alpha = r_1 r_2 \cdots r_i \cdots$ where $r_i = \tau$ or $r_i = \omega_n$ for $n \geq 0$ and $i \geq 1$.

Given a continued fraction α and $M \in \mathbb{N}$, we say that α is *M-weakly bounded* if $a \leq M$ for each character a in the symbolic encoding of α. For example, α is M-weakly bounded for any $M \in \mathbb{N}$ when the symbolic encoding of α is of type (1). When the symbolic encoding is of type (2), there are m characters a in the sequence and α is M-weakly bounded for M large enough. When the symbolic encoding is of type (3), there are infinite characters a in the sequence. The continued fraction α is M-weakly bounded if these characters are bounded by M. Now, we are able to prove the main theorem about the bound of the derivatives $|\sigma'_\alpha(0)|$ and $|\sigma''_\alpha(0)|$.

Theorem 5.1. *Given $\alpha \in (0, 1) \cap \mathbb{Q}^c$ and $M \in \mathbb{N}$, suppose that the continued fraction is $\alpha = [a_1, a_2, \ldots, a_n, \ldots]$ and that α is M-weakly bounded. Denote by $\sigma_n(x)$ the discriminant polynomial of the critical almost Mathieu operator with $\alpha_n = [a_1, a_2, \ldots, a_n]$. There exist constants $\lambda_{1,2,3} = \lambda_{1,2,3}(M) > 0$ so that*

$$|\sigma'_n(0)| + |\sigma''_n(0)| \leq e^{\lambda_1} e^{\lambda_2 n} q_n^{\lambda_3}$$

for $n \geq 1$.

Proof. The proof is a recursive application of the results in the previous sections and we start from the first step. The rational approximation of α is $\alpha_n = [a_1, a_2, \ldots, a_n]$ and we denote the canonical representation by $\alpha_n = p_n / q_n$. We assume that $n \geq 3$ is given throughout the proof.

(1) For $1 \leq i \leq n$, we denote the canonical representation by $t_i = u_i / v_i = [a_i, a_{i+1}, \ldots, a_n]$. By definition, we have $p_n = u_1, q_n = v_1$. Let $t_{n+1} = 0$ and we denote

$A_i = q_i + q_{i-1}t_{i+1}$ for $2 \le i \le n$. We prove $A_i = A_{i-1}t_i^{-1}$ where $3 \le i \le n$. By direct calculation, we obtain

$$A_i = q_i + q_{i-1}t_{i+1} = a_i q_{i-1} + q_{i-2} + q_{i-1}t_{i+1} = q_{i-2} + \frac{q_{i-1}}{t_i} = A_{i-1}t_i^{-1}$$

which implies $q_n = A_n = A_2/(t_3 t_4 \cdots t_n)$ by induction. We now calculate the term A_2. We have $q_1 = a_1, q_2 = 1 + a_1 a_2$ and

$$t_1 = \frac{1}{a_1 + t_2}, t_2 = \frac{1}{a_2 + t_3}, t_1 t_2 = \frac{1}{1 + a_1(a_2 + t_3)}.$$

Combining the results above, we have $A_2 = q_2 + q_1 t_3 = 1 + a_1 a_2 + a_1 t_3 = 1/(t_1 t_2)$ and $q_n = 1/(t_1 t_2 \cdots t_n)$.

(2) Given $z \in \mathbb{Z}$, we construct the array $(\gamma_i, m_i)_{i=1}^n$ in this step. We first set $\gamma_1 = z t_1 + m_1$ where $m_1 \in \mathbb{Z}$ is selected to ensure $2\gamma_1 \in [t_1, 2 + t_1]$. By induction, we can construct $(\gamma_i, m_i)_{i=2}^n$ with the conditions

(2.1) $\gamma_i = m_{i-1}t_i + m_i$,

(2.2) $\gamma_i - \gamma_{i-1}/t_{i-1} \in \mathbb{Z}$,

(2.3) $\gamma_i \in [t_i/2, 1 + t_i/2]$,

where $2 \le i \le n$. Let $\gamma_2 = \gamma_1/t_1 + m_2'$ for some $m_2' \in \mathbb{Z}$ to be determined. By direct calculation, we have

$$\gamma_2 = \frac{z t_1 + m_1}{t_1} + m_2' = m_1(a_1 + t_2) + z + m_2' = m_1 t_2 + m_2$$

where $m_2 = m_1 a_1 + z + m_2'$. We take $m_2' \in \mathbb{Z}$ to ensure that $t_2 \le 2\gamma_2 \le 2 + t_2$. Suppose that (γ_i, m_i) has been constructed. We now construct (γ_{i+1}, m_{i+1}). Let $\gamma_{i+1} = \gamma_i/t_i + m_{i+1}'$ for some $m_{i+1}' \in \mathbb{Z}$ to be determined. We have

$$\gamma_{i+1} = \frac{m_{i-1}t_i + m_i}{t_i} + m_{i+1}' = m_i(a_i + t_{i+1}) + m_{i-1} + m_{i+1}' = m_i t_{i+1} + m_{i+1}$$

where $m_{i+1} = m_i a_i + m_{i-1} + m_{i+1}'$. We take certain $m_{i+1}' \in \mathbb{Z}$ to ensure $t_{i+1} \le 2\gamma_{i+1} \le 2 + t_{i+1}$ and the induction is completed.

(3) We now consider the bound of the first-order derivative $|\sigma_n'(0)|$. When q_n is even, the discriminant polynomial is an even function and we have $\sigma_n'(0) = 0$. Assume q_n is odd and denote $r = (q_n - 1)/2$. For $0 \le \gamma \le r$, the term S_γ has been defined by equation (5). We take $z = -2\gamma$ in (2) and obtain the array $(\gamma_i, m_i)_{i=1}^n$. Proposition 2.3 shows that $S_\gamma = \mathrm{Re}(S(p_n, q_n, -2\gamma p_n/q_n)) = \mathrm{Re}(S(u_1, v_1, \gamma_1))$. By Proposition 3.2, we have

$$|S_\gamma| \le |S(u_1, v_1, \gamma_1)| \le |I(u_1, v_1, \gamma_1)| + |T(u_2, v_2, \gamma_2, a_1 \pmod 2)|.$$

By Proposition 4.2, we also have

$$|S_\gamma| \le |I(u_1, v_1, \gamma_1)| + |J(u_2, v_2, \gamma_2, a_1 \pmod 2)| + \begin{cases} |S(u_3, v_3, \gamma_3)|, & a_1 \pmod 2 = 0, \\ |T(u_3, v_3, \gamma_3, a_2 + 1 \pmod 2)|, & a_1 \pmod 2 = 1. \end{cases}$$

After a recursive application of Propositions 3.2 and 4.2 along the sequence, Proposition 3.3 or Proposition 4.3 is applied at the final step. We thus obtain an upper bound of $|S_\gamma|$, which is a combination of integrals with a residue term R_γ at the end. The residue term can be bounded by $|R_\gamma| \le 2$. We have $|S_\gamma| \le 2 + \sum_{i=1}^n P_i$, where $P_i = |I(u_i, v_i, \gamma_i)|$ or $P_i = |J(u_i, v_i, \gamma_i, \delta_i)|$. By Proposition 3.1 and Proposition 4.1, we also have

$$|S_\gamma| \le 2 + \sum_{i=1}^n L_i \Big(4 \ln \frac{1}{t_i} + \frac{6}{\pi u_i} + \beta\Big),$$

where $L_i = (\sin(\pi t_i/2))^{-1}$ if $P_i = |J(u_i, v_i, \gamma_i, 0)|$, and $L_i = 1$ if $P_i = |I(u_i, v_i, \gamma_i)|$ or $P_i = |J(u_i, v_i, \gamma_i, 1)|$. Note that $L_i = (\sin(\pi t_i/2))^{-1}$ is unbounded when a_i is large enough. To obtain an upper bound for $|S_\gamma|$, we need to consider where the term $|J(u_i, v_i, \gamma_i, 0)|$ (or $|T(u_i, v_i, \gamma_i, 0)|$) appears along the sequence. The symbolic encoding is applied to solve this problem.

(4) For simplicity, the term $S(u_i, v_i, \gamma_i)$ is abbreviated as S and the term $T(u_i, v_i, \gamma_i, \delta_i)$ is abbreviated as $T(\delta_i)$. We claim that the term $T(0)$ appears at the i-th position when and only when a_i is a character a in the symbolic encoding of α. For the sequence $\tau = ea$, we assume that the term S appears at the first character e. Then the second term at a will be $T(e \pmod 2) = T(0)$. For the sequence $\omega_n = oee \cdots eoa$, we assume that the term S appears at the first character o. The second term at e is $T(o \pmod 2) = T(1)$ and the third term at e is $T(e + 1 \pmod 2) = T(1)$. By induction, all the terms after S are $T(1)$ except the final term at the character a, which is $T(o + 1 \pmod 2) = T(0)$. We still need to consider the sequence ε. We also assume that the term S appears at the first character o. The second term at e is $T(o \pmod 2) = T(1)$ and the third term at e is $T(e + 1 \pmod{y2}) = T(1)$. By induction, all the terms after S are $T(1)$. Note that the term after $T(0)$ is always S. Combining the observations above, we prove that the term $T(0)$ appears at the i-th position when and only when a_i is a character a in the symbolic encoding.

(5) For some $1 \le i \le n$, we assume that a_i is a character a in the symbolic encoding of α. We have $a_i \le M$ since α is M-weakly bounded. This shows that $t_i \ge 1/(M+1)$ and $L_i = (\sin(\pi t_i/2))^{-1} \le M + 1$. We are now able to derive an upper bound of the first-order derivative $|\sigma_n'(0)|$. We have obtained $|\sigma_n'(0)| \le \sum_{\gamma=0}^r e^{L_\gamma}$ and

Theorem 2.5 shows that $L_\gamma \le \gamma_0(\ln(q_n)+2)+|S_\gamma|$. We have

$$|S_\gamma| \le 2+\sum_{i=1}^{n}(M+1)\Big(4\ln\frac{1}{t_i}+\frac{6}{\pi u_i}+\beta\Big)$$
$$\le 2+(M+1)\Big(4\ln(q_n)+\Big(\beta+\frac{6}{\pi}\Big)n\Big).$$

Combining the inequalities above, we have

$$|\sigma_n'(0)| \le (r+1)e^{2+(\ln(q_n)+2)\gamma_0+(M+1)(4\ln(q_n)+(\beta+6/\pi)n)} \le e^{\lambda_1}e^{\lambda_2 n}q_n^{\lambda_3}$$

where $\lambda_{1,2,3}=\lambda_{1,2,3}(M)>0$ are constants.

(6) We now consider the bound of the second-order derivative $|\sigma_n''(0)|$. When q_n is odd, the second-order derivative of the discriminant polynomial is $\sigma_n''(0)=0$. We thus assume q_n is even, μ is odd, ν is even, and $1\le\mu<\nu\le q_n$. By Proposition 2.4, we have $S_{\mu\nu}=2(2\mu-2\nu+q_n)/q_n+S_\mu'+S_\nu'$ where

$$S_\mu'=\mathrm{Re}\Big(S'\Big(p_n,q_n,\frac{\mu p_n}{q_n}\Big)\Big),\quad S_\nu'=\mathrm{Re}\Big(S'\Big(p_n,q_n,\frac{\nu p_n}{q_n}\Big)\Big).$$

We first estimate the term S_μ'. We take $z=\mu$ in (2) and thus obtain the array $(\gamma_i,m_i)_{i=1}^n$. We have $|S_\mu'|\le|S'(p_n,q_n,\mu p_n/q_n)|\le|S'(u_1,v_1,\gamma_1)|$. After a recursive application of Proposition 3.4 and Proposition 4.4, we use Proposition 3.5 or Proposition 4.5 at the final step. We thus obtain the upper bound $|S_\mu'|\le\sum_{i=1}^n P_i+Q_i$ where $P_i=|I(u_i,v_i,\gamma_i)|$, $Q_i=|R(u_i,v_i,\gamma_i)|$ or $P_i=|J(u_i,v_i,\gamma_i,\delta_i)|$, $Q_i=|Q(u_i,v_i,\gamma_i,\delta_i)|$. We also have the bound $|Q_i|\le 12$. By Proposition 3.1 and Proposition 4.1, we have

$$|S_\mu'|\le 12n+\sum_{i=1}^{n}L_i\Big(4\ln\frac{1}{t_i}+\frac{6}{\pi u_i}+\beta\Big),$$

where $L_i=(\sin(\pi t_i/2))^{-1}$ if $P_i=|J(u_i,v_i,\gamma_i,0)|$, and where $L_i=1$ if $P_i=|I(u_i,v_i,\gamma_i)|$ or $P_i=|J(u_i,v_i,\gamma_i,1)|$. Similar to the method in (4), we claim that the term $|J(u_i,v_i,\gamma_i,0)|$ appears at the i-th position when and only when a_i is a character a in the symbolic encoding of α. We have $L_i\le M+1$ (for $1\le i\le n$) since α is M-weakly bounded. We obtain the bound

$$|S_\mu'|\le 12n+(M+1)\Big(4\ln(q_n)+\Big(\beta+\frac{6}{\pi}\Big)n\Big).$$

We have the same bound for $|S'_\nu|$. By Proposition 2.1 and Theorem 2.5, we have

$$\begin{aligned}|\sigma''_n(0)| &= \sum_{2\nmid\mu,2|\nu,1\leq\mu<\nu\leq q_n} 2e^{L_{\mu\nu}} \\ &\leq \sum_{2\nmid\mu,2|\nu,1\leq\mu<\nu\leq q_n} 2e^{2\gamma_0(\ln(q_n)+3)+|2(2\mu-2\nu+q_n)/q_n|+|S'_\mu|+|S'_\nu|} \\ &\leq \sum_{2\nmid\mu,2|\nu,1\leq\mu<\nu\leq q_n} 2e^{2\gamma_0(\ln(q_n)+3)+6+|S'_\mu|+|S'_\nu|}.\end{aligned}$$

By the inequalities above, we have

$$|\sigma''_n(0)| \leq e^{\lambda_1} e^{\lambda_2 n} q_n^{\lambda_3}$$

where $\lambda_{1,2,3} = \lambda_{1,2,3}(M) > 0$ are constants.

(7) Combining the bound of $|\sigma'_n(0)|$ in (5) and the bound of $|\sigma''_n(0)|$ in (6), we obtain

$$|\sigma'_n(0)| + |\sigma''_n(0)| \leq e^{\lambda_1} e^{\lambda_2 n} q_n^{\lambda_3}$$

where $\lambda_{1,2,3} = \lambda_{1,2,3}(M) > 0$ are constants. The proof is completed. ∎

6. Application to the central spectral band

In this section, Theorem 5.1 is applied to obtain a bound for the derivatives $|\sigma'_\alpha(0)|$ and $|\sigma''_\alpha(0)|$ under stronger conditions. We demonstrate the relation between the measure of the central spectral band and the derivatives of the discriminant polynomial. We then derive a lower bound for the measure of the central spectral band.

Corollary 6.1. *Given $\alpha \in (0,1)$ with the continued fraction $\alpha = [a_1, a_2, \ldots, a_n, \ldots]$, assume the symbolic encoding is $\alpha = \varepsilon$. We denote by $\sigma_n(x)$ the discriminant polynomial of the critical almost Mathieu operator with $\alpha_n = [a_1, a_2, \ldots, a_n]$. There exist constants $\lambda_{1,2,3} > 0$ independent of α so that*

$$|\sigma'_n(0)| + |\sigma''_n(0)| \leq e^{\lambda_1} e^{\lambda_2 n} q_n^{\lambda_3}$$

for $n \geq 1$.

Proof. There is no character a in the symbolic encoding $\alpha = \varepsilon$ and α is M-weakly bounded for any $M \in \mathbb{N}$. By the proof of Theorem 5.1, we can find the constants $\lambda_{1,2,3} > 0$ independent of M so that

$$|\sigma'_n(0)| + |\sigma''_n(0)| \leq e^{\lambda_1} e^{\lambda_2 n} q_n^{\lambda_3}$$

for $n \geq 1$. The proof is completed. ∎

Corollary 6.2. *Given $\alpha \in (0,1)$ with the continued fraction $\alpha = [a_1, a_2, \ldots, a_n, \ldots]$, assume α is M-weakly bounded for some $M \in \mathbb{N}$. We also assume*

$$\limsup_{m\to\infty} \Big(\prod_{n=1}^{m} a_n\Big)^{1/m} < +\infty. \tag{23}$$

Denote by $\sigma_n(x)$ the discriminant polynomial of the critical almost Mathieu operator with $\alpha_n = [a_1, a_2, \ldots, a_n]$, then there exists a constant $\lambda = \lambda(\alpha) > 0$ so that

$$|\sigma_n'(0)| + |\sigma_n''(0)| \le \lambda^n$$

for $n \ge 1$.

Proof. We denote the canonical representation by $\alpha_n = p_n/q_n$. Given $n \ge 1$, we have $q_{n+1} \le (a_{n+1}+1)q_n$. By condition (23), we have $a_1 a_2 \ldots a_n \le L^n (n \ge 1)$ for some constant $L > 0$. Combining the inequalities above, we have

$$q_n \le \prod_{i=1}^{n}(a_i + 1) \le \prod_{i=1}^{n} 2a_i \le (2L)^n.$$

By Theorem 5.1, there exist constants $\lambda_{1,2,3} = \lambda_{1,2,3}(\alpha) > 0$ so that

$$|\sigma_n'(0)| + |\sigma_n''(0)| \le e^{\lambda_1} e^{\lambda_2 n} q_n^{\lambda_3} \le e^{\lambda_1} e^{\lambda_2 n} (2L)^{\lambda_3 n}$$

for $n \ge 1$. The proof is completed. ∎

Given $\alpha = p/q$ and $(p,q) = 1$, the union of the spectrum $\sigma(\alpha,\theta)$ over $\theta \in \mathbb{R}$ has been denoted by $S(\alpha)$. We have defined the central spectral band of $S(\alpha)$ in Section 2. Denote the central spectral band by $\varDelta$. We now consider its measure. When q is odd, the central spectral band is the band containing the origin and Y. Last demonstrates its measure has the order(see [8])

$$\frac{6}{|\sigma_\alpha'(0)|} \le |\varDelta| \le \frac{8e}{|\sigma_\alpha'(0)|}. \tag{24}$$

An upper bound of the derivative $|\sigma_\alpha'(0)|$ determines a lower bound of the measure $|\varDelta|$. We now assume q is even and we claim the measure of the central spectral band can be bounded from below by the second-order derivative $|\sigma_\alpha''(0)|$.

Lemma 6.3. *Suppose $\alpha = p/q, (p,q) = 1$ and q is even. Denote by $\sigma_\alpha(x)$ the discriminant polynomial of the critical almost Mathieu operator and by $\varDelta$ the central spectral band. We have*

$$|\varDelta| \ge \frac{8}{\sqrt{|\sigma_\alpha''(0)|}}. \tag{25}$$

Proof. Suppose that $\Sigma(x)$ is an n-order polynomial with n distinct real roots x_i (for $1 \le i \le n$). We assume $x_i < x_j$ for $1 \le i < j \le n$. Given $1 \le i \le n-1$, there exists a unique point $x_i' \in (x_i, x_{i+1})$ with $\Sigma'(x_i') = 0$. It is not hard to prove that $\Sigma(x)$ is strictly increasing (or decreasing) on $[x_i, x_i']$ and strictly decreasing (or increasing) on $[x_i', x_{i+1}]$. This observation is significant for the proof since the discriminant polynomial $\sigma_\alpha(x)$ has q distinct real roots. We have $\sigma_\alpha'(0) = 0$ and $|\sigma_\alpha(0)| = 4$. We may assume $\sigma_\alpha(0) = 4$ and the condition $\sigma_\alpha(0) = -4$ is similar. Denote by $x_0 > 0$ the right endpoint of the central spectral band Δ. We have $\sigma_\alpha(x_0) = -4$ and

$$\int_0^{x_0} \sigma_\alpha'(x)\,\mathrm{d}x = -8. \tag{26}$$

We claim $\sigma_\alpha'(x) \ge \sigma_\alpha''(0)x$ for any $x \in [0, x_0]$. This claim is obvious when $q = 2$ and we now assume $q \ge 4$. Denote by $x_1 \ge x_0$ the first critical point of $\sigma_\alpha(x)$ to the right of the origin. There is an inflection point $x_2 \in (0, x_1)$ of the discriminant polynomial. The second-order derivative $\sigma_\alpha''(t)$ is negative on $(0, x_2)$ and positive on (x_2, x_1). We have $\sigma_\alpha''(t) \ge \sigma_\alpha''(0)$ for any $t \in [0, x_1]$. For $x \in [0, x_0]$, we obtain the inequality

$$\int_0^{x} \sigma_\alpha''(t)\,\mathrm{d}t \ge \int_0^{x} \sigma_\alpha''(0)\,\mathrm{d}t$$

which shows that $\sigma_\alpha'(x) \ge \sigma_\alpha''(0)x$. Combining this with equation (26), we have $|\Delta| \ge 8/\sqrt{|\sigma_\alpha''(0)|}$ and the proof is completed. ∎

We have obtained an upper bound for the derivatives $|\sigma_\alpha'(0)|$ and $|\sigma_\alpha''(0)|$ in Theorem 5.1. By inequalities (24) and (25), we can derive a lower bound for the measure of the central spectral band.

Corollary 6.4. *Given $\alpha \in (0,1) \cap \mathbb{Q}^c$ and $M \in \mathbb{N}$, suppose the continued fraction is $\alpha = [a_1, a_2, \ldots, a_n, \ldots]$ and α is M-weakly bounded. Denote by Δ_n the central spectral band of the critical almost Mathieu operator with $\alpha_n = [a_1, a_2, \ldots, a_n]$, then there exist constants $\lambda_{1,2,3} = \lambda_{1,2,3}(M) > 0$ so that*

$$|\Delta_n| \ge (e^{\lambda_1} e^{\lambda_2 n} q_n^{\lambda_3})^{-1}$$

for $n \ge 1$.

Proof. By Theorem 5.1, there exist constants $\lambda_{1,2,3} = \lambda_{1,2,3}(M) > 0$ so that

$$|\sigma_n'(0)| + |\sigma_n''(0)| \le e^{\lambda_1} e^{\lambda_2 n} q_n^{\lambda_3}$$

for $n \ge 1$. By inequality (24), we have $|\Delta_n| \ge 6(e^{\lambda_1} e^{\lambda_2 n} q_n^{\lambda_3})^{-1}$ when q_n is odd. By inequality (25), we have $|\Delta_n| \ge 8(e^{\lambda_1} e^{\lambda_2 n} q_n^{\lambda_3})^{-1/2}$ when q_n is even. Combining these inequalities, the proof is completed. ∎

Suppose $\alpha \in (0,1) \cap \mathbb{Q}^c$ satisfies the condition in Corollary 6.1 or Corollary 6.2. Similar to Corollary 6.4, we can also derive a lower bound for the measure of the central spectral band and the details are omitted.

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