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On Minima of Sum of Theta Functions and Application to Mueller–Ho Conjecture

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Abstract

Let $z = x + iy \in \mathbb{H} := \{z = x + iy \in \mathbb{C} : y > 0\}$ and $\theta(s; z) = \sum_{(m,n)\in\mathbb{Z}^2} e^{-s\frac{\pi}{y}|mz+n|^2}$ be the theta function associated with the lattice $\Lambda = \mathbb{Z}\oplus z\mathbb{Z}$. In this paper we consider minimization problems

$$\begin{aligned} &\min_{\mathbb{H}} \theta\left(2; \frac{z+1}{2}\right) + \rho\theta(1; z), \quad \rho \in [0, \infty), \\ &\min_{\mathbb{H}} \theta\left(1; \frac{z+1}{2}\right) + \rho\theta(2; z), \quad \rho \in [0, \infty), \end{aligned} \tag{0.1}$$

where the parameter $\rho \in [0, \infty)$ represents the competition of two intertwining lattices, and the particular selection of the parameters $s = 1, 2$ is determined by the physical model, which can be generalized by our strategy and method proposed here. We find that as ρ varies, the optimal lattices admit a novel pattern: they move from rectangular (the ratio of long and short sides changes from $\sqrt{3}$ to 1 continuously), square and rhombus (the angle changes from $\pi/2$ to $\pi/3$ continuously) to hexagonal continuously; geometrically, up to an invariant group (a subgroup of the classical modular group), they move continuously on a special curve; furthermore, there exists a closed interval of ρ such that the optimal lattices is always a square lattice. This is the first, novel and also the complete result on the minimizer problem for theta functions with parameter ρ. This is in sharp contrast to optimal lattice shapes for a single theta function ($\rho = \infty$ case), for which the hexagonal lattice prevails. As a consequence, we give a partial and positive answer to optimal lattice arrangements of vortices in competing systems of Bose–Einstein condensates as conjectured (and numerically and experimentally verified) by Mueller and Ho (Phys Rev Lett 88:180403, 2002); this is the first progress on the Mueller–Ho conjecture. Lastly, we mention that the strategy and method we propose here is general, and can be used in much more general minimization problems on the lattices.

1. Introduction and Statement of Main Results

Let $z \in \mathbb{H} := \{z = x + iy \in \mathbb{C} : y > 0\}$ and $\Lambda = \sqrt{\frac{1}{y}}\Big(\mathbb{Z} \oplus z\mathbb{Z}\Big)$ with area of unit cell is 1 be the lattice in $\mathbb{R}^2$ parameterized by z. The theta function associated with the lattice Λ is defined as

$$\theta(s; \Lambda) := \sum_{\mathbb{P}\in\Lambda} e^{-\pi s|\mathbb{P}|^2}.$$

By $\Lambda = \sqrt{\frac{1}{y}}\Big(\mathbb{Z} \oplus z\mathbb{Z}\Big)$, one has

$$\theta(s; z) := \theta(s; \Lambda) = \sum_{(m,n)\in\mathbb{Z}^2} e^{-s\frac{\pi}{y}|mz+n|^2}. \tag{1.1}$$

In 1988, Montgomery [28] proved the following celebrated result:

Theorem 1.1. *For all $s > 0$ and $z \in \mathbb{H}$,*

$$Minima\ \theta(s; z)_{z\in\mathbb{H}} = z_0, \tag{1.2}$$

where $z_0 = \frac{1}{2} + i\frac{\sqrt{3}}{2}$ (the triangular lattice, or called hexagonal lattice is the lattice $A_2 = \mathbb{Z} \oplus z_0\mathbb{Z}$.). Equality holds if and only if $z = z_0$ (up to the group $\mathcal{G}_1$ [see (3.2), Section 3)].

For the higher dimensional cases, the corresponding minimization problems on lattices was first investigated by Sarnak and Strombergsson [30] and recently by Cohn et al. [12,13]. For relations with sphere packing problems, see Viazovska [34] and Cohn et al. [12] and the references therein. We mention that minimization problems for Dedekind eta function (equivalent to the theta function (1.1) via Mellin transform) also arise in the extremal determinants of Laplace–Beltrami Operators. See Osgood et al. [27], Faulhuber [16], Bétermin and Sandier [3], and the reference therein.

The celebrated Theorem 1.1 laid the foundations for many optimal lattice problems in number theory and has been frequently used in applied mathematical and physical models such as crystallizations of particle interactions (Blanc and Lewin [10]; Bétermin [5,6]; Bétermin and Zhang [4]), Ginzburg–Landau theory in superconductors (Abrikosov [1]; Sandier and Serfaty [31,32], Serfaty [33]), Ohta–Kawasaki models in di-block copolymers (Chen and Oshita [11]; Goldman et al. [17]; Ren and Wei [29]), minimal frame operator norms (Faulhuber [15]) and many others. The related minimization of theta and eta functions on lattices has application to Gross–Pitaevskii theory in superfluids or Bose–Einstein condensates, Ohta–Kawasaki models triblock copolymers (Luo et al. [24]) and many others.

In this paper, we consider a minimization problem with sum of **two** theta functions, which represent **two** intertwining lattices, one lattice shifted by the center of the other lattice; See Fig. 1 and the physical explanation in the next section.

Let $\rho > 0$ denote the relative strength of the two lattices. Consider the functional

$$\mathcal{W}_{1,\rho}(z) := \theta\left(2; \frac{z+1}{2}\right) + \rho\theta(1; z). \tag{1.3}$$

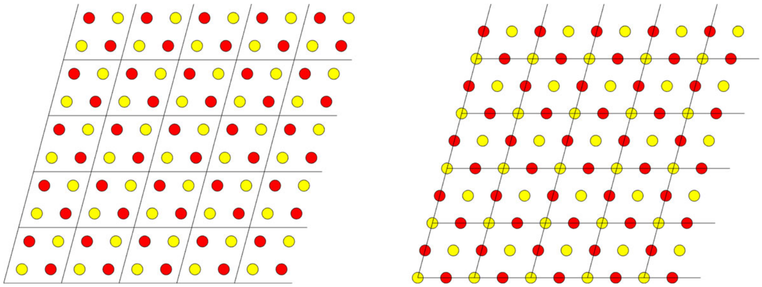

Fig. 1. Two lattices with centers at the lattice points and the half lattice points

It is easy to see that $\mathcal{W}_{1,\rho}(z)$ is invariant under the group (see Section 3)

$$\mathcal{G}_2 : \text{the group generated by } \ z \mapsto -\frac{1}{z}, \quad z \mapsto z+2, \quad z \mapsto -\overline{z}. \tag{1.4}$$

The new minimization problem we consider is the following:

$$\min_{z\in\mathbb{H}} \mathcal{W}_{1,\rho}(z), \quad \rho \in [0,\infty). \tag{1.5}$$

Our first main result is the following theorem which gives a complete characterization of the minimization problem (1.5), as ρ varies:

Theorem 1.2. *The minimization problem* (1.5) *admits a unique minimizer $z_{1,\rho}$ which moves continuously on a special curve as the parameter ρ varies (up to the group $\mathcal{G}_2$). The trajectory curve of the minimizer, denoted by Ω_e* (see Fig. 2)*, is given by*

$$\begin{aligned} \Omega_e &:= \Omega_{ea} \cup \Omega_{eb}, \\ \Omega_{ea} &:= \{z : x = 0, 1 \leqq y \leqq \sqrt{3}\}, \\ \Omega_{eb} &:= \left\{ z : |z| = 1, 0 \leqq x < \frac{1}{2} \right\}. \end{aligned} \tag{1.6}$$

More precisely, there exist two thresholds $\sigma_{1,a} = 0.04016 \cdots < \sigma_{1,b} = 0.83972 \cdots$ such that

(1) *if ρ varies in $[0, \sigma_{1,a}]$, the minimizer $z_{1,\rho}$ moves from $\sqrt{3}i$ to i along the vertical line segment Ω_{ea} correspondingly;*
(2) *if $\rho \in [\sigma_{1,a}, \sigma_{1,b}]$, the minimizer $z_{1,\rho}$ stays fixed on the corner of the curve Ω_e, that is,*

$$z_{1,\rho} \equiv i, \quad \textit{if} \ \ \rho \in [\sigma_{1,a}, \sigma_{1,b}];$$

(3) *if ρ varies in $[\sigma_{1,b}, \infty)$, the minimizer $z_{1,\rho}$ moves from i to $\frac{1}{2} + i\frac{\sqrt{3}}{2}$ along the unit arc Ω_{eb}. Moreover*

$$\textit{as } \rho \to \infty, \quad z_{1,\rho} \to \frac{1}{2} + i\frac{\sqrt{3}}{2} \ \ \textit{from left hand side of } \ \Omega_{eb}.$$

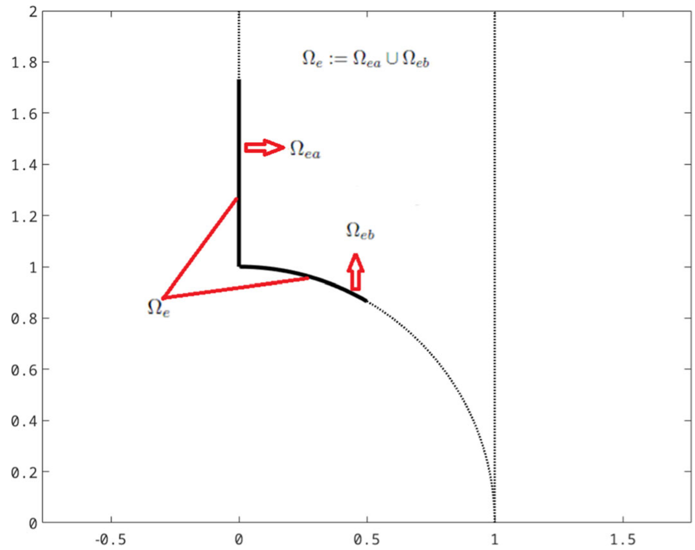

Fig. 2. The curve Ω_e

Remark 1.1. In [24], with X. Ren, we studied another minimization problem:

$$\min_{z\in\mathbb{H}} -\left((1-b)\left(\frac{1}{2}\log(\sqrt{y}|\eta(z)|^2)\right)\right)+b\left(\frac{1}{2}\log\left(\sqrt{y}\left|\eta\left(\frac{z+1}{2}\right)\right|^2\right)\right), \tag{1.7}$$
$$z=x+iy,\quad b\in[0,1],$$

where η is the Dedekind eta function

$$\eta(z)=e^{\frac{\pi}{3}\pi i}\prod_{n=1}^{\infty}(1-e^{2\pi nzi})^4. \tag{1.8}$$

When $b=0$, this is the minimization problem studied by Chen and Oshita [11] and Sandier and Serfaty [32]. While Chen and Oshita used analytical method to prove that the triangular lattice is the optimal, Sandier and Serfaty made use of a relation between the Dedekind eta function and the Epstein zeta function (Mellin transform), and then Theorem 1.1 to arrive at the same conclusion. When $0<b<1$, we have showed a similar transition phenomenon from rectangle lattice to hexagonal lattice to Theorem 1.2 in [24] for the functional in (1.7).

We also consider another minimization problem, which can be viewed as a "conjugate" problem to (1.5):

$$\begin{aligned}&\min_{z\in\mathbb{H}} \mathcal{W}_{2,\rho}(z),\quad \rho\in[0,\infty),\\ &\text{where } \mathcal{W}_{2,\rho}(z):=\theta\left(1;\frac{z+1}{2}\right)+\rho\theta(2;z).\end{aligned} \tag{1.9}$$

The precise relation between $\mathcal{W}_{1,\rho}$ and $\mathcal{W}_{2,\rho}$ can be found in Lemma 3.3. The minimizers of (1.9) can be characterized as follows:

Theorem 1.3. *The minimization problem* (1.9) *admits a unique minimizer* $z_{2,\rho}$ *which lies on the curve* Ω_e (1.6) (*up to the group* $\mathcal{G}_2$ (1.4)). *There exist two thresholds* $\sigma_{2,a} = 1.190861337\cdots$, $\sigma_{2,b} = 24.89618074\cdots$ *such that*

(1) *if* ρ *varies from left to right on* $[0, \sigma_{2,a}]$, *the minimizer* $z_{2,\rho}$ *moves from* $\sqrt{3}i$ *to* i *on the vertical line segment* Ω_{ea};
(2) *if* $\rho \in [\sigma_{2,a}, \sigma_{2,b}]$, *the minimizer* $z_{2,\rho}$ *stays fixed on the corner of curve* (1.6), *that is* $z_{2,\rho} \equiv i$;
(3) *if* ρ *moves from left to right on* $[\sigma_{2,a}, \infty)$, *the minimizer* $z_{2,\rho}$ *moves from left to right along the unit curve* Ω_{eb}. *Furthermore,*

$$\text{as } \rho \to \infty,\ z_{2,\rho} \to \frac{1}{2} + i\frac{\sqrt{3}}{2} \text{ from left hand side of } \Omega_{eb}.$$

Remark 1.2. The values of $\sigma_{1,a}, \sigma_{1,b}, \sigma_{2,a}$ and $\sigma_{2,b}$ are given explicitly in terms of Jacobi Theta functions (See Theorem 1.4 below.)

Remark 1.3. We found that the minimizers of the minimization problems (1.5) and (1.9) admit a novel pattern: they bond together in a very special way and form a nice geometric shape and move with the parameter in a monotone way. It is remarkable that in a suitable range of the parameter, the minimizer is always a square lattice. The optimal lattices have richer structures than that of Theorem 1.1.

There are some hidden connections revealed later between the two minimization problems (1.5) and (1.9). They are like "a pair" as shown in Table 1 below. The following theorem gives more qualitative behaviors of minimizers in Theorems 1.2 and 1.3, and is our major theorem of this paper:

Theorem 1.4. *We state the almost exact formulas on the minimizers of* (1.5) *and* (1.9) *for* $\rho \in [0, \infty)$.

(1) *The minima of* $\mathcal{W}_{j,\rho}(z)$, $j = 1, 2$ *is unique for each* $\rho \in [0, \infty)$ *up to the group* $\mathcal{G}_2$. *Furthermore,*

$$Minima_{z\in\mathbb{H}}\mathcal{W}_{1,\rho}(z) = \begin{cases} iy_{1,\rho}, & \text{if } \rho \in [0, \rho_1), \\ i, & \text{if } \rho \in [\rho_1, 1/\rho_2], \\ e^{i\theta_{2,\rho}}, \theta_{2,\rho} = \arctan\frac{2y_{2,1/\rho}}{y_{2,1/\rho}^2 - 1}, & \text{if } \rho \in (1/\rho_2, \infty). \end{cases} \tag{1.10}$$

and

$$Minima_{z\in\mathbb{H}}\mathcal{W}_{2,\rho}(z) = \begin{cases} iy_{2,\rho}, & \text{if } \rho \in [0, \rho_2), \\ i, & \text{if } \rho \in [\rho_2, 1/\rho_1], \\ e^{i\theta_{1,\rho}}, \theta_{1,\rho} = \arctan\frac{2y_{1,1/\rho}}{y_{1,1/\rho}^2 - 1}, & \text{if } \rho \in (1/\rho_1, \infty). \end{cases} \tag{1.11}$$

Here $y_{1,\rho}, y_{2,\rho} \in (1, \sqrt{3}]$ *for* $\rho \in [0, \rho_1)$ *and* $\rho \in [0, \rho_2)$ *respectively,* $\theta_{1,\rho}, \theta_{2,\rho} \in (\frac{\pi}{3}, \frac{\pi}{2})$ *for* $\rho \in (1/\rho_1, \infty)$ *and* $\rho \in (1/\rho_2, \infty)$ *respectively. For the qualitative behaviors of* $y_{j,\rho}, \theta_{j,\rho}$, $j = 1, 2$, *we have*

$$\frac{\mathrm{d}}{\mathrm{d}\rho} y_{j,\rho} < 0, \textit{for } \rho \in [0, \rho_j); \ \frac{\mathrm{d}}{\mathrm{d}\rho}\theta_{j,\rho} < 0, \textit{for } \rho \in (1/\rho_j, \infty).$$

See more on this theorem in (3).

(2) ρ_1, ρ_2 *in* (1.10) *and* (1.11), *respectively, are determined explicitly by*

$$\rho_1 = -\frac{\mathcal{Y}''(1)}{\mathcal{X}''(1)}, \quad \rho_2 = -1 - \frac{\mathcal{B}''(1)}{\mathcal{A}''(1)}.$$

Here

$$\begin{aligned} &\mathcal{X}(y) := \vartheta_3(y)\vartheta_3\left(\frac{1}{y}\right), \qquad \mathcal{Y}(y) := 2\left(\vartheta_3(4y)\vartheta_3\left(\frac{4}{y}\right) + \vartheta_2(4y)\vartheta_2\left(\frac{4}{y}\right)\right) \\ &\mathcal{A}(y) := \sqrt{2}\vartheta_3(2y)\vartheta_3(\frac{2}{y}), \quad \mathcal{B}(y) := \sqrt{2}\vartheta_2(2y)\vartheta_2(\frac{2}{y}) \end{aligned} \tag{1.12}$$

and the Jacobi theta functions are defined as

$$\vartheta_2(y) = \sum_{n\in\mathbb{Z}} e^{-\pi(n-\frac{1}{2})^2 y}, \quad \vartheta_3(y) = \sum_{n\in\mathbb{Z}} e^{-\pi n^2 y}, \quad \vartheta_4(y) = \sum_{n\in\mathbb{Z}} (-1)^n e^{-\pi n^2 y}. \tag{1.13}$$

The thresholds in Theorems 1.2 *and* 1.3 *are given by*

$$\sigma_{1,a} = \frac{1}{\sigma_{2,b}} = \rho_1, \quad \sigma_{1,b} = \frac{1}{\sigma_{2,a}} = \frac{1}{\rho_2},$$

(3) The $y_{1,1/\rho}$ *and* $y_{2,1/\rho}$ *in* (1.10) *and* (1.11) *are implicitly determined by*

$$\begin{aligned} &y_{1,1/\rho} \ \textit{ is the unique solution of } \ \frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)} + 1/\rho = 0, \ y \in (1, \sqrt{3}] \\ &y_{2,1/\rho} \ \textit{ is the unique solution of } \ 1 + \frac{\mathcal{B}'(y)}{\mathcal{A}'(y)} + 1/\rho = 0, \ y \in (1, \sqrt{3}]. \end{aligned} \tag{1.14}$$

Furthermore, it holds that

$$\frac{\mathrm{d}}{\mathrm{d}\rho} y_{1,\rho} < 0, \forall \rho \in [0, \rho_1] \ \textit{ and } \ \frac{\mathrm{d}}{\mathrm{d}\rho} y_{2,\rho} < 0, \forall \rho \in [0, \rho_2].$$

The existence and uniqueness of $y_{1,1/\rho}, y_{2,1/\rho}$ in the Theorems 1.2 and 1.3 are consequences of the following theorem whose proof will be given by Theorems 6.1 and 7.1 . (Here $\mathcal{X}(y)$, $\mathcal{Y}(y)$ and $\mathcal{A}(y)$, $\mathcal{B}(y)$ are defined in (1.12).)

Theorem 1.5. *The critical points and monotonicity of quotients of derivatives.*

- *The function* $y \mapsto \frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)}$, $y > 0$ *has only one critical point at* $y = 1$, *and it holds that*

$$\left(\frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)}\right)' < 0, \quad y \in (0, 1) \textit{ and } \left(\frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)}\right)' > 0, \quad y \in (1, \infty).$$

• *The function* $y \mapsto \frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}$, $y > 0$ *has only one critical point at* $y = 1$, *and it holds that*

$$\Big(\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}\Big)' < 0, \quad y \in (0, 1) \;\; \textit{and} \; \Big(\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}\Big)' > 0, \quad y \in (1, \infty).$$

Theorem 1.2 has direct applications to the Mueller–Ho functional and Mueller–Ho Conjecture in vortices arrangements for competing systems of Bose-Einstein condensates, as we explain in the next section.

We should also point out that, our strategy and method in proving Theorems 1.2 and 1.4 can be used in solving more general minimization problems

$$\begin{aligned} &\min_{\mathbb{H}} \theta\left(2t; \frac{z+1}{2}\right) + \rho\theta(t; z), \quad \rho \in [0, \infty), \\ &\min_{\mathbb{H}} \theta\left(t; \frac{z+1}{2}\right) + \rho\theta(2t; z), \quad \rho \in [0, \infty), \end{aligned} \tag{1.15}$$

with arbitrary $t > 0$. We have a pattern similar to Theorem 1.4 for the problem (1.15).

It is natural to consider the following pair of minimization problems from the point of view pure mathematical interest:

$$\begin{aligned} &\min_{\mathbb{H}} \theta\left(s; \frac{z+1}{2}\right) + \rho\theta(t; z), \quad \rho \in [0, \infty), \\ &\min_{\mathbb{H}} \theta\left(t; \frac{z+1}{2}\right) + \rho\theta(s; z), \quad \rho \in [0, \infty), \end{aligned} \tag{1.16}$$

with arbitrary $s, t > 0$.

It turns out that the minimization problem (1.15) is the critical case of problem (1.16) in the sense of the parameters s, t to have the completely continuous phase transitions as found in Theorem 1.4.

The minimization results of problems (1.15) and (1.16) can be generalized directly to the sum of two completely monotone functions on the lattices.

These are left to further work.

2. Applications to Mueller–Ho Conjecture

As we have mentioned in Section 1, the problem of finding optimal lattice shapes arises in many physical models. Besides those examples mentioned in Section 1, other examples is the so-called vortices in Bose–Einstein condensates. Vortices in Bose–Einstein condensates are also called topological defects, correspond to a zero of the order parameter with a circulation of the phase. When they get numerous, these vortices arrange themselves on a lattice. In fact, in rotating Bose–Einstein condensates (BEC), vortices were first observed in two-component BEC's (Matthews et al. [25]); it is observed experimentally that the shape of the lattice can be either hexagonal or square depending on the rotational velocity of the condensate. Since then, following the pioneering work of Mueller and Ho [26], many authors have investigated the lattice shape in two component BEC's and for instance Kasamatsu et al. [20,21]; related works include Keeli and Oktel [19] who numerically calculate the elastic coefficients of the lattice. In Kuokanportti et al. [22], the authors investigate the case of different masses and attractive interactions.

The ground state of a two-component condensate is well described by a Gross-Pitaevskii energy depending on the wave functions of each component which are coupled by an interaction term. The construction of the Bose–Einstein condensates with large number of vortices was deduced in Ho [18] (one-component case) and Mueller and Ho [26] (two-component case), with the potential energy given by

$$\mathcal{V} = \frac{1}{2}g_1|\Psi_1|^4 + \frac{1}{2}g_2|\Psi_2|^4 + g_{12}|\Psi_1|^2|\Psi_2|^2,$$

where g_{12} represents the competing strength between the two components of Bose gas. We omit the details of the construction of the model here. In Mueller and Ho [26] they have reduced the minimization problems on lattices to the minimization problems for the Mueller–Ho functional

$$\min_{z\in\mathbb{H},(a,b)} \mathcal{E}_{MH}(z;a,b), \alpha\in[-1,1], \text{ where } \mathcal{E}_{MH}(z) := \theta(1;z) + \alpha\mathcal{J}(z;a,b). \tag{2.1}$$

Here $\Lambda = \sqrt{\frac{1}{y}}\Big(\mathbb{Z}\oplus z\mathbb{Z}\Big)$ denotes the lattice of one-component Bose gas A, and the theta function $\theta(1;z)$ (defined at (1.1)) represents the self-interaction part of single component of A or B, that is, the so-called Abrikosov energy (See Abrikosov [1]). The functional

$$\mathcal{J}(z;a,b) = \sum_{(m,n)\in\mathbb{Z}^2} e^{-\frac{\pi}{y}|mz-n|^2}\cos(2\pi(ma+nb)) \tag{2.2}$$

characterizes the competing strength of two-component A and B. $\alpha = \frac{g_{12}}{\sqrt{g_1 g_2}}$ represents the strength of competition between two competing components A and B. The vector (a,b) characterizes the relative position of the these lattice shape. See Fig. 1 when $(a,b)=(\frac{1}{2},\frac{1}{2})$.

Mathematically, by Poisson Summation Formula, the energy functional $\mathcal{J}(z;a,b)$ is the energy of translated lattice by the vector $\{a,b\}$, namely

$$\mathcal{J}(z;a,b) = \theta(1;\Lambda+\{a,b\}). \tag{2.3}$$

Here the lattice Λ is parameterized by $\Lambda = \sqrt{\frac{1}{y}}\Big(\mathbb{Z}\oplus z\mathbb{Z}\Big)$. The formula (2.3) is also pointed out in Mueller and Ho [26].

It is interesting to compare the two-component case with the single-component case. In the latter system, energy minimization reduces to minimizing $\theta(1;z)$ whose only local minimum is the triangular lattice, where $z = z_0 = e^{i\frac{\pi}{3}}$ and $\theta(1;z_0) = 1.1596$ (by Theorem 1.1); the square lattice $z = i$ is a saddle point with $\theta(1;i) = 1.1803$. For two-component case, the minimum of $\mathcal{E}_{MH}(z;a,b)$ depends on the relative strength α and the relative position of the lattices, as conjectured by Mueller and Ho [26] (supported by numerical computations and experimental results).

Mueller–Ho Conjecture: For a two-component Bose gas, the most favorable lattice minimizing $\theta(1; z) + \alpha\mathcal{J}(z; a, b)$ are

(a) $\alpha < 0$: the vortices of the two components coincide with each other ($a = b = 0$) to form a triangular lattice ($z = e^{i\frac{\pi}{3}}$).
(b) $0 < \alpha < 0.172$: the vortex lattice in each component remains triangular. However one lattice is displaced to the center of the triangle of the other $a = b = \frac{1}{3}$. The lattice type (characterized by $z = z_0 = e^{i\frac{\pi}{3}}$) remains constant within this interval.
(c) $0.172 < \alpha < 0.373$: (a, b) jumps from the center of the triangle (that is, half of the unit cell) to the center of the rhombic unit cell $a = b = \frac{1}{2}$. The angle jumps from 60^o to 67.95^o at $\alpha = 0.172$, and increases continuously to 90^o as α increases to 0.372. As a result, the lattice shape type is no longer fixed and the unit cell is rhombus. The modulus $\frac{b}{a}$, however, remains fixed across this region.
(d) $0.373 < \alpha < 0.926$: the two lattices are "mode locked" into a centered square structure throughout the entire interval ($z = i, a = b = \frac{1}{2}$).
(e) $0.926 < \alpha < 1$: the lattice type again varies continuously with interaction α. Each component's vortex lattice has a rectangular unit cell (angle$= \frac{\pi}{2}$) whose aspect ratio $|z|$ increases with α. At $\alpha = 1$, the aspect ratio is $\sqrt{3}$.

Remark 2.1. Both Rb^{87} and Na^{23} have interaction parameters with the range (d), that is, $0.373 < \alpha < 0.926$ (see Mueller and Ho [26] and the references therein).

For more on the vortex shape and Bose–Einstein condensates, including the construction of theoretical models and numerical and experimental results, we refer to [20,21,25] and the references therein. In [19] the authors considered Tkachenko modes and verified the same numerical results as in Mueller–Ho Conjecture. It seems that the Mueller–Ho conjecture is a universal phenomenon, as commented by Bétermin [7] that *"the same phenomenon in Mueller–Ho results is also expected in other physical and biological models involving infinite lattices and competitive interactions"*. See also numerical computations in Bétermin et al. [9] for systems with alternating charges ± 1.

To study the minimizer of the Muller–Ho functional $\mathcal{E}_{MH}(z; a, b) = \theta(1; z) + \alpha\mathcal{J}(z; a, b)$ with respect to $(z; a, b)$, we first need to identify the critical points of $\mathcal{E}_{MH}$ which satisfy

$$\nabla_z\theta(1; z) + \alpha\nabla_z\mathcal{J}(z; a, b) = 0, \tag{2.4}$$

$$\nabla_{(a,b)}\mathcal{J}(z; a, b) = 0. \tag{2.5}$$

To consider the global minimum of $\theta(1; z)+\alpha\mathcal{J}(z; a, b)$, a necessary condition is that (a, b) must be a minimum of $\mathcal{J}(z; a, b)$. Thus we first focus on critical point equation (2.5).

For the function $\mathcal{J}(z; a, b)$ with respect to (a, b), one sees clearly that

$$\mathcal{J}(z; a + 1, b) = \mathcal{J}(z; a, b), \quad \mathcal{J}(z; a, b + 1) = \mathcal{J}(z; a, b) \tag{2.6}$$

$$\mathcal{J}(z; 1 - a, 1 - b) = \mathcal{J}(z; a, b). \tag{2.7}$$

The periodicity and symmetry imply that $(a, b) \mapsto \mathcal{J}(z; a, b)$ has four universal critical points, which are denoted by

$$w_0 := (0, 0),\ w_1 := \left(\frac{1}{2}, 0\right),\ w_2 := \left(0, \frac{1}{2}\right),\ w_3 := w_1 + w_2 = \left(\frac{1}{2}, \frac{1}{2}\right) \tag{2.8}$$

We call "universal" here since they are independent of the lattice structures that is, z. Clearly, the critical point w_0 is the global maxima of $\mathcal{J}(z; a, b)$ with respect to (a, b). For critical points w_1, w_2, w_3, we have the following partial classification result (the proof will be given in Section 9):

Lemma 2.1. *Let $z = iy$, $y > 0$. It holds that*

- *w_1, w_2 are the saddle points of $\mathcal{J}(z; a, b)$ with respect to (a, b). Explicitly, the Hessian at each point can be expressed by*

$$D^2 J(z; a, b) \mid_{\{z=iy,(a,b)=w_1\}} = 16\pi^2 \vartheta_3\left(\frac{1}{y}\right)\vartheta_3'\left(\frac{1}{y}\right)\vartheta_4(y)\vartheta_4'(y) < 0$$

$$D^2 J(z; a, b) \mid_{\{z=iy,(a,b)=w_2\}} = 16\pi^2 \vartheta_3(y)\vartheta_3'(y)\vartheta_4\left(\frac{1}{y}\right)\vartheta_4'\left(\frac{1}{y}\right) < 0.$$

- *w_3 is the local minimum of $\mathcal{J}(z; a, b)$ with respect to (a, b). Explicitly, one has the Hessian expression*

$$D^2 J(z; a, b) \mid_{\{z=iy,(a,b)=w_3\}} = 16\pi^2 \vartheta_4(y)\vartheta_4'(y)\vartheta_4\left(\frac{1}{y}\right)\vartheta_4'\left(\frac{1}{y}\right) > 0.$$

For $(a, b) = (0, 0)$, $\mathcal{J}(z; 0, 0) = \theta(1; z)$. Combining Theorem 1.1 and using the fact that w_0 is the global maxima of $\mathcal{J}(z; a, b)$, we have the following proposition which confirms the (a) part of Mueller–Ho Conjecture:

Proposition 2.1. *For $\alpha \in [-1, 0]$, the minimizer of the functional $\mathcal{E}_{MH}(z; a, b) = \theta(1; z) + \alpha\mathcal{J}(z; a, b)$ is achieved at $z_0 = \frac{1}{2} + i\frac{\sqrt{3}}{2}$ and $(a, b) = (0, 0)$.*

Besides the above 4 universal critical points, there may be other additional pair critical points. (Note that by symmetry if (a, b) is a critical point then $(1-a, 1-b)$ is also a critical point.) We have

Lemma 2.2. *If $z = i$, then $(a, b) = (\frac{1}{3}, \frac{1}{3})$ is not a critical point of $\mathcal{J}(z; a, b)$; while $(a, b) = (\frac{1}{3}, \frac{1}{3})$ (and $(a, b) = (\frac{2}{3}, \frac{2}{3})$) is a critical point of $\mathcal{J}(z; a, b)$ if $z = \frac{1}{2} + i\frac{\sqrt{3}}{2}$.*

The proof of Lemma 2.2 will be given in "Appendix 1".

On the critical point equation (2.5), the numerical simulation suggests the following conjecture:

Conjecture 2.1. *The function $\mathcal{J}(z; a, b)$ with respect to the a, b has either 4 or 6 critical points depending on modulus of the tori z. Let Ω_4 (resp. Ω_6) be the subset of $\mathbb{H}$ which corresponds to tori z having four (resp. six) critical points. It holds that* *a : Alterative: either 4 or 6 critical points, that is,*

$$\mathbb{H} = \Omega_4 \cup \Omega_6, \quad \Omega_4 \cap \Omega_6 = \emptyset.$$

b : Rectangular tori has only four critical points and the hexagonal one has six.

$$i \in \{z \,|: \mathrm{Re}(z) = 0, \mathrm{Im}(z) > 0\} \subset \Omega_4, \frac{1}{2} + i\frac{\sqrt{3}}{2} \in \Omega_6.$$

c : Invariance:

$$z \in \Omega_4 \Rightarrow \Gamma(z) \in \Omega_4; z \in \Omega_6 \Rightarrow \Gamma(z) \in \Omega_6.$$

Here the modular group is

$$\Gamma := SL_2(\mathbb{Z}) = \{\begin{pmatrix} a & b \\ c & d \end{pmatrix}, ad - bc = 1, a, b, c, d \in \mathbb{Z}\}. \tag{2.9}$$

Remark 2.2. This conjecture has some similarity to the discovery in Lin and Wang [23], in which they showed surprisingly that the Green function on the two-dimensional torus has either 3 or 5 critical points. Furthermore, once Conjecture (2.1) is proved, we can recover Lin–Wang's Theorem ([23]).

In summary, we see that $(a, b) = (\frac{1}{3}, \frac{1}{3})$ is not always a critical point of $\mathcal{J}(z; a, b)$ for $z \in \mathbb{H}$, while $(a, b) = (\frac{1}{2}, \frac{1}{2})$ is always a critical point of $\mathcal{J}(z; a, b)$ for all $z \in \mathbb{H}$. Moreover $(a, b) = (\frac{1}{2}, \frac{1}{2})$ is a local minimum at least for $z = iy$, $y > 0$.

When $(a, b) = w_3 = (\frac{1}{2}, \frac{1}{2})$ we can simplify the Mueller–Ho functional using the following (whose proof will be given in Section 9):

Lemma 2.3.

$$\mathcal{J}\left(z; \frac{1}{2}, \frac{1}{2}\right) = 2\theta\left(2, \frac{z+1}{2}\right) - \theta(1; z).$$

As a consequence the Mueller–Ho functional becomes

$$\mathcal{E}_{MH}\left(z; \frac{1}{2}, \frac{1}{2}\right) = (1-\alpha)\theta(1; z) + 2\alpha\theta\left(2, \frac{z+1}{2}\right). \tag{2.10}$$

Applying Theorem 1.4 with $\rho = \frac{1-\alpha}{2\alpha}$, we have the following:

Theorem 2.1. *For the Mueller–Ho functional $\mathcal{E}_{MH}(z; \frac{1}{2}, \frac{1}{2})$, there exist thresholds $\sigma_a, \sigma_b \in (0, 1)$ such that*

(A) *For $\alpha \in [0, \sigma_a]$, the minimizer is rhombic lattice$(e^{i\theta_\alpha})$, and the angle increase from $\frac{\pi}{3}$ to $\frac{\pi}{2}$;*
(B) *For $\alpha \in [\sigma_a, \sigma_b]$, the minimizer is square lattice;*
(C) *For $\alpha \in [\sigma_b, 1]$, the minimizer is rectangular lattice$(iy_{1, \frac{1-\alpha}{2\alpha}})$ and the ratio of long side and short side increases from 1 to $\sqrt{3}$.*

Table 1. Minimizers of $\mathcal{E}_{MH}(z; \frac{1}{2}, \frac{1}{2})$: numerical aspect by the minimizer formulas (2.12)

values of α $\alpha \in [0, \sigma_a]$	Lattice shape Rhombic lattice=$e^{i\theta_\alpha}$	Values of α $\alpha \in [\sigma_b, 1]$	Lattice shape Rectangular lattice=$iy_{1,\frac{1-\alpha}{2\alpha}}$
$\alpha = 0$	$\theta_\alpha = \frac{\pi}{3}$	$\alpha = \sigma_b$	i
$\alpha = 0.05$	$\theta_\alpha = 1.083383631\cdots$	$\alpha = 0.93$	$i1.145857964\cdots$
$\alpha = 0.1$	$\theta_\alpha = 1.122437655\cdots$	$\alpha = 0.94$	$i1.280334718\cdots$
$\alpha = 0.15$	$\theta_\alpha = 1.165251963\cdots$	$\alpha = 0.95$	$i1.378964867\cdots$
$\alpha = 0.20$	$\theta_\alpha = 1.213239200\cdots$	$\alpha = 0.96$	$i1.463132141\cdots$
$\alpha = 0.25$	$\theta_\alpha = 1.268922810\cdots$	$\alpha = 0.97$	$i1.538538467\cdots$
$\alpha = 0.30$	$\theta_\alpha = 1.337831332\cdots$	$\alpha = 0.98$	$i1.607675336\cdots$
$\alpha = 0.35$	$\theta_\alpha = 1.439448210\cdots$	$\alpha = 0.99$	$i1.671897256\cdots$
$\alpha = \sigma_a$	$\theta_\alpha = \frac{\pi}{2}$	$\alpha = 1$	$i\sqrt{3}$

(D) *The thresholds σ_a and σ_b are determined by*

$$\sigma_a = \frac{\sigma_{2,a}}{2+\sigma_{2,a}} = \frac{\mathcal{B}''(1)+\mathcal{A}''(1)}{\mathcal{B}''(1)-\mathcal{A}''(1)}, \quad \sigma_b = \frac{1}{1+2\sigma_{1,a}} = \frac{\mathcal{X}''(1)}{\mathcal{X}''(1)-2\mathcal{Y}''(1)}. \tag{2.11}$$

See $\mathcal{A}, \mathcal{B}, \mathcal{X}, \mathcal{Y}$ in (1.12). *Within these relations, the approximate values with arbitrary accuracy can be calculated,*

$$\sigma_a = 0.3732155067\cdots, \quad \sigma_b = 0.9256496973\cdots.$$

(E) *An alternative expression of rhombic lattice,*

$$z_{\min} = \frac{y^2_{2,\frac{1-\alpha}{2\alpha}}-1}{y^2_{2,\frac{1-\alpha}{2\alpha}}+1} + i\frac{2y_{2,\frac{1-\alpha}{2\alpha}}}{y^2_{2,\frac{1-\alpha}{2\alpha}}+1} = e^{i\theta_\alpha}, \theta_\alpha = \arctan\left(\frac{2y_{2,\frac{1-\alpha}{2\alpha}}}{y^2_{2,\frac{1-\alpha}{2\alpha}}-1}\right), \quad \alpha \in (0, \sigma_a). \tag{2.12}$$

Qualitatively, there has

$$\begin{aligned} &\frac{d}{d\alpha}\theta_\alpha > 0, \quad \alpha \in (0, \sigma_a) \\ &\frac{d}{d\alpha}y_{1,\frac{1-\alpha}{2\alpha}} > 0, \quad \alpha \in (\sigma_b, 1). \end{aligned} \tag{2.13}$$

Here $y_{j,\frac{1-\alpha}{2\alpha}}$, $j = 1, 2$ are located precisely in (1.14).

To illustrate the pattern of the vortices shape, we calculate some particular values by the theoretical analysis(minimizer formula (2.12)) in Table 1.

Proposition 2.1 and Theorem 2.1 give a partial answer to the (a), (c), (d) and (e) part of Mueller–Ho Conjecture. We also locate the precise formulas of the numerical thresholds in the Conjecture. Theorem 2.1 shows that as the competition strength between the two Bose gases increases the lattice structures moves from hexagonal, rhombus, square to rectangular. (See Figs. 3, 4).

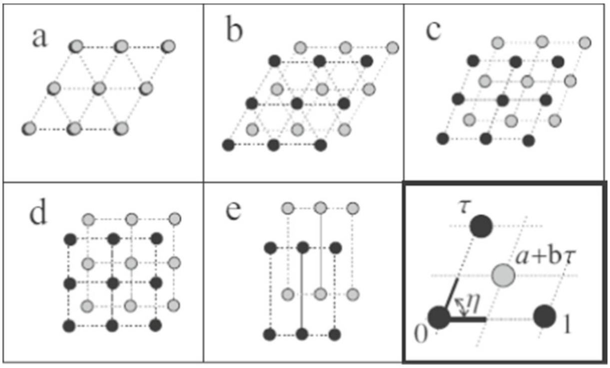

Fig. 3. The lattice shape predicted and drew by Mueller and Ho [26]

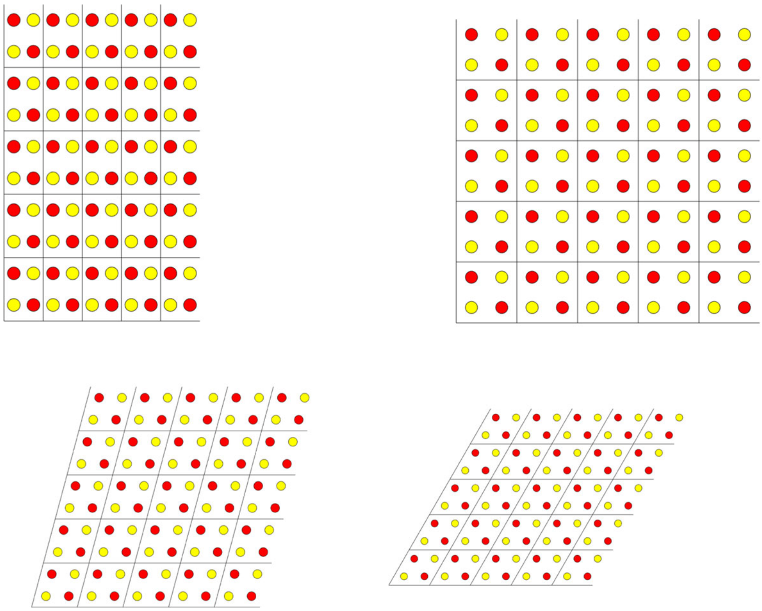

Fig. 4. Two-component Bose gas in lattices. First row from left to right: a rectangular lattice and a square lattice. Second row from left to right: a rhombic lattice and a hexagonal lattice

Finally we discuss the (b) part of Mueller–Ho Conjecture. In the Mueller–Ho Conjecture, the expected lattice structure when α is small is triangular lattice, and the relative position of the two components A, B is characterized by $(a, b) = (\frac{1}{3}, \frac{1}{3})$. To see this, there is a clear competition between $\theta(1; z) + \alpha\mathcal{J}(z; \frac{1}{2}, \frac{1}{2})$ and $\theta(1; z) + \alpha\mathcal{J}(z; \frac{1}{3}, \frac{1}{3})$ when α is small. Thus the upper bound of α preserving the triangular lattice structure is determined by

$$\alpha_0 := \max_{\alpha\in[0,1]}\Big\{\alpha \mid \theta\Big(1;\frac{1}{2}+i\frac{\sqrt{3}}{2}\Big)+\alpha\mathcal{J}\Big(\frac{1}{2}+i\frac{\sqrt{3}}{2};\frac{1}{3},\frac{1}{3}\Big) \\ \leqq \min_{z\in\mathbb{H}}\Big(\theta(1;z)+\alpha\mathcal{J}\Big(z;\frac{1}{2},\frac{1}{2})\Big)\Big\}. \tag{2.14}$$

To find α_0, one first uses $\min_{z\in\mathbb{H}}\big(\theta(1;z)+\alpha\mathcal{J}(z;w_3)\big)\leqq\theta(1;i)+\alpha\mathcal{J}(i;\frac{1}{2},\frac{1}{2})$ to obtain a rough bound

$$\alpha_0 \leqq \frac{\theta(1;i)-\theta(1;\frac{1}{2}+i\frac{\sqrt{3}}{2})}{\mathcal{J}\left(\frac{1}{2}+i\frac{\sqrt{3}}{2};\frac{1}{2},\frac{1}{2}\right)-\mathcal{J}\left(i;\frac{1}{2},\frac{1}{2}\right)} := 0.2419435012\cdots. \tag{2.15}$$

By Theorem 2.1, one deduces that

$$\max_{\alpha\in[0,1]}\Big\{\alpha \mid \theta\Big(1;\frac{1}{2}+i\frac{\sqrt{3}}{2}\Big)+\alpha\mathcal{J}\Big(\frac{1}{2}+i\frac{\sqrt{3}}{2};\frac{1}{3},\frac{1}{3}\Big) \\ \leqq \Big(\theta(1;e^{i\theta_\alpha})+\alpha\mathcal{J}\Big(e^{i\theta_\alpha};\frac{1}{2},\frac{1}{2}\Big)\Big)\Big\}. \tag{2.16}$$

In view of (2.15), the upper bound α_0 satisfies the equation

$$\theta\Big(1;\frac{1}{2}+i\frac{\sqrt{3}}{2}\Big)+\alpha\mathcal{J}\Big(\frac{1}{2}+i\frac{\sqrt{3}}{2};\frac{1}{3},\frac{1}{3}\Big)=\theta(1;e^{i\theta_\alpha})+\alpha\mathcal{J}\Big(e^{i\theta_\alpha};\frac{1}{2},\frac{1}{2}\Big). \tag{2.17}$$

Equation (2.17) gives the upper bound in (b) of Mueller–Ho Conjecture which is

$$\alpha_0 = 0.1726645\cdots, \theta_{\alpha_0} = 1.186248384\cdots. \tag{2.18}$$

Remark 2.3. Several comments on Mueller–Ho conjecture are in order.

- The bounds 0.172, 0.373 and 0.926 are located exactly by the explicit or implicit equation in (2.11) and (2.17).
- The case (a) in Mueller–Ho conjecture is confirmed by Proposition 2.1.
- The cases (c,d,e) in Mueller–Ho conjecture are confirmed by Theorem 2.1. All the expressions have exact formulas by implicit variable determined by explicit equations.
- The behaviors of lattice shapes varying with parameter α is proved in (E) of Theorem 2.1.
- A complete proof Mueller–Ho conjecture is still needed. The Theorem 2.1 answers the main cases positively, however, it remains open to prove that the minimizers of $\{\mathcal{I}(z)+\alpha\mathcal{J}(z;a,b)\}$ admit only three possibilities, that is,
  (1) $(a,b)=(0,0)$.
  (2) $(a,b)=(\frac{1}{3},\frac{1}{3})$.

(3) $(a, b) = (\frac{1}{2}, \frac{1}{2})$.

In case (2), the corresponding z is $\frac{1}{2} + i\frac{\sqrt{3}}{2}$. Cases (1), (3) are universal critical points but have significant meaning.

Remark 2.4. (*Alternative meaning of Theorem* 2.1) The Theorem 2.1 serves to prove Mueller—Ho conjecture firstly as seen in Remark 2.3. However, we would like to point out, Theorem 2.1 can be seen as an independent Theorem to describe the lattice structures. Recall that $(a, b) \in [0, 1]^2$ which characterizes the relative displacement between the two lattices corresponding to the two components. Assume that the component has relative displacement $(a, b) = (\frac{1}{2}, \frac{1}{2})$(vortices of one component on the center of another), then lattice structures are completely classified by Theorem 2.1.

In summary, we give the exact expressions and locate analytically the behaviors of the lattice shapes in Mueller–Ho conjecture. Our result is only a partial result, however, we have a complete proof of Mueller–Ho Conjecture as long as the conjecture on the critical points (Conjecture (2.1)) is proved.

The rest of the paper is organized as follows: in Section 3, we collect some basic invariance properties of the functionals $\mathcal{W}_{1,\rho}(z)$ and $\mathcal{W}_{2,\rho}(z)$ and discuss the intricate relations between these two functionals. In Section 4, we prove a fundamental monotonicity property of the theta function $\theta(s; \frac{z+1}{2})$. The conjugate monotonicity of $\mathcal{W}_{1,\rho}(z)$ and $\mathcal{W}_{2,\rho}(z)$ are established in Section 5. In Sects. 6 and 7, we classify the shape of $\mathcal{W}_{1,\rho}(z)$ and $\mathcal{W}_{2,\rho}(z)$ on the $y-$axis for all $\rho \in [0, \infty)$ respectively. In Section 8, we prove Theorems 1.2, 1.3 and 1.4 , the method of the proof relies on the properties established in Sections 3–7. In Section 9, we prove the properties on Mueller–Ho functional and Theorem 2.1.

In the remaining part of the paper we use the common notation $\sum_{m,n} := \sum_{(m,n)\in\mathbb{Z}^2}$ so that the theta function becomes $\theta(s; z) = \sum_{(m,n)} e^{-s\pi\frac{1}{y}|mz+n|^2}$. We also use the notation

$$\pi = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Leftrightarrow \pi(\tau) = \frac{a\tau + b}{c\tau + d}. \tag{2.19}$$

3. Some Preliminaries

In this section we present some simple symmetries of the two theta functions $\theta(s; z)$ and $\theta(s; \frac{z+1}{2})$ and the associated fundamental domains. As a result we establish the precise connection between $\mathcal{W}_{1,\rho}(z)$ and $\mathcal{W}_{2,\rho}(z)$.

Let $\mathbb{H}$ denote the upper half plane and Γ denote the modular group (defined at (2.9)).

We use the following definition of fundamental domain which is slightly different from the classical definition (see [28]):

Definition 3.1. (page 108, [14]) The fundamental domain associated to group G is a connected domain $\mathcal{D}$ satisfies that

- For any $z \in \mathbb{H}$, there exists an element $\pi \in G$ such that $\pi(z) \in \overline{\mathcal{D}}$;

- Suppose $z_1, z_2 \in \mathcal{D}$ and $\pi(z_1) = z_2$ for some $\pi \in G$, then $z_1 = z_2$ and $\pi = \pm Id$.

By Definition 3.1, the fundamental domain associated to modular group Γ is

$$\mathcal{D}_\Gamma := \left\{ z \in \mathbb{H} : |z| > 1,\ -\frac{1}{2} < x < \frac{1}{2} \right\}, \tag{3.1}$$

which is open. Note that the fundamental domain can be open. (see [p. 30, [2]]).

Next we introduce another two groups related to the functionals $\mathcal{W}_{1,\rho}$ and $\mathcal{W}_{2,\rho}$. The generators of these groups are given by

$$\mathcal{G}_1 : \text{the group generated by } \tau \mapsto -\frac{1}{\tau},\quad \tau \mapsto \tau + 1,\quad \tau \mapsto -\overline{\tau}, \tag{3.2}$$

$$\mathcal{G}_2 : \text{the group generated by } \tau \mapsto -\frac{1}{\tau},\quad \tau \mapsto \tau + 2,\quad \tau \mapsto -\overline{\tau}. \tag{3.3}$$

It is easy to see that the fundamental domains associated to group $\mathcal{G}_j$, $j = 1, 2$ denoted by $\mathcal{D}_{\mathcal{G}_1}, \mathcal{D}_{\mathcal{G}_2}$ are

$$\mathcal{D}_{\mathcal{G}_1} := \left\{ z \in \mathbb{H} : |z| > 1,\ 0 < x < \frac{1}{2} \right\} \tag{3.4}$$

$$\mathcal{D}_{\mathcal{G}_2} := \{ z \in \mathbb{H} : |z| > 1,\ 0 < x < 1 \}. \tag{3.5}$$

Clearly we have that

$$\mathcal{G}_1 \supseteq \mathcal{G}_2, \quad \mathcal{D}_{\mathcal{G}_1} \subseteq \mathcal{D}_{\mathcal{G}_2}.$$

As in [28], the fundamental domain for the single theta function $\theta(s; z)$ is $\mathcal{D}_{\mathcal{G}_1}$. As we will show in this section the fundamental domain for the sum of two theta functions $\mathcal{W}_{1,\rho}, \mathcal{W}_{2,\rho}$ is $\mathcal{D}_{\mathcal{G}_2}$, which is larger. This leads to fundamental difficulty in finding the minimizers.

The next lemma characterizes the basic symmetries of the theta functions $\theta(s; z)$ and $\theta(s; \frac{z+1}{2})$. The proof is trivial so we omit it.

Lemma 3.1. *There are two invariant properties for $\theta(s; z), \theta(s; \frac{z+1}{2})$:*

- *For any $s > 0$, any $\gamma \in \mathcal{G}_1$ and $z \in \mathbb{H}$, $\theta(s; \gamma(z)) = \theta(s; z)$.*
- *For any $s > 0$, any $\gamma \in \mathcal{G}_2$ and $z \in \mathbb{H}$, $\theta(s; \frac{\gamma(z)+1}{2}) = \theta(s; \frac{z+1}{2})$.*

A corollary of Lemma 3.1 yields

Lemma 3.2. *For any $\rho \in \mathbb{R}$, $\gamma \in \mathcal{G}_2$ and $z \in \mathbb{H}$,*

$$\mathcal{W}_{1,\rho}(\gamma(z)) = \mathcal{W}_{1,\rho}(z),\ \ \mathcal{W}_{2,\rho}(\gamma(z)) = \mathcal{W}_{2,\rho}(z).$$

Next, we introduce the nonlinear connection between the two functionals $\mathcal{W}_{1,\rho}(\tau)$ and $\mathcal{W}_{2,\rho}(\tau)$.

Let $w \in \mathcal{G}_2$ be $w : \tau \mapsto \frac{\tau-1}{\tau+1}$ and its the inverse be $\tau : w \mapsto \frac{1+w}{1-w}$. We have

Lemma 3.3.

$$\theta\left(s;\frac{\tau+1}{2}\right)=\theta(s;w),\quad \theta(s;\tau)=\theta\left(s;\frac{w+1}{2}\right). \tag{3.6}$$

$$\mathcal{W}_{1,\rho}(\tau)=\rho\cdot\mathcal{W}_{2,1/\rho}(w),\ \mathcal{W}_{2,\rho}(\tau)=\rho\cdot\mathcal{W}_{1,1/\rho}(w). \tag{3.7}$$

Or, equivalently,

$$\mathcal{W}_{1,\rho}(w)=\rho\cdot\mathcal{W}_{2,1/\rho}(\tau),\ \mathcal{W}_{2,\rho}(w)=\rho\cdot\mathcal{W}_{1,1/\rho}(\tau).$$

Proof. We check that $\theta(s;\frac{\tau+1}{2})=\theta(s;\frac{\frac{1+w}{1-w}+1}{2})=\theta(s;\frac{1}{1-w})=\theta(s;w)$ since the map $w\mapsto\frac{1}{1-w}\in\mathcal{G}_1$. Similarly $\theta(s;\frac{w+1}{2})=\theta(s;\frac{\frac{\tau-1}{\tau+1}+1}{2})=\theta(s;\frac{\tau}{\tau+1})=\theta(s;\tau)$ since the map $\tau\mapsto\frac{\tau}{1+\tau}\in\mathcal{G}_1$. This proves (3.6), (3.7) and (3.8) follows from (3.6). □

Lemma 3.3 builds a connection between the two functionals $\mathcal{W}_{1,\rho}(\tau)$ and $\mathcal{W}_{2,\rho}(\tau)$ via a special element in $\mathcal{G}_2$. As an application of Lemma 3.3, we have the following lemma which transfers the computations on unit circles to straight lines:

Lemma 3.4. *Suppose* $|w|=1$, $w=w_1+iw_2$, $w_2>0$. *It holds that*

$$\frac{\partial}{\partial w_1}\mathcal{W}_{p,\rho}(w)=\rho\frac{\sqrt{1-w_1^2}}{1-w_1}\frac{\partial}{\partial\tau_2}\mathcal{W}_{q,1/\rho}\left(i\frac{\sqrt{1-w_1^2}}{1-w_1}\right)$$

$$\frac{\partial}{\partial w_2}\mathcal{W}_{p,\rho}(w)=-\rho\frac{w_1}{1-w_1}\frac{\partial}{\partial\tau_2}\mathcal{W}_{q,1/\rho}\left(i\frac{\sqrt{1-w_1^2}}{1-w_1}\right),$$

where $p\neq q\in\{1,2\}$.

Proof. Let $\tau:=\tau(w)=\frac{1+w}{1-w}$. We use Lemma 3.3. Let $\tau=\tau_1+i\tau_2$, then

$$\tau_1=\frac{1-w_1^2-w_2^2}{(1-w_1)^2+w_2^2},\quad \tau_2=\frac{2w_2}{(1-w_1)^2+w_2^2}, \tag{3.8}$$

and

$$\frac{\partial\tau_2}{\partial w_1}=\frac{4(1-w_1)w_2}{((1-w_1)^2+w_2^2)^2},\quad \frac{\partial\tau_2}{\partial w_2}=\frac{2((1-w_1)^2-w_2^2)}{((1-w_1)^2+w_2^2)^2}. \tag{3.9}$$

Differentiating the identities in Lemma 3.3, we get

$$\frac{\partial}{\partial w_j}\mathcal{W}_{p,\rho}(w)=\rho\sum_{k=1}^{2}\frac{\partial}{\partial\tau_k}\mathcal{W}_{q,1/\rho}(\tau)\frac{\partial\tau_k}{\partial w_j},\ j=1,2. \tag{3.10}$$

On the other hand, for $|w|=1$, $w_2>0$, by (3.8) and (3.9)

$$\tau_1|_{|w|=1,w_2>0}=0,\quad \tau_2|_{|w|=1,w_2>0}=\frac{\sqrt{1-w_1^2}}{1-w_1} \tag{3.11}$$

and

$$\frac{\partial \tau_2}{\partial w_1}|_{|w|=1,w_2>0} = \frac{\sqrt{1-w_1^2}}{1-w_1}, \quad \frac{\partial \tau_2}{\partial w_2}|_{|w|=1,w_2>0} = -\frac{w_1}{1-w_1}. \tag{3.12}$$

From Theorem 3.2, $\mathcal{W}_{p,\rho}(-\overline{\tau}) = \mathcal{W}_{p,\rho}(\tau)$, $p = 1, 2$. It follows that

$$\frac{\partial}{\partial \tau_1}\mathcal{W}_{p,\rho}(i\tau_2) = 0, \quad \forall \tau_2 > 0, \, p = 1, 2. \tag{3.13}$$

Plugging (3.11), (3.12) and (3.13) into (3.10), one gets the result.

□

4. Monotonicity of $\theta\left(s; \frac{z+1}{2}\right)$

The main purpose of this section is to establish the monotonicity of the functional $\theta(s; \frac{z+1}{2})$ on its fundamental domain $\mathcal{D}_{\mathcal{G}_2}$ (defined at (3.3)), which is

Theorem 4.1. • *For any $s > 0$, it holds that*

$$\frac{\partial}{\partial x}\theta\left(s; \frac{z+1}{2}\right) > 0, \quad \forall \, z \in \mathcal{D}_{\mathcal{G}_2}.$$

- *Or equivalently, via the map $z \mapsto \frac{z+1}{2}$, for any $s > 0$,*

$$\frac{\partial}{\partial x}\theta(s; z) < 0, \quad \forall \, z \in \Omega_{\mathcal{C}_1}.$$

Here

$$\Omega_{\mathcal{C}_1} := \{z \mid 0 < x < \frac{1}{2}, y > \sqrt{x - x^2}\}.$$

Remark 4.1. In Lemma 1 of [28] Montgomery proved that

$$\frac{\partial}{\partial x}\theta(s; z) < 0, \quad \forall \, z \in \Omega_{\mathcal{C}_0} := \left\{z \in \mathbb{H} : y > \frac{1}{2}, \; 0 < x < \frac{1}{2}\right\} \tag{4.1}$$

Theorem 4.1 improves this result to a larger domain $\Omega_{\mathcal{C}_1}$ as $\Omega_{\mathcal{C}_0} \subset \Omega_{\mathcal{C}_1}$. Furthermore, $\Omega_{\mathcal{C}_1}$ contains a corner at $z = 0$, which makes the proof much more involved. We have to divide $\Omega_{\mathcal{C}_1}$ into four different cases to overcome this difficulty.

We state two corollaries related to the functionals $\mathcal{W}_{j,\rho}(z)$, $j = 1, 2$.

Corollary 4.1. *For any $s > 0$,*

$$\frac{\partial}{\partial x}\theta(s; z) > 0, \; \forall z \in \Omega_{\mathcal{C}_2}.$$

Here

$$\Omega_{\mathcal{C}_2} := \left\{z \mid \frac{1}{2} < x < 1, y > \sqrt{x - x^2}\right\}.$$

Proof. Since $z \mapsto 1-\overline{z} \in \mathcal{G}_1$, by Lemma 3.1, we have $\theta(s; 1-\overline{z}) = \theta(s; z)$. Thus

$$\frac{\partial}{\partial x}\theta(s; 1-\overline{z}) = -\frac{\partial}{\partial x}\theta(s; z). \tag{4.2}$$

The result follows by (4.2) and Theorem 4.1.

□

By Theorem 4.1 and Corollary 4.1 we have

Corollary 4.2. *For any* $\rho > 0$,

$$\frac{\partial}{\partial x}\mathcal{W}_{j,\rho}(z) > 0, \ \forall z \in \mathcal{R}_L, \, j = 1, 2.$$

Here

$$\mathcal{R}_L := \Omega_{\mathcal{C}_2} \cap \mathcal{D}_{\mathcal{G}_2} = \left\{ z \mid \frac{1}{2} < x < 1, |z| > 1 \right\}.$$

In the remaining part of this section, we prove Theorem 4.1. To prove Theorem 4.1, we use some delicate analysis of the Jacobi theta function and Poisson summation formula.

We first recall the following well-known Jacobi triple product formula:

$$\prod_{m=1}^{\infty}(1-x^{2m})(1+x^{2m-1}y^2)\left(1+\frac{x^{2m-1}}{y^2}\right) = \sum_{n=-\infty}^{\infty} x^{n^2}y^{2n}, \tag{4.3}$$

for complex numbers x, y with $|x| < 1$, $y \neq 0$.

The Jacob theta function is defined as

$$\vartheta_J(z; \tau) := \sum_{n=-\infty}^{\infty} e^{i\pi n^2\tau + 2\pi i n z},$$

and the classical one-dimensional theta function is given by

$$\vartheta(X; Y) := \vartheta_J(Y; iX) = \sum_{n=-\infty}^{\infty} e^{-\pi n^2 X} e^{2n\pi i Y}. \tag{4.4}$$

Hence by the Jacobi triple product formula (4.3), it holds that

$$\vartheta(X; Y) = \prod_{n=1}^{\infty}(1-e^{-2\pi n X})(1+e^{-2(2n-1)\pi X} + 2e^{-(2n-1)\pi X}\cos(2\pi Y)). \tag{4.5}$$

The next two Lemmas improve the bounds in Montgomery [28]. We provide the proof of Lemma 4.1 and omit the proof of Lemma 4.2 which is similar.

Lemma 4.1. *Assume* $X > \frac{1}{5}$. *If* $\sin(2\pi Y) > 0$, *then*

$$-\overline{\vartheta}(X)\sin(2\pi Y) \leqq \frac{\partial}{\partial Y}\vartheta(X;Y) \leqq -\underline{\vartheta}(X)\sin(2\pi Y).$$

If $\sin(2\pi Y) < 0$, *then*

$$-\underline{\vartheta}(X)\sin(2\pi Y) \leqq \frac{\partial}{\partial Y}\vartheta(X;Y) \leqq -\overline{\vartheta}(X)\sin(2\pi Y).$$

Here

$$\underline{\vartheta}(X) := 4\pi e^{-\pi X}(1-\mu(X)), \quad \overline{\vartheta}(X) := 4\pi e^{-\pi X}(1+\mu(X)),$$

and

$$\mu(X) := \sum_{n=2}^{\infty} n^2 e^{-\pi(n^2-1)X}. \tag{4.6}$$

The proof is almost the same as in Lemma 1 of [28]. However, to show the method and show how the bounds can be improved, we provide the details here. The new thing here is we introduce the new function $\mu(X)$ (in (4.6)) in estimating the bounds, this provides more accurate and powerful tool in the proof of our monotonicity theorem (Theorem 4.1).

Proof. Taking logarithmic on both sides of (4.5) and differentiating $\frac{\partial}{\partial Y}$, we have

$$\begin{aligned}
-\frac{\frac{\partial}{\partial Y}\vartheta(X;Y)}{\sin(2\pi Y)} &= 4\pi\sum_{n=1}^{\infty} e^{-(2n-1)\pi X}\frac{\vartheta(X;Y)}{1+e^{-2(2n-1)\pi X}+2e^{-(2n-1)\pi X}\cos(2\pi Y)}\\
&= 4\pi\sum_{n=1}^{\infty} e^{-(2n-1)\pi X}\prod_{m\neq n, m=1}^{\infty}(1-e^{-2\pi m X})(1+e^{-2(2m-1)\pi X}\\
&\quad + 2e^{-(2m-1)\pi X}\cos(2\pi Y)).
\end{aligned} \tag{4.7}$$

One sees from (4.7) that the function $-\frac{\frac{\partial}{\partial Y}\vartheta(X;Y)}{\sin(2\pi Y)}$ has a period 1, is decreasing on $[0,\frac{1}{2}]$ and is an even function for Y.

Thus

$$\lim_{Y\to\frac{1}{2}} -\frac{\frac{\partial}{\partial Y}\vartheta(X;Y)}{\sin(2\pi Y)} \leqq -\frac{\frac{\partial}{\partial Y}\vartheta(X;Y)}{\sin(2\pi Y)} \leqq \lim_{Y\to 0} -\frac{\frac{\partial}{\partial Y}\vartheta(X;Y)}{\sin(2\pi Y)}. \tag{4.8}$$

By L'Hospital's rule we have

$$\frac{1}{2\pi}\frac{\partial^2}{\partial Y^2}\vartheta(X;Y)\mid_{Y=\frac{1}{2}} \leqq -\frac{\frac{\partial}{\partial Y}\vartheta(X;Y)}{\sin(2\pi Y)} \leqq -\frac{1}{2\pi}\frac{\partial^2}{\partial Y^2}\vartheta(X;Y)\mid_{Y=0} \tag{4.9}$$

From (4.4), we have that

$$\begin{aligned}\frac{\partial^2}{\partial Y^2}\vartheta(X;Y)\mid_{Y=0} &= 4\pi e^{-\pi X}(1+\sum_{n=2}^{\infty}n^2e^{-\pi(n^2-1)X})\\ \frac{1}{2\pi}\frac{\partial^2}{\partial Y^2}\vartheta(X;Y)\mid_{Y=\frac{1}{2}} &= 4\pi\sum_{n=1}^{\infty}(-1)^{n-1}n^2e^{-n^2\pi X} \\ &\geqq 4\pi e^{-\pi X}\left(1-\sum_{n=2}^{\infty}n^2e^{-\pi(n^2-1)X}\right).\end{aligned} \tag{4.10}$$

Combining (4.8), (4.9) and (4.10), we obtain the proof of the Lemma.

□

Lemma 4.2. *Assume* $X<\min\{\frac{\pi}{\pi+2},\frac{\pi}{4\log\pi}\}=\frac{\pi}{\pi+2}$. *If* $\sin(2\pi Y)>0$, *then*

$$-\overline{\vartheta}(X)\sin(2\pi Y)\leqq\frac{\partial}{\partial Y}\vartheta(X;Y)\leqq-\underline{\vartheta}(X)\sin(2\pi Y).$$

If $\sin(2\pi Y)<0$, *then*

$$-\underline{\vartheta}(X)\sin(2\pi Y)\leqq\frac{\partial}{\partial Y}\vartheta(X;Y)\leqq-\overline{\vartheta}(X)\sin(2\pi Y).$$

Here

$$\underline{\vartheta}(X):=\pi e^{-\frac{\pi}{4X}}X^{-\frac{3}{2}};\quad \overline{\vartheta}(X):=X^{-\frac{3}{2}}.$$

In view of (4.4), by Poisson Summation Formula, one has

$$\vartheta(X;Y)=X^{-\frac{1}{2}}\sum_{n\in\mathbb{Z}}e^{-\frac{\pi(n-Y)^2}{X}}. \tag{4.11}$$

Thus the two-dimensional theta function can be written in terms of one-dimensional theta function as follows:

$$\begin{aligned}\theta(s;z) &= \sum_{(m,n)\in\mathbb{Z}^2}e^{-s\pi\frac{1}{y}|nz+m|^2}=\sum_{n\in\mathbb{Z}}e^{-s\pi yn^2}\sum_{m\in\mathbb{Z}}e^{-\frac{s\pi(nx+m)^2}{y}}\\ &=\sqrt{\frac{y}{s}}\sum_{n\in\mathbb{Z}}e^{-s\pi yn^2}\vartheta\left(\frac{y}{s};-nx\right)=\sqrt{\frac{y}{s}}\sum_{n\in\mathbb{Z}}e^{-s\pi yn^2}\vartheta\left(\frac{y}{s};nx\right)\\ &=2\sqrt{\frac{y}{s}}\sum_{n=1}^{\infty}e^{-s\pi yn^2}\vartheta\left(\frac{y}{s};nx\right).\end{aligned} \tag{4.12}$$

Now we are ready to prove Theorem 4.1.

Proof. By Mellin transform, (see [28]), $\theta(\frac{1}{s}; z) = s\theta(s; z)$. Thus we only need to consider the case $s \geqq 1$. For simplicity, we use $\sum_{n\leqq\frac{1}{2x}}, \sum_{n>\frac{1}{2x}}$ to denote $\sum_{n\leqq\frac{1}{2x}, n\geqq 1}, \sum_{n>\frac{1}{2x}, n\geqq 1}$ respectively. From (4.12), we have

$$\begin{aligned} -\frac{\partial}{\partial x}\theta(s;z) &= -2\sqrt{\frac{y}{s}}\sum_{n=1}^{\infty} n e^{-\pi s y n^2}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{s};Y\right)|_{Y=nx} \\ &= 2\sqrt{\frac{y}{s}}\left(-\sum_{n\leqq\frac{1}{2x}} n e^{-\pi s y n^2}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{s};Y)|_{Y=nx} - \sum_{n>\frac{1}{2x}} n e^{-\pi s y n^2}\frac{\partial}{\partial Y}\vartheta(\frac{y}{s};Y\right)|_{Y=nx}\right) \\ &= 2\sqrt{\frac{y}{s}}\left(\mathcal{E}^a_{s,x}(z) + \mathcal{E}^b_{s,x}(z)\right), \end{aligned} \tag{4.13}$$

where

$$\begin{aligned} \mathcal{E}^a_{s,x}(z) &:= -\sum_{n\leqq\frac{1}{2x}} n e^{-\pi s y n^2}\frac{\partial}{\partial Y}\vartheta(\frac{y}{s};Y)|_{Y=nx}, \quad \mathcal{E}^b_{s,x}(z) \\ &:= -\sum_{n>\frac{1}{2x}} n e^{-\pi s y n^2}\frac{\partial}{\partial Y}\vartheta(\frac{y}{s};Y)|_{Y=nx}. \end{aligned} \tag{4.14}$$

For $\mathcal{E}^a_{s,x}(z)$, by Lemma 4.1, we have that

$$\mathcal{E}^a_{s,x}(z) \geqq \sum_{n\leqq\frac{1}{2x}} n e^{-\pi s y n^2}\underline{\vartheta}(\frac{y}{s})\sin(2\pi n x) \geqq e^{-\pi s y}\underline{\vartheta}(\frac{y}{s})\sin(2\pi x). \tag{4.15}$$

Notice that all the terms in the summation of (4.15) are nonnegative.

Let n_0 be the smallest integer such that $n > \frac{1}{2x}$. By Lemma 4.1,

$$\begin{aligned} |\mathcal{E}^b_{s,x}(z)| &\leqq \sum_{n>\frac{1}{2x}} n e^{-\pi s y n^2}\overline{\vartheta}\left(\frac{y}{s}\right)|\sin(2\pi n x)| \\ &\leqq \sum_{n>\frac{1}{2x}} n^2 e^{-\pi s y n^2}\overline{\vartheta}\left(\frac{y}{s}\right)|\sin(2\pi x)| \\ &= n_0^2 e^{-\pi s y n_0^2}\overline{\vartheta}(\frac{y}{s})\sin(2\pi x)\cdot(1+\delta(x)), \text{ with} \\ \delta(x) &:= \sum_{k=1}^{\infty}\left(1+\frac{k}{n_0}\right)^2 e^{-\pi s y(2kn_0+k^2)}. \end{aligned} \tag{4.16}$$

To estimate $\delta(x)$, note that $yn_0 > \frac{\sqrt{1-x}}{2\sqrt{x}}$,

$$\begin{aligned} \delta(x) &\leqq \sum_{k=1}^{\infty}\left(1+\frac{2k}{n_0}+\frac{k^2}{n_0^2}\right)e^{-2\pi s y k n_0} \leqq \sum_{k=1}^{\infty}\left(1+\frac{2k}{n_0}+\frac{k^2}{n_0^2}\right)e^{-\pi\frac{\sqrt{1-x}}{\sqrt{x}}k} \\ &= \frac{e^{-q(x)}}{1-e^{-q(x)}} + \frac{2}{n_0}\frac{e^{-q(x)}}{(1-e^{-q(x)})^2} + \frac{1}{n_0^2}\frac{e^{-q(x)}(1+e^{-q(x)})}{(1-e^{-q(x)})^3} \\ &\leqq \frac{e^{-q(x)}}{1-e^{-q(x)}} + 4x\frac{e^{-q(x)}}{(1-e^{-q(x)})^2} + 4x^2\frac{e^{-q(x)}(1+e^{-q(x)})}{(1-e^{-q(x)})^3} \end{aligned} \tag{4.17}$$

with $q(x) := \pi\frac{\sqrt{1-x}}{\sqrt{x}}$. Denote that

$$\delta_q(x) := \frac{e^{-q(x)}}{1-e^{-q(x)}} + 4x\frac{e^{-q(x)}}{(1-e^{-q(x)})^2} + 4x^2\frac{e^{-q(x)}(1+e^{-q(x)})}{(1-e^{-q(x)})^3}.$$

It is easy to see that $\delta_q(x)$ is monotonically increasing on $[0, \frac{1}{2}]$ and hence $\delta(x) \leqq \delta_q(\frac{1}{2}) = 0.188822585\cdots < \frac{1}{5}$. Then by (4.16) and (4.17), one has

$$|\mathcal{E}^b_{s,x}(z)| \leqq \frac{6}{5}n_0^2 e^{-\pi s y n_0^2}\overline{\vartheta}(\frac{y}{s})\sin(2\pi x). \tag{4.18}$$

Combining (4.13), (4.15) with (4.18), one gets

$$-\frac{\partial}{\partial x}\theta(s;z) \geqq 2\sqrt{\frac{y}{s}}\sin(2\pi x)e^{-\pi s y}\overline{\vartheta}\left(\frac{y}{s}\right)\left(\frac{\underline{\vartheta}\left(\frac{y}{s}\right)}{\overline{\vartheta}(\frac{y}{s})} - \frac{6}{5}n_0^2 e^{-\pi s y(n_0^2-1)}\right), \tag{4.19}$$

with $n_0 = [\frac{1}{2x}] + 1$.

Let

$$\mathcal{E}_{s,x}(z) := \frac{\underline{\vartheta}(\frac{y}{s})}{\overline{\vartheta}(\frac{y}{s})} - \frac{6}{5}n_0^2 e^{-\pi s y(n_0^2-1)}. \tag{4.20}$$

By (4.19) it suffices to prove that $\mathcal{E}_{s,x}(z) > 0$.

$\Omega_{\mathcal{C}_1}$ has a corner $z = 0$ which induces the difficulty to get the lower bound estimate for $\mathcal{E}_{s,x}(z)$. Thus we divide the proof into four cases.

Case a: $\frac{y}{s} \leqq \frac{1}{2}, x \in (0, \frac{1}{3}]$. In this case, $\frac{s}{y} \geqq 2$ and $\frac{\sqrt{1-x}(1-4x^2)}{x^{\frac{3}{2}}} - \frac{1}{\sqrt{x-x^2}} > 0$. By Lemma 4.2,

$$\begin{aligned}
\mathcal{E}_{s,x}(z) &\geqq \left(\frac{\pi s}{y} - 2\right)e^{-\frac{\pi s}{4y}} - \frac{6}{5}n_0^2 e^{-\pi s y(n_0^2-1)}\\
&\geqq (2\pi - 2)e^{-\frac{\pi s}{4\sqrt{x-x^2}}} - \frac{3}{10x^2}e^{-\pi s\sqrt{x-x^2}\left(\frac{1}{4x^2}-1\right)}\\
&= \frac{3}{10x^2}e^{-\pi s\sqrt{x-x^2}\left(\frac{1}{4x^2}-1\right)}\left(\frac{20\pi-20}{3}x^2 e^{\frac{\pi s}{4}\left(\frac{\sqrt{1-x}(1-4x^2)}{x^{\frac{3}{2}}} - \frac{1}{\sqrt{x-x^2}}\right)} - 1\right)\\
&\geqq \frac{3}{10x^2}e^{-\pi s\sqrt{x-x^2}\left(\frac{1}{4x^2}-1\right)}\left(\frac{20\pi-20}{3}x^2 e^{\frac{\pi}{4}\left(\frac{\sqrt{1-x}(1-4x^2)}{x^{\frac{3}{2}}} - \frac{1}{\sqrt{x-x^2}}\right)} - 1\right)\\
&> 0
\end{aligned} \tag{4.21}$$

where the last inequality follows from elementary calculus because $x \in (0, \frac{1}{3})$.

Case b: $\frac{y}{s} \leqq \frac{1}{2}$, $x \in [\frac{1}{3}, \frac{1}{2}]$. In this case, $n_0 = [\frac{1}{2x}] + 1 \geqq \frac{1}{2x} + \frac{1}{2}$ and we have

$$\begin{aligned}
\mathcal{E}_{s,x}(z) &\geqq \left(\frac{\pi s}{y} - 2\right) e^{-\frac{\pi s}{4y}} - \frac{6}{5} n_0^2 e^{-\pi s y (n_0^2 - 1)} \\
&\geqq (2\pi - 2) e^{-\frac{\pi s}{4y}} - \frac{6}{5}\left(\frac{1}{2x} + \frac{1}{2}\right)^2 e^{-\pi s y\left(\left(\frac{1}{2x}+\frac{1}{2}\right)^2 - 1\right)} \\
&= \frac{3(1+x)^2}{10x^2} e^{-\pi s y\left(\left(\frac{1}{2x}+\frac{1}{2}\right)^2 - 1\right)} \left(\frac{(20\pi - 20)x^2}{9(1+x)^2} e^{\pi s\left(y\frac{(1+x)^2 - 4x^2}{4x^2} - \frac{1}{4y}\right)} - 1\right) \\
&\geqq \frac{3(1+x)^2}{10x^2} e^{-\pi s y((\frac{1}{2x}+\frac{1}{2})^2 - 1)} \left(\frac{(20\pi - 20)x^2}{9(1+x)^2} e^{\pi s\left(\sqrt{x - x^2}\frac{(1+x)^2 - 4x^2}{4x^2} - \frac{1}{4\sqrt{x-x^2}}\right)} - 1\right) \\
&\geqq \frac{3(1+x)^2}{10x^2} e^{-\pi s y((\frac{1}{2x}+\frac{1}{2})^2 - 1)} \left(\frac{(20\pi - 20)x^2}{9(1+x)^2} e^{\pi\left(\sqrt{x - x^2}\frac{(1+x)^2 - 4x^2}{4x^2} - \frac{1}{4\sqrt{x-x^2}}\right)} - 1\right) \\
&> 0
\end{aligned}$$

where we have used the following inequalities whose computation is left to the reader:

$$\begin{aligned}
&\sqrt{x - x^2}\frac{(1+x)^2 - 4x^2}{4x^2} - \frac{1}{4\sqrt{x - x^2}} > 0, \quad x \in \left[0, \frac{1}{2}\right], \\
&\frac{(20\pi - 20)x^2}{9(1+x)^2} e^{\pi\left(\sqrt{x-x^2}\frac{(1+x)^2-4x^2}{4x^2} - \frac{1}{4\sqrt{x-x^2}}\right)} - 1 > 0, \quad x \in \left[0, \frac{1}{2}\right].
\end{aligned} \tag{4.22}$$

Case c: $\frac{y}{s} \geqq \frac{1}{2}$, $x \in [0, \frac{2}{5}]$. In this case, $ys \geqq \frac{s^2}{2} \geqq \frac{1}{2}$. By Lemma 4.1,

$$\begin{aligned}
\mathcal{E}_{s,x}(z) &\geqq \frac{1 - \mu(\frac{y}{s})}{1 + \mu(\frac{y}{s})} - \frac{6}{5} n_0^2 e^{-\pi s y (n_0^2 - 1)} \geqq \frac{1 - \mu(\frac{1}{2})}{1 + \mu(\frac{1}{2})} - \frac{3}{10x^2} e^{-\frac{\pi(1-4x^2)}{8x^2}} \\
&\geqq \left(\frac{1 - \mu(\frac{1}{2})}{1 + \mu(\frac{1}{2})} - \frac{3}{10x^2} e^{-\frac{\pi(1-4x^2)}{8x^2}}\right) |_{x=\frac{2}{5}} = 0.1556238052 > 0.
\end{aligned}$$

The monotonically increasing of $\frac{3}{10x^2} e^{-\frac{\pi(1-4x^2)}{8x^2}}$ on $(0, \frac{2}{5}]$ is used here; similarly, we use $\frac{3(1+x)^2}{10x^2} e^{-\frac{\pi}{2}\left((\frac{1+x}{2x})^2 - 1\right)}$ is monotonically increasing on $[\frac{1}{3}, \frac{1}{2}]$ in the Case d.

Case d: $\frac{y}{s} \geqq \frac{1}{2}$, $x \in [\frac{1}{3}, \frac{1}{2}]$. In this case, $n_0 = [\frac{1}{2x}] + 1 \geqq \frac{1}{2x} + \frac{1}{2}$ and $y \geqq \frac{s^2}{2} \geqq \frac{1}{2}$. By Lemma 4.1,

$$\begin{aligned}
\mathcal{E}_{s,x}(z) &\geqq \frac{1 - \mu(\frac{y}{s})}{1 + \mu(\frac{y}{s})} - \frac{6}{5} n_0^2 e^{-\pi s y (n_0^2 - 1)} \geqq \frac{1 - \mu(\frac{1}{2})}{1 + \mu(\frac{1}{2})} - \frac{3(1+x)^2}{10x^2} e^{-\frac{\pi}{2}\left((\frac{1+x}{2x})^2 - 1\right)} \\
&\geqq \left(\frac{1 - \mu(\frac{1}{2})}{1 + \mu(\frac{1}{2})} - \frac{3(1+x)^2}{10x^2} e^{-\frac{\pi}{2}\left((\frac{1+x}{2x})^2 - 1\right)}\right) |_{x=\frac{1}{2}} = 0.7866071958 \cdots > 0.
\end{aligned}$$

Combining cases (a)–(d), (4.19) and (4.20), the proof of Theorem 4.1 is complete.

□

5. Monotonicity of $\mathcal{W}_{1,\rho}(z)$ and $\mathcal{W}_{2,\rho}(z)$

Let the closure of the left-half fundamental domain corresponding to $\mathcal{G}_2$ be

$$\mathcal{R}_2 = \left\{ z \in \mathbb{H} : 0 \leqq x \leqq \frac{1}{2}, |z| \geqq 1 \right\}.$$

In this section, we aim to establish the following property of the pair $\mathcal{W}_{j,\rho}(z)$, $j = 1, 2$: there exists ρ_* such that for $\forall z \in \mathcal{R}_2$, $\frac{\partial}{\partial x}\mathcal{W}_{1,\rho}(z) \geqq 0$ when $0 \leqq \rho \leqq \rho_*$, and $\frac{\partial}{\partial x}\mathcal{W}_{2,\rho}(z) \geqq 0$ when $0 \leqq \rho \leqq \frac{1}{\rho_*}$. (In fact we will choose $\rho_* = \frac{1}{20}$). We call this pair monotonicity is the conjugate monotonicity of the functionals. This property plays an important role in finding the minimizers and will be proved in Propositions 5.1 and 5.2 .

We begin with

Proposition 5.1. *For* $0 \leqq \rho \leqq \rho_* := 1/20$*, it holds that*

$$\frac{\partial}{\partial x}\mathcal{W}_{1,\rho}(z) \geqq 0$$

for $\forall z \in \mathcal{R}_2$*. The equality holds only when* $x = 0$ *or* $\frac{1}{2}$.

Proof. From (4.12), we obtain that

$$\begin{aligned}
\frac{\partial}{\partial x}\mathcal{W}_{1,\rho}(z) &= \frac{\partial}{\partial x}\left(\sqrt{\frac{y}{4}}\sum_n e^{-\pi y n^2}\vartheta\left(\frac{y}{4}; n\frac{x+1}{2}\right) + \rho\sqrt{y}\sum_n e^{-\pi y n^2}\vartheta(y; nx)\right)\\
&= \frac{\sqrt{y}}{2}\sum_{n=1}^{\infty} n e^{-\pi y n^2}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{4}; Y\right)|_{Y=n\frac{x+1}{2}} + 2\rho\sqrt{y}\sum_{n=1}^{\infty} n e^{-\pi y n^2}\frac{\partial}{\partial Y}\vartheta(y; Y)|_{Y=nx}\Big)\\
&= \frac{\sqrt{y}}{2}e^{-\pi y}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{4}; Y\right)|_{Y=\frac{x+1}{2}} + \sqrt{y}e^{-4\pi y}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{4}; Y\right)|_{Y=x+1}\\
&\quad + 2\rho\sqrt{y}e^{-\pi y}\frac{\partial}{\partial Y}\vartheta(y; Y)|_{Y=x} + 4\rho\sqrt{y}e^{-4\pi y}\frac{\partial}{\partial Y}\vartheta(y; Y)|_{Y=2x}\\
&\quad + \frac{\sqrt{y}}{2}\sum_{n=3}^{\infty} n e^{-\pi y n^2}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{4}; Y\right)|_{Y=n\frac{x+1}{2}} + 2\rho\sqrt{y}\sum_{n=3}^{\infty} n e^{-\pi y n^2}\frac{\partial}{\partial Y}\vartheta(y; Y)|_{Y=nx}\\
&= \mathcal{W}_{1,x}^a(z) + \mathcal{W}_{1,x}^b(z) + \mathcal{W}_{1,x}^c(z)
\end{aligned} \tag{5.1}$$

where $\mathcal{W}_{1,x}^a(z)$, $\mathcal{W}_{1,x}^b(z)$ and $\mathcal{W}_{1,x}^c(z)$ are defined at the last equality.

By Lemma 4.1, we see that

$$\begin{aligned}
\mathcal{W}_{1,x}^a(z) + \mathcal{W}_{1,x}^b(z) \geqq\ & \frac{\sqrt{y}}{2}e^{-\pi y}\underline{\vartheta}\left(\frac{y}{4}\right)\sin(\pi x) - \sqrt{y}e^{-4\pi y}\overline{\vartheta}\left(\frac{y}{4}\right)\sin(2\pi x)\\
& - 2\rho\sqrt{y}e^{-\pi y}\overline{\vartheta}(y)\sin(2\pi x) - 4\rho\sqrt{y}e^{-4\pi y}\overline{\vartheta}(y)|\sin(4\pi x)|.
\end{aligned} \tag{5.2}$$

Since $|\sin(nx)| \leqq n|\sin(x)|$ for any $x \in \mathcal{R}_2$, again by Lemma 4.1, we have

$$\begin{aligned}
\mathcal{W}_{1,x}^c(z) \geqq & -\frac{\sqrt{y}}{4}\sum_{n=3}^{\infty} n^2 e^{-\pi y n^2}\overline{\vartheta}\left(\frac{y}{4}\right)\sin(2\pi x)\\
& - 2\rho\sqrt{y}\sum_{n=3}^{\infty} n^2 e^{-\pi y n^2}\overline{\vartheta}(y)\sin(2\pi x).
\end{aligned} \tag{5.3}$$

Plugging (5.2) and (5.3) in (5.1), we get

$$
\begin{aligned}
\frac{\partial}{\partial x}\mathcal{W}_{1,\rho}(z) \geqq\ & \frac{\sqrt{y}}{2}e^{-\pi y}\underline{\vartheta}\left(\frac{y}{4}\right)\sin\pi x - \sqrt{y}e^{-4\pi y}\overline{\vartheta}\left(\frac{y}{4}\right)\sin(2\pi x)\\
&\left(1+\frac{1}{4}\sum_{n=3}^{\infty}n^2e^{-\pi y(n^2-4)}\right)\\
&-2\rho\sqrt{y}e^{-\pi y}\overline{\vartheta}(y)\sin(2\pi x)\left(1+\sum_{n=2}^{\infty}n^2e^{-\pi y\left(n^2-1\right)}\right)\\
=\ & \sqrt{y}e^{-\pi y}\sin(\pi x)\left(\frac{1}{2}\underline{\vartheta}(\frac{y}{4}) - 2e^{-3\pi y}\overline{\vartheta}(\frac{y}{4})\cos(\pi x)(1+\sigma_1)\right.\\
&\left.-4\rho\overline{\vartheta}(y)\cos(\pi x)(1+\sigma_2)\right)\\
\geqq\ & \sqrt{y}e^{-\pi y}\sin(\pi x)\\
&\times\left(\frac{1}{2}\underline{\vartheta}\left(\frac{y}{4}\right) - 2e^{-3\pi y}\overline{\vartheta}\left(\frac{y}{4}\right)(1+\sigma_1) - 4\rho\overline{\vartheta}(y)(1+\sigma_2)\right),
\end{aligned}
\tag{5.4}
$$

where

$$
\sigma_1(y) := \frac{1}{4}\sum_{n=3}^{\infty}n^2e^{-\pi y(n^2-4)},\quad \sigma_2(y) := \sum_{n=2}^{\infty}n^2e^{-\pi y(n^2-1)},
$$

and $\sigma_1(y), \sigma_1(y)$ are small. (In fact $\sigma_1(\frac{\sqrt{3}}{2}) \approx 2.781\cdot 10^{-6},\ \sigma_2(\frac{\sqrt{3}}{2}) \approx 1.14105\cdot 10^{-3}$.)

By the lower and upper bound estimates in Lemma 4.1, from (5.4), we see that

$$
\begin{aligned}
\frac{\partial}{\partial x}\mathcal{W}_{1,\rho}(z) \geqq\ & \sqrt{y}e^{-\pi y}\sin(\pi x)\left(2\pi\left(1-\mu\left(\frac{y}{4}\right)\right)e^{-\frac{\pi y}{4}}\right.\\
&-8\pi e^{-3\pi y}\left(1+\mu\left(\frac{y}{4}\right)\right)e^{-\frac{\pi y}{4}}(1+\sigma_1)\\
&\left.-16\rho\pi(1+\mu(y))e^{-\pi y}(1+\sigma_2)\right)\\
=\ & 4\pi\sqrt{y}e^{-\frac{5\pi y}{4}}\sin(\pi x)\left(\frac{1}{2}\left(1-\mu\left(\frac{y}{4}\right)\right) - 2(1+\sigma_1)e^{-3\pi y}\right.\\
&\left(1+\mu\left(\frac{y}{4}\right)\right)\\
&\left.-4\rho(1+\sigma_2)e^{-\frac{3\pi y}{4}}(1+\mu(y))\right)\\
=\ & 4\pi\sqrt{y}e^{-\frac{5\pi y}{4}}\sin(\pi x)\vartheta_{\mathcal{W}_{1,\rho}}(y)
\end{aligned}
\tag{5.5}
$$

where $\vartheta_{\mathcal{W}_{1,\rho}}(y)$ is defined at the last equality.

It suffices to prove that

$$
\vartheta_{\mathcal{W}_{1,\rho}}(y) > 0.
$$

First it is easy to see that

$$
\frac{\partial}{\partial\rho}\vartheta_{\mathcal{W}_{1,\rho}}(y) > 0,\ \ y > 0. \tag{5.6}
$$

Since the functions $\mu(y), \sigma_1, \sigma_2$ are decreasing on $y > 0$, it follows that

$$\frac{\partial}{\partial y}\vartheta_{\mathcal{W}_{1,\rho}}(y) > 0, \ \ y > 0. \tag{5.7}$$

A direct calculation gives

$$\vartheta_{\mathcal{W}_{1,\rho}}(y)|_{y=\frac{\sqrt{3}}{2},\rho=\frac{1}{20}} = 0.1933\cdots > 0,$$

which implies

$$\vartheta_{\mathcal{W}_{1,\rho}} > 0, \ \text{for } y \geqq \frac{\sqrt{3}}{2}, \rho \leqq \frac{1}{20}$$

by the monotonicity properties (5.6) and (5.7). $\frac{\partial}{\partial x}\mathcal{W}_{1,\rho}(y)$ vanishes only when $x = 0$ or $\frac{1}{2}$ by (5.5). The proof is completed.

□

We then have a similar monotonicity for $\mathcal{W}_{2,\rho}(z)$.

Proposition 5.2. *For $\rho \leqq \frac{1}{\rho_*} = 20$, it holds that*

$$\frac{\partial}{\partial x}\mathcal{W}_{2,\rho}(z) \geqq 0$$

for $\forall z \in \mathcal{R}_2$. The equality holds only when $x = 0$ or $\frac{1}{2}$.

Proof. The proof is similar to Proposition 5.1. Using (4.12), we see that

$$\begin{aligned}
\frac{\partial}{\partial x}\mathcal{W}_{2,\rho_\Gamma}(z) &= \frac{\partial}{\partial x}\left(\sqrt{\frac{y}{2}}\sum_n e^{-\frac{1}{2}\pi y n^2}\vartheta\left(\frac{y}{2}; n\frac{x+1}{2}\right) + \rho\sqrt{\frac{y}{2}}\sum_n e^{-2\pi y n^2}\vartheta\left(\frac{y}{2}; nx\right)\right)\\
&= \sqrt{\frac{y}{2}}\sum_{n=1}^{\infty} n e^{-\frac{1}{2}\pi y n^2}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{2}; Y\right)|_{Y=n\frac{x+1}{2}}\\
&\quad + 2\rho\sqrt{\frac{y}{2}}\sum_{n=1}^{\infty} n e^{-2\pi y n^2}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{2}; Y\right)|_{Y=nx}\\
&= \sqrt{\frac{y}{2}}e^{-\frac{1}{2}\pi y}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{2}; Y\right)|_{Y=\frac{x+1}{2}} + 2\sqrt{\frac{y}{2}}e^{-2\pi y}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{2}; Y\right)|_{Y=x+1}\\
&\quad + 2\rho\sqrt{\frac{y}{2}}e^{-2\pi y}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{2}; Y\right)|_{Y=x}\\
&\quad + \sqrt{\frac{y}{2}}\sum_{n=3}^{\infty} n e^{-\frac{1}{2}\pi y n^2}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{2}; Y\right)|_{Y=n\frac{x+1}{2}}\\
&\quad + 2\rho\sqrt{\frac{y}{2}}\sum_{n=2}^{\infty} n e^{-2\pi y n^2}\frac{\partial}{\partial Y}\vartheta\left(\frac{y}{2}; Y\right)|_{Y=nx}\\
&= \mathcal{W}_{2,x}^{a}(z) + \mathcal{W}_{2,x}^{b}(z) + \mathcal{W}_{2,x}^{c}(z),
\end{aligned} \tag{5.8}$$

where $\mathcal{W}_{2,x}^{a}(z)$, $\mathcal{W}_{2,x}^{b}(z)$ and $\mathcal{W}_{2,x}^{c}(z)$ are defined at the last equality.

By Lemma 4.1, we also have

$$\begin{aligned}\mathcal{W}_{2,x}^{a}(z)+\mathcal{W}_{2,x}^{b}(z) &\geqq \sqrt{\frac{y}{2}}e^{-\frac{1}{2}\pi y}\underline{\vartheta}\left(\frac{y}{2}\right)\sin(\pi x)\\ &\quad -(2+2\rho)\sqrt{\frac{y}{2}}e^{-2\pi y}\overline{\vartheta}\left(\frac{y}{2}\right)\sin(2\pi x).\end{aligned}$$

Since $|\sin(nx)|\leqq n|\sin(x)|$ for any $x\in\mathcal{R}_2$, again by Lemma 4.1, we see that

$$\begin{aligned}\mathcal{W}_{2,x}^{c}(z) &\geqq -\frac{1}{2}\sqrt{\frac{y}{2}}\sum_{n=3}^{\infty}n^2e^{-\frac{1}{2}\pi yn^2}\overline{\vartheta}\left(\frac{y}{2}\right)\sin(2\pi x)\\ &\quad -\rho\sqrt{\frac{y}{2}}\sum_{n=2}^{\infty}n^2e^{-2\pi yn^2}\overline{\vartheta}\left(\frac{y}{2}\right)\sin(2\pi x).\end{aligned}$$

Plugging the above inequality into (5.8), we get that

$$\begin{aligned}\frac{\partial}{\partial x}\mathcal{W}_{2,\rho}(z) &\geqq \sqrt{\frac{y}{2}}e^{-\frac{1}{2}\pi y}\underline{\vartheta}\left(\frac{y}{2}\right)\sin(\pi x)-(2+2\rho+\sigma_3(y)\\ &\quad +\rho\sigma_4(y))\sqrt{\frac{y}{2}}e^{-2\pi y}\overline{\vartheta}\left(\frac{y}{2}\right)\sin(2\pi x)\\ &=\sqrt{\frac{y}{2}}e^{-\frac{1}{2}\pi y}\sin(\pi x)\left(\underline{\vartheta}\left(\frac{y}{2}\right)-(4+4\rho\right.\\ &\quad \left.+2\sigma_3(y)+2\rho\sigma_4(y))\cos(\pi x)e^{-\frac{3}{2}\pi y}\overline{\vartheta}\left(\frac{y}{2}\right)\right),\end{aligned}\tag{5.9}$$

where

$$\sigma_3(y):=\frac{1}{2}\sum_{n=3}^{\infty}n^2e^{-\frac{1}{2}\pi y(n^2-4)},\quad \sigma_4(y):=\sum_{n=2}^{\infty}n^2e^{-2\pi y(n^2-1)}.$$

$\sigma_3(y),\sigma_4(y)$ are functions with small L^∞ norm. (In fact $\sigma_3(\frac{\sqrt{3}}{2})\approx 5.00388\cdot 10^{-3}$, $\sigma_4(\frac{\sqrt{3}}{2})\approx 3.255011\cdot 10^{-7}$.)

By the lower and upper bound estimates in Lemma 4.1, from (5.9) one deduces that

$$\begin{aligned}\frac{\partial}{\partial x}\mathcal{W}_{2,\rho}(z) &\geqq \sqrt{\frac{y}{2}}e^{-\frac{1}{2}\pi y}\sin(\pi x)\left(4\pi\left(1-\mu\left(\frac{y}{2}\right)\right)e^{-\frac{\pi y}{2}}\right.\\ &\quad \left.-4\pi(4+4\rho+2\sigma_3(y)+2\rho\sigma_4(y))\cos(\pi x)e^{-2\pi y}\left(1+\mu\left(\frac{y}{2}\right)\right)\right)\\ &\geqq 4\pi\sqrt{\frac{y}{2}}e^{-\pi y}\sin(\pi x)\left(\left(1-\mu\left(\frac{y}{2}\right)\right)\right.\\ &\quad \left.-(4+4\rho+2\sigma_3(y)+2\rho\sigma_4(y))\cos(\pi x)e^{-\frac{3}{2}\pi y}\left(1+\mu\left(\frac{y}{2}\right)\right)\right).\end{aligned}$$

Let

$$\vartheta_{\mathcal{W}_{2,\rho}}(z) := \left(1-\mu\left(\frac{y}{2}\right)\right) - (4+4\rho+2\sigma_3(y)+2\rho\sigma_4(y)) \cos(\pi x)e^{-\frac{3}{2}\pi y}\left(1+\mu\left(\frac{y}{2}\right)\right).$$

Then

$$\frac{\partial}{\partial x}\mathcal{W}_{2,\rho}(z) \geqq 4\pi\sqrt{\frac{y}{2}}e^{-\pi y}\sin(\pi x)\cdot\vartheta_{\mathcal{W}_{2,\rho}}(y) \tag{5.10}$$

It suffices to prove that

$$\vartheta_{\mathcal{W}_{2,\rho}}(z) > 0, \quad \text{for } z \in \mathcal{R}_\Gamma,\ \rho \leqq \frac{1}{\rho_\Gamma} = 20.$$

Now obviously

$$\frac{\partial}{\partial \rho}\vartheta_{\mathcal{W}_{2,\rho}}(y) < 0;\ \forall y > 0,\ \text{ and } \frac{\partial}{\partial x}\vartheta_{\mathcal{W}_{2,\rho}}(z) > 0;\ \forall x \in \left[0, \frac{1}{2}\right],\ \forall y > 0. \tag{5.11}$$

Observe that the functions $\mu(y), \sigma_3, \sigma_4$ are decreasing on $y > 0$. It follows that

$$\frac{\partial}{\partial y}\vartheta_{\mathcal{W}_{2,\rho}}(z) > 0,\ \forall y > 0. \tag{5.12}$$

To complete the proof, we prove that $\vartheta_{\mathcal{W}_{2,\rho}}(z)$ is positive on the following three unbounded rectangular domains:

$$\mathcal{R}_a = \left\{z \mid x \in \left[0, \frac{1}{4}\right], y \geqq \frac{\sqrt{15}}{4}\right\};\ \mathcal{R}_b = \left\{z \mid x \in \left[\frac{1}{4}, \frac{3}{8}\right], y \geqq \frac{\sqrt{55}}{8}\right\};$$
$$\mathcal{R}_c = \left\{z \mid x \in \left[\frac{3}{8}, \frac{1}{2}\right], y \geqq \frac{\sqrt{3}}{2}\right\}.$$

It is clear that

$$\mathcal{R}_2 \subset \mathcal{R}_a \cup \mathcal{R}_b \cup \mathcal{R}_c. \tag{5.13}$$

A direct calculation gives

$$\vartheta_{\mathcal{W}_{2,\rho}}(z)|_{x=0, y=\frac{\sqrt{15}}{4}, \rho=20} = 0.0450964128\cdots > 0$$
$$\vartheta_{\mathcal{W}_{2,\rho}}(z)|_{x=\frac{1}{4}, y=\frac{\sqrt{55}}{8}, \rho=20} = 0.1583739562\cdots > 0$$
$$\vartheta_{\mathcal{W}_{2,\rho}}(z)|_{x=\frac{3}{8}, y=\frac{\sqrt{3}}{2}, \rho=20} = 0.3525036217\cdots > 0.$$

This yields

$$\vartheta_{\mathcal{W}_{2,\rho}}(z) > 0,\ \text{ for } z \in \mathcal{R}_a \cup \mathcal{R}_b \cup \mathcal{R}_c$$

by the monotonicity properties (5.11) and (5.12). Therefore by (5.13)

$$\vartheta_{\mathcal{W}_{2,\rho}}(z) > 0,\ \text{ for } z \in \mathcal{R}_2.$$

By (5.10) $\frac{\partial}{\partial x}\mathcal{W}_{2,\rho_*}(z)$ vanishes only at $x = 0$ or $\frac{1}{2}$. This completes the proof.

□

6. The Behavior of $\mathcal{W}_{1,\rho}(z)$ on the $y-$Axis

In this section, we study the property of the functional $\mathcal{W}_{1,\rho}$ on the $y-$axis. We will prove that on the $y-$axis, depending on ρ, $\mathcal{W}_{1,\rho}(z)$ has either 1 or 3 critical points. This gives the precise characterization of the minimizers of $\mathcal{W}_{1,\rho}(z)$ on the $y-$axis. The proof relies crucially on a novel property of Jacob theta function proved in Theorem 6.1 below.

Proposition 6.1. *There exists a threshold ρ_1 which is the unique solution of $\frac{\partial^2}{\partial y^2}\mathcal{W}_{1,\rho}(yi)\mid_{y=1}=0$, (in fact, $\rho_1=-\frac{\mathcal{Y}''(1)}{\mathcal{X}''(1)}\sim 0.04016680351\cdots$), such that*

1. *if $\rho\in[\rho_1,+\infty)$, the function $y\to\mathcal{W}_{1,\rho}(yi)$, $y>0$ admits only one critical point at $y=1$, and $\frac{\partial}{\partial y}\mathcal{W}_{1,\rho}(yi)<0$ if $y\in(0,1)$ and $\frac{\partial}{\partial y}\mathcal{W}_{1,\rho}(yi)>0$ if $y\in(1,\infty)$;*
2. *if $\rho\in[0,\rho_1)$, the function $y\to\mathcal{W}_{1,\rho}(yi)$, $y>0$ admits only three critical points at $y_{1,\rho}$, 1 and $\frac{1}{y_{1,\rho}}$, where $y_{1,\rho}\in(1,\sqrt{3}]$. Moreover*

$$
\begin{aligned}
&\frac{\partial}{\partial y}\mathcal{W}_{1,\rho}(yi)<0 \text{ if } y\in\left(0,\frac{1}{y_{1,\rho}}\right),\\
&\frac{\partial}{\partial y}\mathcal{W}_{1,\rho}(yi)>0 \text{ if } y\in\left(\frac{1}{y_{1,\rho}},1\right),\\
&\frac{\partial}{\partial y}\mathcal{W}_{1,\rho}(yi)<0 \text{ if } y\in\left(1,y_{1,\rho}\right),\\
&\frac{\partial}{\partial y}\mathcal{W}_{1,\rho}(yi)>0 \text{ if } y\in\left(y_{1,\rho},\infty\right).
\end{aligned}
$$

The critical point $y_{1,\rho}$ is the unique solution of $\frac{\partial}{\partial y}\mathcal{W}_{1,\rho}(yi)=0,\ \ y\in(1,\sqrt{3}]$. Furthermore if $\rho\in[0,\rho_1]$, then

$$
\frac{\partial y_{1,\rho}}{\partial\rho}<0. \tag{6.1}
$$

To prove Proposition 6.1, we need to use some properties of the Jacobi theta functions defined at (1.12)–(1.13). They satisfy the transformation properties

$$
\begin{aligned}
&\vartheta_3\left(\frac{1}{y}\right)=\sqrt{y}\vartheta_3(y),\ \ \vartheta_2\left(\frac{1}{y}\right)=\sqrt{y}\vartheta_4(y)\\
&\vartheta_4\left(\frac{1}{y}\right)=\sqrt{y}\vartheta_2(y),\quad \vartheta_4(y)=\vartheta_3(4y)-\vartheta_2(4y).
\end{aligned}
\tag{6.2}
$$

It is easy to see that for $z=yi$

$$
\theta(s;yi)=\sum_m\sum_n e^{-s\frac{\pi}{y}(n^2+m^2y^2)},\ \ \theta\left(s;\frac{yi+1}{2}\right)=\sum_m\sum_n e^{-2s\frac{\pi}{y}((\frac{m}{2}+n)^2+\frac{m^2}{4}y^2)}.
\tag{6.3}
$$

We first express $\theta(s;yi)$, $\theta(s;\frac{yi+1}{2})$ as products of Jacobi theta functions, which is a starting point of our analysis.

Lemma 6.1. *It holds that*

$$\theta(s; yi) = \vartheta_3(sy)\vartheta_3\left(\frac{s}{y}\right), \ \theta(s; \frac{yi+1}{2}) = \vartheta_3(2sy)\vartheta_3\left(\frac{2s}{y}\right) + \vartheta_2(2sy)\vartheta_2\left(\frac{2s}{y}\right).$$

Proof. The first one is straightforward:

$$\theta(s; yi) = \sum_n e^{-s\frac{\pi}{y}n^2} \sum_m e^{-s\pi y m^2} = \vartheta_3(sy)\vartheta_3\left(\frac{s}{y}\right).$$

For the second one,

$$\begin{aligned}\theta\left(s; \frac{yi+1}{2}\right) &= \sum_m \sum_n e^{-2s\frac{\pi}{y}((\frac{m}{2}+n)^2+\frac{m^2}{4}y^2)} = \sum_{p\equiv q(\mod 2)} e^{-\frac{s\pi}{2}(\frac{1}{y}p^2+yq^2)}\\ &= \sum_{p=2m',q=2n'} e^{-\frac{s\pi}{2}(\frac{1}{y}p^2+yq^2)} + \sum_{p=2m'+1,q=2n'+1} e^{-\frac{s\pi}{2}(\frac{1}{y}p^2+yq^2)}\\ &= \sum_{m'} e^{-2s\pi\frac{1}{y}m'^2} \sum_{n'} e^{-2s\pi y n'^2}\\ &\quad + \sum_{m'} e^{-\frac{2s\pi}{4}\frac{1}{y}(2m'+1)^2} \sum_{n'} e^{-\frac{2s\pi}{4}y(2n'+1)^2}\\ &= \vartheta_3(2sy)\vartheta_3\left(\frac{2s}{y}\right) + \vartheta_2(2sy)\vartheta_2\left(\frac{2s}{y}\right).\end{aligned}$$

□

The next Lemma follows from Lemma 3.1. We single it out for the convenience of our analysis here.

Lemma 6.2. *For any* $s > 0$*,* $\theta(s; yi)$ *and* $\theta(s; \frac{yi+1}{2})$ *both satisfy the functional equation*

$$\mathcal{H}\left(\frac{1}{y}\right) = \mathcal{H}(y). \tag{6.4}$$

Consequently, $\mathcal{H}'(\frac{1}{y}) = -y^2\mathcal{H}'(y)$*. In particular,* $\mathcal{H}'(1) = 0$*, that is,* $y = 1$ *is always a critical point of* $\theta(s; yi), \theta(s; \frac{yi+1}{2})$*.*

For $s = 1$, by Lemma 6.1 and transformation (6.2), we obtain

Lemma 6.3.

$$\begin{aligned}\theta(1; yi) &= \sqrt{y}\vartheta_3^2(y),\\ \theta\left(2; \frac{yi+1}{2}\right) &= \frac{\sqrt{y}}{2}\left(\vartheta_3(4y)\vartheta_3\left(\frac{y}{4}\right) + \vartheta_2(4y)\vartheta_4\left(\frac{y}{4}\right)\right).\end{aligned} \tag{6.5}$$

To prove Proposition 6.1, we first prove a monotonicity property of $\theta(1; yi)$ and $\theta(2; \frac{yi+1}{2})$ in Lemma 6.4, which can be viewed as the particular case of Proposition 6.1. Then we establish the key Theorem 6.1, in which a novel property about the quotient of Jacobi theta functions is proved.

The following Lemma is known in [8,28]:

Lemma 6.4. • *The function $y \to \theta(s; yi)$, $y > 0$, has only one critical point at $y = 1$. Furthermore*

$$\frac{\partial}{\partial y}\theta(s; yi) < 0 \text{ for } y \in (0, 1); \quad \frac{\partial}{\partial y}\theta(s; yi) > 0 \text{ for } y \in (1, \infty).$$

• *For any $s > 0$, the function $y \to \theta(s; \frac{yi+1}{2})$, $y > 0$, has three critical points at $\frac{\sqrt{3}}{3}$, 1 and $\sqrt{3}$.*

We now state Theorem 6.1 whose proof is much involved. We use a combination of functional equations, error terms analysis and several new observations. Let

$$\begin{aligned}
\mathcal{X}(y) &:= \vartheta_3(y)\vartheta_3\left(\frac{1}{y}\right) = \sqrt{y}\vartheta_3^2(y),\\
\mathcal{Y}(y) &:= 2\left(\vartheta_3(4y)\vartheta_3\left(\frac{4}{y}\right) + \vartheta_2(4y)\vartheta_2\left(\frac{4}{y}\right)\right)\\
&= \sqrt{y}\left(\vartheta_3(4y)\vartheta_3\left(\frac{y}{4}\right) + \vartheta_2(4y)\vartheta_4\left(\frac{y}{4}\right)\right).
\end{aligned}$$

Theorem 6.1. *The function $y \mapsto \frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)}$, $y > 0$ has only one critical point at $y = 1$. Furthermore $\left(\frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)}\right)' < 0$ for $y \in (0, 1)$ and $\left(\frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)}\right)' > 0$ for $y \in (1, \infty)$.*

Proof. Denote $\mathcal{Z}(y) := \frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)}$. By Lemma 6.4, the function $\mathcal{Z}(y)$ is well-defined. By Lemma 6.2, we also have

$$\mathcal{X}'\left(\frac{1}{y}\right) = -y^2\mathcal{X}'(y), \; \mathcal{Y}'\left(\frac{1}{y}\right) = -y^2\mathcal{Y}'(y). \tag{6.6}$$

Hence

$$\mathcal{Z}\left(\frac{1}{y}\right) = \mathcal{Z}(y),$$

and

$$\mathcal{Z}'\left(\frac{1}{y}\right) = -y^2\mathcal{Z}'(y). \tag{6.7}$$

Consequently, $\mathcal{Z}'(1) = 0$, that is, $y = 1$ is the critical point of $\mathcal{Z}(y)$.

By (6.7), it suffices to prove that

$$\mathcal{Z}'(y) > 0, \quad \text{for } y \in (1, \infty). \tag{6.8}$$

By the explicit expression of Jacobi theta functions (1.13) and (6.2), we start with

$$
\begin{aligned}
\mathcal{X}(y) &= \sqrt{y}\left(1+2\sum_{n=1}^{\infty} e^{-\pi n^2 y}\right)^2 \\
&= \left(\sqrt{y}+4\sqrt{y}e^{-\pi y}+4\sqrt{y}e^{-2\pi y}+4\sqrt{y}e^{-4\pi y}\right) \\
&\quad+\left(4\sqrt{y}\sum_{n=3}^{\infty} e^{-\pi n^2 y}+4\sqrt{y}\left(\sum_{n=2}^{\infty} e^{-\pi n^2 y}\right)^2+8\sqrt{y}\sum_{n=2}^{\infty} e^{-\pi(n^2+1)y}\right) \\
&:= \mathcal{X}_a(y)+\mathcal{X}_e(y)
\end{aligned}
$$

where $\mathcal{X}_a(y)$ and $\mathcal{X}_e(y)$ are defined at the last equality. $\mathcal{X}_a$ is the major part and $\mathcal{X}_e$ is the error part. In fact, we have that, for some constant $C > 0$,

$$
\|\mathcal{X}_e(y)\|_{C^2} \leqq C\sqrt{y}e^{-5\pi y}, \ \text{for } y > 1. \tag{6.9}
$$

For $\mathcal{Y}(y)$, again by (1.13) and (6.2), one first has

$$
\begin{aligned}
\sqrt{y}\vartheta_3(4y)\vartheta_3(\frac{y}{4}) &= \sqrt{y}\left(1+2\sum_{n=1}^{\infty} e^{-4\pi n^2 y}\right)\left(1+2\sum_{n=1}^{\infty} e^{-\frac{1}{4}\pi n^2 y}\right) \\
&= \sqrt{y}+2\sqrt{y}e^{-\frac{1}{4}\pi y}+2\sqrt{y}e^{-\pi y}+2\sqrt{y}e^{-\frac{9}{4}\pi y}+4\sqrt{y}e^{-4\pi y} \\
&\quad+2\sqrt{y}\sum_{n=2}^{\infty} e^{-4\pi n^2 y}+2\sqrt{y}\sum_{n=5}^{\infty} e^{-\frac{1}{4}\pi n^2 y} \\
&\quad+4\sqrt{y}\sum_{n=1}^{\infty} e^{-4\pi n^2 y}\sum_{n=1}^{\infty} e^{-\frac{1}{4}\pi n^2 y}.
\end{aligned}
$$

We regroup the terms as

$$
\begin{aligned}
&\sqrt{y}\vartheta_2(4y)\vartheta_4\left(\frac{y}{4}\right) = \sqrt{\vartheta}_2(4y)\big(\vartheta_3(y)-\vartheta_2(y)\big) = \sqrt{y}\vartheta_2(4y)\vartheta_3(y) \\
&-\sqrt{y}\vartheta_2(4y)\vartheta_2(y) \\
&= 2\sqrt{y}\sum_{n=1}^{\infty} e^{-\pi(2n-1)^2 y}+4\sqrt{y}\sum_{n=1}^{\infty} e^{-\pi(2n-1)^2 y}\sum_{n=1}^{\infty} e^{-\pi n^2 y} \\
&\quad-4\sqrt{y}e^{-\frac{5}{4}\pi y}\left(1+\sum_{n=2}^{\infty} e^{-\pi((n-\frac{1}{2})^2-\frac{1}{4})y}\right)\left(1+\sum_{n=2}^{\infty} e^{-\pi((2n-1)^2-1)y}\right) \\
&= 2\sqrt{y}e^{-\pi y}+4\sqrt{y}e^{-2\pi y}-4\sqrt{y}e^{-\frac{5}{4}\pi y}-4\sqrt{y}e^{-\frac{13}{4}\pi y} \\
&\quad+4\sqrt{y}\left(\sum_{n=2}^{\infty} e^{-\pi((2n-1)^2+1)y}+\sum_{n=2}^{\infty} e^{-\pi(n^2+1)y}+\sum_{n=2}^{\infty} e^{-\pi(2n-1)^2 y}\sum_{n=2}^{\infty} e^{-\pi n^2 y}\right) \\
&\quad-4\sqrt{y}e^{-\frac{5}{4}\pi y}\left(\sum_{n=3}^{\infty} e^{-\pi((n-\frac{1}{2})^2-\frac{1}{4})y}+\sum_{n=2}^{\infty} e^{-\pi((2n-1)^2-1)y}\right.
\end{aligned}
$$

$$+\sum_{n=2}^{\infty} e^{-\pi((n-\frac{1}{2})^2-\frac{1}{4})y} \cdot \sum_{n=2}^{\infty} e^{-\pi((2n-1)^2-1)y}\Bigg).$$

Now let the approximate part of $\mathcal{Y}(y)$ be

$$\begin{aligned}\mathcal{Y}_a(y) &:= \sqrt{y} + 2\sqrt{y}e^{-\frac{1}{4}\pi y} + 4\sqrt{y}e^{-\pi y} + 2\sqrt{y}e^{-\frac{9}{4}\pi y} + 4\sqrt{y}e^{-2\pi y}\\ &\quad + 4\sqrt{y}e^{-4\pi y} - 4\sqrt{y}e^{-\frac{5}{4}\pi y} - 4\sqrt{y}e^{-\frac{13}{4}\pi y}\end{aligned}$$

and the error part by

$$\begin{aligned}\mathcal{Y}_e(y) &:= 2\sqrt{y}\sum_{n=2}^{\infty} e^{-4\pi n^2 y} + 2\sqrt{y}\sum_{n=5}^{\infty} e^{-\frac{1}{4}\pi n^2 y} + 4\sqrt{y}\sum_{n=1}^{\infty} e^{-4\pi n^2 y}\sum_{n=1}^{\infty} e^{-\frac{1}{4}\pi n^2 y}\\ &\quad + 4\sqrt{y}\left(\sum_{n=2}^{\infty} e^{-\pi((2n-1)^2+1)y} + \sum_{n=2}^{\infty} e^{-\pi(n^2+1)y} + \sum_{n=2}^{\infty} e^{-\pi(2n-1)^2 y}\sum_{n=2}^{\infty} e^{-\pi n^2 y}\right)\\ &\quad - 4\sqrt{y}e^{-\frac{5}{4}\pi y}\Bigg(\sum_{n=3}^{\infty} e^{-\pi((n-\frac{1}{2})^2-\frac{1}{4})y} + \sum_{n=2}^{\infty} e^{-\pi((2n-1)^2-1)y}\\ &\quad + \sum_{n=2}^{\infty} e^{-\pi((n-\frac{1}{2})^2-\frac{1}{4})y} \cdot \sum_{n=2}^{\infty} e^{-\pi((2n-1)^2-1)y}\Bigg).\end{aligned}$$

Then

$$\mathcal{Y}(y) = \mathcal{Y}_a(y) + \mathcal{Y}_e(y) \tag{6.10}$$

and we have following estimate for $\mathcal{Y}_e(y)$:

$$\|\mathcal{Y}_e(y)\|_{C^2} \leqq C\sqrt{y}e^{-\frac{17}{4}\pi y}.$$

To prove (6.8), we divide the proof into two regions of y: the large y case $y \in [1.1, \infty)$ and the small y case $y \in (1, 1.1)$.
Case (a): $y \in [1.1, \infty)$. In this case we have

$$\mathcal{Z}'(y) = \frac{\mathcal{Y}''(y)\mathcal{X}'(y) - \mathcal{X}''(y)\mathcal{Y}'(y)}{(\mathcal{X}'(y))^2}.$$

By Lemma 6.4, to prove Case (a) it suffices to prove that

$$\mathcal{Y}''(y)\mathcal{X}'(y) - \mathcal{X}''(y)\mathcal{Y}'(y) > 0 \ \text{ if } \ y \in (1.1, \infty).$$

By (6.9) and (6.10), there holds

$$\mathcal{Y}''\mathcal{X}' - \mathcal{Y}'\mathcal{X}'' = \left(\mathcal{Y}_a''\mathcal{X}_a' - \mathcal{X}_a''\mathcal{Y}_a'\right) + \left(\mathcal{Y}_e''\mathcal{X}' - \mathcal{Y}_e'\mathcal{X}'' + \mathcal{Y}_a''\mathcal{X}_e' - \mathcal{X}_e''\mathcal{Y}_a'\right)$$

where $\left(\mathcal{Y}_a''\mathcal{X}_a' - \mathcal{X}_a''\mathcal{Y}_a'\right)$ and $\left(\mathcal{Y}_e''\mathcal{X}' - \mathcal{Y}_e'\mathcal{X}'' + \mathcal{Y}_a''\mathcal{X}_e' - \mathcal{X}_e''\mathcal{Y}_a'\right)$ are the approximate part and the error part of $\mathcal{Y}''\mathcal{X}' - \mathcal{Y}''\mathcal{X}'$ respectively. We shall use the approximate part to control the error part.

To obtain the lower bound of $\left(\mathcal{Y}_a''\mathcal{X}_a' - \mathcal{X}_a''\mathcal{Y}_a'\right)$, after subtracting some proper factor($\frac{16y}{\pi}e^{\frac{1}{4}\pi y}$), one finds that

$$y \to \frac{16y}{\pi}e^{\frac{1}{4}\pi y}\left(\mathcal{Y}_a''\mathcal{X}_a' - \mathcal{X}_a''\mathcal{Y}_a'\right)(y) \tag{6.11}$$

is monotonically increasing.

For the error part $\left(\mathcal{Y}_e''\mathcal{X}' - \mathcal{Y}_e'\mathcal{X}'' + \mathcal{Y}_a''\mathcal{X}_e' - \mathcal{X}_e''\mathcal{Y}_a'\right)$, one has the estimate

$$|\left(\mathcal{Y}_e''\mathcal{X}' - \mathcal{Y}_e'\mathcal{X}'' + \mathcal{Y}_a''\mathcal{X}_e' - \mathcal{X}_e''\mathcal{Y}_a'\right)(y)| \leqq C\sqrt{y}e^{-\frac{17}{4}\pi y}, \tag{6.12}$$

which decays to zero very fast.

Combining (6.11) with (6.12), one deduces that

$$\mathcal{Y}''\mathcal{X}' - \mathcal{X}''\mathcal{Y}' > 0 \ \text{ if } \ y \in [1.1, \infty). \tag{6.13}$$

The detailed proof of (6.11), (6.12) and (6.13) will be provided in the Appendix 2.

This proves that

$$\mathcal{Z}'(y) > 0 \ \text{ if } \ y \in [1.1, \infty). \tag{6.14}$$

Case (b): $y \in (1, 1.1)$. In this case $0 < 1 - y < 0.1$. To prove

$$\mathcal{Z}'(y) = \left(\frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)}\right)' > 0, \text{on } y \in (1, 1.1), \tag{6.15}$$

it suffices to prove that

$$\left(\frac{\mathcal{Y}''(y)}{\mathcal{X}''(y)}\right)' > 0, \forall\ y \in (1, 1.1),$$

given that

$$\mathcal{X}'(1) = \mathcal{Y}'(1) = 0 \tag{6.16}$$

which follows from (6.6). In fact, there exists $y_1, y_2 \in (1, y)$ such that

$$\begin{aligned}\left(\frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)}\right)' &= \frac{\mathcal{Y}''(y)\mathcal{X}'(y) - \mathcal{Y}'(y)\mathcal{X}''(y)}{\mathcal{X}'^2(y)} = \frac{\mathcal{X}''(y)}{\mathcal{X}'(y)}\left(\frac{\mathcal{Y}''(y)}{\mathcal{X}''(y)} - \frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)}\right)\\ &= \frac{\mathcal{X}''(y)}{\mathcal{X}'(y) - \mathcal{X}'(1)}\left(\frac{\mathcal{Y}''(y)}{\mathcal{X}''(y)} - \frac{\mathcal{Y}'(y) - \mathcal{Y}'(1)}{\mathcal{X}'(y) - \mathcal{X}'(1)}\right)\\ &= \frac{\mathcal{X}''(y)}{\mathcal{X}''(y_2)(y-1)}\left(\frac{\mathcal{Y}''(y)}{\mathcal{X}''(y)} - \frac{\mathcal{Y}''(y_1)}{\mathcal{X}''(y_1)}\right)\end{aligned} \tag{6.17}$$

using (6.16).

We also have that

$$\mathcal{X}''(y) > 0, \quad \text{if } y \in (1, \infty) \tag{6.18}$$

by the same decomposition method as used above. We omit the details here. (Actually, we only need (6.18) holds for small interval such as $(1, 1.2]$).

Moreover, $\left(\frac{\mathcal{Y}''(y)}{\mathcal{X}''(y)}\right)' > 0$ implies

$$\frac{\mathcal{Y}''(y)}{\mathcal{X}''(y)} - \frac{\mathcal{Y}''(y_1)}{\mathcal{X}''(y_1)} > 0. \tag{6.19}$$

Then the claim follows from (6.19), (6.18) and (6.17).

For the derivative of the quotient of second order derivatives, one has

$$\left(\frac{\mathcal{Y}''(y)}{\mathcal{X}''(y)}\right)' = \frac{\mathcal{Y}'''(y)\mathcal{X}''(y) - \mathcal{Y}''(y)\mathcal{X}'''(y)}{\mathcal{X}''^2(y)}.$$

Define

$$f_{\mathcal{X}\mathcal{Y}}(y) := \mathcal{Y}'''(y)\mathcal{X}''(y) - \mathcal{Y}''(y)\mathcal{X}'''(y).$$

Equivalently, to show (6.15) one needs to show that

$$f_{\mathcal{X}\mathcal{Y}}(y) > 0 \quad \text{for} \quad y \in (1, 1.1). \tag{6.20}$$

Differrentiating(6.6), the functions $\mathcal{X}(y)$ and $\mathcal{Y}(y)$ both satisfy the following functional equations

$$\begin{aligned}\mathcal{H}''\left(\frac{1}{y}\right) &= 2y^3\mathcal{H}'(y) + y^4\mathcal{H}''(y)\\ \mathcal{H}'''\left(\frac{1}{y}\right) &= -6y^4\mathcal{H}'(y) - 6y^5\mathcal{H}''(y) - y^6\mathcal{H}'''(y).\end{aligned} \tag{6.21}$$

Plugging $y = 1$ in (6.21) and using (6.16), one deduces

$$\mathcal{X}'''(1) = -3\mathcal{X}''(1), \quad \mathcal{Y}'''(1) = -3\mathcal{Y}''(1). \tag{6.22}$$

From (6.22), one has

$$f_{\mathcal{X}\mathcal{Y}}(1) = 0. \tag{6.23}$$

Then to prove (6.20), by (6.23), it suffices to prove that

$$f'_{\mathcal{X}\mathcal{Y}}(y) > 0 \quad \text{for} \quad y \in (1, 1.1). \tag{6.24}$$

Proceed by (6.9) and (6.10)

$$\begin{aligned}f'_{\mathcal{X}\mathcal{Y}} &= \mathcal{Y}''''\mathcal{X}'' - \mathcal{Y}''\mathcal{X}''''\\ &= \left(\mathcal{Y}_a''''\mathcal{X}_a'' - \mathcal{Y}_a''\mathcal{X}_a''''\right) + \left(\mathcal{X}_e''\mathcal{Y}'''' + \mathcal{Y}_e''''\mathcal{X}_a'' - \mathcal{X}_e''''\mathcal{Y}'' - \mathcal{Y}_e''\mathcal{X}_a''''\right).\end{aligned} \tag{6.25}$$

We use $\left(\mathcal{Y}_a''''\mathcal{X}_a'' - \mathcal{Y}_a''\mathcal{X}_a''''\right)$ and $\left(\mathcal{X}_e''\mathcal{Y}'''' + \mathcal{Y}_e''''\mathcal{X}_a'' - \mathcal{X}_e''''\mathcal{Y}'' - \mathcal{Y}_e''\mathcal{X}_a''''\right)$ as the approximate and error parts of $f'_{\mathcal{X}\mathcal{Y}}$ respectively.

For the approximate part, after subtracting some proper factor, one finds

$$y \to \frac{512y^4}{\pi} e^{\frac{1}{4}\pi y} \Big(\mathcal{Y}_a'''' \mathcal{X}_a'' - \mathcal{Y}_a'' \mathcal{X}_a'''' \Big)(y) \tag{6.26}$$

is monotonically decreasing on (1, 1.2).

For the error part, one has the following estimate

$$|\Big(\mathcal{X}_e'' \mathcal{Y}'''' + \mathcal{Y}_e'''' \mathcal{X}_a'' - \mathcal{X}_e'''' \mathcal{Y}'' - \mathcal{Y}_e'' \mathcal{X}_a'''' \Big)(y)| \leqq C y e^{-5\pi y}, \tag{6.27}$$

which has fast decay.

Combining (6.26), (6.27) and (6.25), we can prove that

$$f'_{\mathcal{X}\mathcal{Y}}(y) > 0 \ \text{ if } \ y \in (1, 1.11]. \tag{6.28}$$

The detailed proof of (6.26), (6.27) and (6.28) will be given in the Appendix 2. This completes the proof.

□

Finally we give the proof of Proposition 6.1.

Proof. By Lemma 6.2, $y = 1$ is a critical point of $\mathcal{W}_{1,\rho}(yi)$. Furthermore

$$\frac{\partial}{\partial y} \mathcal{W}_{1,\rho} \left(\frac{1}{y} i \right) = -y^2 \frac{\partial}{\partial y} \mathcal{W}_{1,\rho}(yi)(y). \tag{6.29}$$

By Lemma 6.4, we have

$$\mathcal{X}'(y) > 0 \ \text{ if } \ y \in (1, \infty) \quad \text{and} \quad \mathcal{Y}'(\sqrt{3}) = 0. \tag{6.30}$$

Hence we obtain that

$$\frac{\partial}{\partial y} \mathcal{W}_{1,\rho}(yi) > 0 \ \text{ if } \ y \in (\sqrt{3}, \infty). \tag{6.31}$$

To study the monotonicity of $\mathcal{W}_{1,\rho}(yi)$ on the interval $(1, \sqrt{3})$, we rewrite $\frac{\partial}{\partial y} \mathcal{W}_{1,\rho}(yi)$ as

$$\begin{aligned} \frac{\partial}{\partial y} \mathcal{W}_{1,\rho}(yi) &= \frac{\partial}{\partial y} \left(\theta \left(2; \frac{yi+1}{2} \right) + \rho \theta(1; yi) \right) = \mathcal{Y}'(y) + \rho \mathcal{X}'(y) \\ &= \mathcal{X}'(y) \cdot \Big(\frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)} + \rho \Big). \end{aligned} \tag{6.32}$$

By (6.30), the zeroes of $\frac{\partial}{\partial y} \mathcal{W}_{1,\rho}(yi)$ on $(1, \sqrt{3})$ satisfy the following functional equation

$$\frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)} + \rho = 0, \quad y \in (1, \sqrt{3}). \tag{6.33}$$

Furthermore, by Theorem 6.1, we see that

$$\frac{\mathcal{Y}'(y)}{\mathcal{X}'(y)} + \rho \ \text{ is strictly increasing on } \ (1, \sqrt{3}). \tag{6.34}$$

(6.34) and (6.33) imply that $\frac{\partial}{\partial y}\mathcal{W}_{1,\rho}(yi)$ admits at most one zero on $(1, \sqrt{3})$. This fact combined with (6.31) yields that $\frac{\partial}{\partial y}\mathcal{W}_{1,\rho}(yi)$ admits either one or three critical points on $(0, \infty)$.

Since $\mathcal{X}'(1) = \mathcal{Y}'(1) = 0$, $\frac{\mathcal{Y}'(1)}{\mathcal{X}'(1)} = \frac{\mathcal{Y}''(1)}{\mathcal{X}''(1)}$.

At the other end point $\sqrt{3}$, since $\mathcal{Y}'(\sqrt{3}) = 0$ (see (6.30)), we have that

$$\frac{\mathcal{Y}'(\sqrt{3})}{\mathcal{X}'(\sqrt{3})} + \rho = 0 + \rho > 0, \quad \rho > 0.$$

By (6.34), we see that the Equation (6.33) has a zero if and only if

$$\frac{\mathcal{Y}''(1)}{\mathcal{X}''(1)} + \rho < 0. \tag{6.35}$$

The condition in (6.35) is

$$\rho < \rho_1 := -\frac{\mathcal{Y}''(1)}{\mathcal{X}''(1)}. \tag{6.36}$$

Combining (6.35),(6.36) with (6.31), one has

$$\frac{\partial}{\partial y}\mathcal{W}_{1,\rho}(yi) > 0 \ \text{ on } \ (1, \infty) \ \text{ provided } \ \rho \geqq \rho_1.$$

This and (6.29) give the proof of part 1 of Proposition 6.1. (For the case $\rho = 0$, $y_{1,\rho} = \sqrt{3}$ by (6.30).)

In the case when $\rho \in (0, \rho_1)$, there exists an unique root of (6.33) as $y_{1,\rho} \in (1, \sqrt{3})$. By duality (6.29), there exists another root $\frac{1}{y_{1,\rho}} \in (\frac{\sqrt{3}}{3}, 1)$. Therefore part 2 of Proposition 6.1 follows from (6.29) and (6.34).

Finally (6.1) follows from (6.34).

This completes the proof.

□

7. The Behavior of $\mathcal{W}_{2,\rho}(z)$ on the $y-$Axis

Let $\mathcal{W}_{2,\rho}(z) := \theta(1; \frac{z+1}{2}) + \rho\theta(2; z)$ be the conjugate of $\mathcal{W}_{1,\rho}(z)$. In this section we prove similar properties of Section 6 for $\mathcal{W}_{2,\rho}$. As in Section 6, $\mathcal{W}_{2,\rho}(yi)$ admits either 1 or 3 three critical points depending on different vales of ρ. These are stated in Proposition 7.1. The proof relies critically on a novel property of the classical theta functions proved in Theorem 7.1.

Proposition 7.1. *There exists a threshold ρ_2 which is the unique solution of*

$$\frac{\partial^2}{\partial y^2}\mathcal{W}_{2,\rho}(yi) \mid_{y=1} = 0$$

(in fact $\rho_2 = -1 - \frac{\mathcal{B}''(1)}{\mathcal{A}''(1)}$, numerically, $\rho_2 = 1.190861337\cdots$) such that

1. *when* $\rho \in [0, \rho_2)$*, the function* $y \to \mathcal{W}_{2,\rho}(yi), y > 0$ *admits only three critical points at* $y_{2,\rho}$*, 1 and* $\frac{1}{y_{2,\rho}}$*, where* $y_{2,\rho} \in (1, \sqrt{3}]$*. Furthermore we have* $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi) < 0$ *if* $y \in (0, \frac{1}{y_{2,\rho}})$*,* $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi) > 0$ *if* $y \in (\frac{1}{y_{2,\rho}}, 1)$*,* $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi) < 0$ *if* $y \in (1, y_{2,\rho})$*, and* $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi) > 0$ *if* $y \in (y_{2,\rho}, \infty)$

The critical point $y_{2,\rho}$ *is the unique solution of* $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi) = 0,\ \ y \in (1, \sqrt{3}]$*. Moreover, if* $\rho \in (0, \rho_2)$*, then*

$$\frac{\partial y_{2,\rho}}{\partial \rho} < 0. \tag{7.1}$$

2. *when* $\rho \in [\rho_2, +\infty)$*, the function* $y \to \mathcal{W}_{2,\rho}(yi), y > 0$ *admits only one critical point at 1, and we have* $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi) < 0$ *if* $y \in (0, 1)$*,* $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi) > 0$ *if* $y \in (1, \infty)$.

As in Section 6, by Lemma 6.1 and transformation (6.2), we have that

Lemma 7.1.

$$\theta(2; yi) = \sqrt{\frac{y}{2}}\vartheta_3(2y)\vartheta_3(\frac{y}{2}),\ \ \theta(1; \frac{yi+1}{2}) = \sqrt{\frac{y}{2}}\big(\vartheta_3(2y)\vartheta_3(\frac{y}{2}) + \vartheta_2(2y)\vartheta_4(\frac{y}{2})\big).$$

Recall by (1.13) and (6.2),

$$\mathcal{A}(y) := \sqrt{2}\vartheta_3(2y)\vartheta_3(\frac{2}{y}) = \sqrt{y}\vartheta_3(2y)\vartheta_3(\frac{y}{2}),\ \mathcal{B}(y) := \sqrt{2}\vartheta_2(2y)\vartheta_2(\frac{2}{y}) = \sqrt{y}\vartheta_2(2y)\vartheta_4(\frac{y}{2}).$$

Next we state Theorem 7.1, which provides the key argument to prove Proposition 7.1.

Theorem 7.1. *The function* $y \mapsto \frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}, y > 0$ *has only one critical point at* $y = 1$*, and furthermore* $\left(\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}\right)' < 0,\quad y \in (0, 1)$ *and* $\left(\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}\right)' > 0,\quad y \in (1, \infty)$.

Proof. By Lemma 6.2,

$$\mathcal{A}'\left(\frac{1}{y}\right) = -y^2\mathcal{A}'(y),\ \mathcal{B}'\left(\frac{1}{y}\right) = -y^2\mathcal{B}'(y). \tag{7.2}$$

Let

$$\mathcal{C}(y) := \frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}.$$

Then

$$\mathcal{C}\left(\frac{1}{y}\right) = \mathcal{C}(y).$$

Hence

$$\mathcal{C}'(\frac{1}{y}) = -y^2\mathcal{C}'(y). \tag{7.3}$$

In particular, $\mathcal{C}'(1) = 0$, that is, $y = 1$ is the critical point of $\mathcal{C}(y)$. This, combining with Lemma 6.4, shows that the $\mathcal{C}(y)$ by the quotient form is well defined.

By (7.3), it suffices to prove that

$$\mathcal{C}'(y) > 0 \quad y \in (1, \infty).$$

To prove this, we need to divide it into two parts of y: the small case $y \in [k, \infty)$ and the large case $y \in (1, k)$, where the parameter k is sightly bigger than 1 and will be determined later. (In fact $k = 1.05$.)

Case (a): $y \in [k, \infty)$. One has

$$\mathcal{C}'(y) = \frac{\mathcal{B}''(y)\mathcal{A}'(y) - \mathcal{A}''(y)\mathcal{B}'(y)}{(\mathcal{A}'(y))^2}.$$

Then we need to estimate the lower bound of $\mathcal{B}''(y)\mathcal{A}'(y) - \mathcal{A}''(y)\mathcal{B}'(y)$.

By (1.13),

$$\begin{aligned}
\mathcal{A}(y) &= \sqrt{y}\left(1 + 2\sum_{n=1}^{\infty} e^{-2\pi n^2 y}\right)\left(1 + 2\sum_{n=1}^{\infty} e^{-\frac{\pi}{2}n^2 y}\right) \\
&= \Big(\sqrt{y} + 2\sqrt{y}e^{-\frac{\pi y}{2}} + 4\sqrt{y}e^{-2\pi y} + 4\sqrt{y}e^{-\frac{5}{2}\pi y} + 4\sqrt{y}e^{-4\pi y} \\
&\quad + 2\sqrt{y}e^{-\frac{9}{2}\pi y} \\
&\quad + 2\sqrt{y}\left(\sum_{n=2}^{\infty} e^{-2\pi n^2 y} + \sum_{n=4}^{\infty} e^{-\frac{\pi}{2}n^2 y}\right)\Big) \\
&\quad + \Bigg(4\sqrt{y}e^{-\frac{5}{2}\pi y}\Bigg(\sum_{n=2}^{\infty} e^{-\frac{1}{2}\pi(n^2-1)y} + \sum_{n=2}^{\infty} e^{-2\pi(n^2-1)y} \\
&\quad + \sum_{n=2}^{\infty} e^{-\frac{1}{2}\pi(n^2-1)y} \cdot \sum_{n=2}^{\infty} e^{-2\pi(n^2-1)y}\Bigg)\Bigg) \\
&:= \mathcal{A}_a(y) + \mathcal{A}_e(y)
\end{aligned} \tag{7.4}$$

where $\mathcal{A}_a(y)$ and $\mathcal{A}_e(y)$ are defined at the last equality. $\mathcal{A}_e(y)$ is the error part which will be proved to satisfy

$$\|\mathcal{A}_e\|_{C^2} \leqq C\sqrt{y}e^{-\frac{13}{2}\pi y}.$$

For $\mathcal{B}(y)$, by (1.13), we rewrite as

$$\begin{aligned}
\mathcal{B}(y) &= \sqrt{y}\vartheta_2(2y)\Big(\vartheta_3(2y)-\vartheta_2(2y)\Big)\\
&= 2\sqrt{y}\sum_{n=1}^{\infty}e^{-2\pi y(n-\frac{1}{2})^2}+4\sqrt{y}\sum_{n=1}^{\infty}e^{-2\pi y(n-\frac{1}{2})^2}\sum_{n=1}^{\infty}e^{-2\pi n^2 y}\\
&\quad -4\sqrt{y}\left(\sum_{n=1}^{\infty}e^{-2\pi y(n-\frac{1}{2})^2}\right)^2\\
&= \Big(2\sqrt{y}e^{-\frac{1}{2}\pi y}+4\sqrt{y}e^{-\frac{5}{2}\pi y}+2\sqrt{y}e^{-\frac{9}{2}\pi y}-4\sqrt{y}e^{-\pi y}\Big)\\
&\quad +(2\sqrt{y}\sum_{n=3}^{\infty}e^{-\frac{1}{2}(2n-1)^2\pi y}+4\sqrt{y}e^{-\frac{5}{2}\pi y}\Big(\sum_{n=2}^{\infty}e^{-\frac{1}{2}((2n-1)^2-1)\pi y}\\
&\quad +\sum_{n=2}^{\infty}e^{-2(n^2-1)\pi y}\\
&\quad +\sum_{n=2}^{\infty}e^{-\frac{1}{2}((2n-1)^2-1)\pi y}\sum_{n=2}^{\infty}e^{-2(n^2-1)\pi y}\Big)-8\sqrt{y}\sum_{n=2}^{\infty}e^{-\frac{1}{2}(2n-1)^2\pi y}\\
&\quad -4\sqrt{y}\Big(\sum_{n=2}^{\infty}e^{-\frac{1}{2}(2n-1)^2\pi y}\Big)^2\Big)\\
&:= \mathcal{B}_a(y)+\mathcal{B}_e(y),
\end{aligned}$$

where $\mathcal{B}_a(y)$ and $\mathcal{B}_e(y)$ are defined at the last equality. That is, we have

$$\mathcal{B}(y)=\mathcal{B}_a(y)+\mathcal{B}_e(y), \tag{7.5}$$

where $\mathcal{B}_a(y)$, $\mathcal{B}_e(y)$ is the approximate part and the error part of $\mathcal{B}(y)$ respectively.
We have the following estimate

$$\|\mathcal{B}_e\|_{C^2}\leqq C\sqrt{y}e^{-\frac{13}{2}\pi y},\quad y\geqq 1.$$

To prove that

$$\mathcal{C}'(y)>0 \text{ if } y\in(k,\infty), \tag{7.6}$$

it suffices to prove that

$$\mathcal{B}''(y)\mathcal{A}'(y)-\mathcal{A}''(y)\mathcal{B}'(y)>0 \text{ if } y\in(k,\infty).$$

By (7.4), there holds

$$\mathcal{B}''\mathcal{A}'-\mathcal{A}''\mathcal{B}'=\Big(\mathcal{B}_a''\mathcal{A}_a'-\mathcal{A}_a''\mathcal{B}_a'\Big)+\Big(\mathcal{B}_e''\mathcal{A}'-\mathcal{B}_e'\mathcal{A}''+\mathcal{B}_a''\mathcal{A}_e'-\mathcal{A}_e''\mathcal{B}_a'\Big).$$

Here $\Big(\mathcal{B}_a''\mathcal{A}_a'-\mathcal{A}_a''\mathcal{B}_a'\Big)$ and $\Big(\mathcal{B}_e''\mathcal{A}'-\mathcal{B}_e'\mathcal{A}''+\mathcal{B}_a''\mathcal{A}_e'-\mathcal{A}_e''\mathcal{B}_a'\Big)$ are the approximate and error part of $\mathcal{B}''\mathcal{A}'-\mathcal{A}''\mathcal{B}'$ respectively.

To estimate the approximate part, we use the monotonicity of a weighted function, that is

$$y \to \frac{4y}{\pi} e^{\frac{1}{2}\pi y} \Big(\mathcal{B}_a'' \mathcal{A}_a' - \mathcal{A}_a'' \mathcal{B}_a' \Big)(y) \tag{7.7}$$

is strictly increasing.

For the error term, we have the following control

$$\left| \left(\mathcal{B}_e'' \mathcal{A}' - \mathcal{B}_e' \mathcal{A}'' + \mathcal{B}_a'' \mathcal{A}_e' - \mathcal{A}_e'' \mathcal{B}_a' \right)(y) \right| \leqq C\sqrt{y} e^{-\frac{13}{2}\pi y}, \quad y \geqq 1 \tag{7.8}$$

which decays fast.

Combining (7.7) and (7.8), one deduces that

$$\Big(\mathcal{B}'' \mathcal{A}' - \mathcal{A}'' \mathcal{B}' \Big)(y) > \quad \text{if} \ \ y \in [1.05, \infty). \tag{7.9}$$

This proves that

$$\mathcal{C}'(y) > 0 \ \ \text{if} \ \ y \in [1.05, \infty). \tag{7.10}$$

The detailed proofs of (7.7), (7.8) and (7.9) will be given in the Appendix 2.

Case (b): $y \in (1, k)$.

To prove

$$\left(\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)} \right)' > 0, \text{on } y \in (1, k), \tag{7.11}$$

by (6.17), it suffices to prove that

$$\left(\frac{\mathcal{B}''(y)}{\mathcal{A}''(y)} \right)' > 0, \text{on } y \in (1, k),$$

given that

$$\mathcal{A}'(1) = \mathcal{B}'(1) = 0 \tag{7.12}$$

which follows from (7.2). Here as in (6.18), we need $\mathcal{A}''(y) > 0$ in small interval such as $(1, 1.2]$ (we omit the details here).

To proceed, we notice that

$$\left(\frac{\mathcal{B}''(y)}{\mathcal{A}''(y)} \right)' = \frac{\mathcal{B}'''(y)\mathcal{A}''(y) - \mathcal{B}''(y)\mathcal{A}'''(y)}{\mathcal{A}''^2(y)}. \tag{7.13}$$

Define

$$f_{\mathcal{A}\mathcal{B}}(y) := \mathcal{B}'''(y)\mathcal{A}''(y) - \mathcal{B}''(y)\mathcal{A}'''(y).$$

Same as (6.23), we see that

$$f_{\mathcal{A}\mathcal{B}}(1) = 0. \tag{7.14}$$

Then to prove (7.11), it suffices to prove that

$$f'_{\mathcal{AB}}(y) > 0 \quad \text{for} \quad y \in (1, k). \tag{7.15}$$

Now by (7.4) and (7.5) we can write as

$$\begin{aligned} f'_{\mathcal{AB}} &= \mathcal{B}'''' \mathcal{A}'' - \mathcal{B}'' \mathcal{A}'''' \\ &= \left(\mathcal{B}_a'''' \mathcal{A}_a'' - \mathcal{B}_a'' \mathcal{A}_a''''\right) + \left(\mathcal{B}_e'''' \mathcal{A}'' - \mathcal{B}_e'' \mathcal{A}'''' + \mathcal{B}_a'''' \mathcal{A}_e'' - \mathcal{A}_e'''' \mathcal{B}_a''\right). \end{aligned} \tag{7.16}$$

The main part is $\left(\mathcal{B}_a'''' \mathcal{A}_a'' - \mathcal{B}_a'' \mathcal{A}_a''''\right)$ which is is not monotonically decreasing or increasing. Instead, a weighted

$$y \to \frac{32y^4}{\pi} e^{\frac{1}{2}\pi y} \left(\mathcal{B}_a'''' \mathcal{A}_a'' - \mathcal{B}_a'' \mathcal{A}_a''''\right)(y) \tag{7.17}$$

is strictly decreasing on $(1, \infty)$.

For the error part in (7.16), one deduces the following upper bound estimate,

$$\left| \left(\mathcal{B}_e'''' \mathcal{A}'' - \mathcal{B}_e'' \mathcal{A}'''' + \mathcal{B}_a'''' \mathcal{A}_e'' - \mathcal{A}_e'''' \mathcal{B}_a''\right)(y) \right| \leqq C\sqrt{y} e^{-\frac{13}{2}\pi y},\ y \geqq 1 \tag{7.18}$$

which decays very fast.

Combining (7.17), (7.18) and (7.16), we can show that

$$f'_{\mathcal{AB}}(y) > 0 \quad \text{if} \quad y \in (1, 1.12]. \tag{7.19}$$

The detailed proof of (7.17), (7.18) and (7.19) is tedious and will be given in the Appendix 2. This completes the proof.

□

Finally we give the proof of Proposition 7.1.

Proof. By Lemma 6.2, the functional $\mathcal{W}_{2,\rho}(yi)$ satisfies the functional equations

$$\mathcal{H}'\left(\frac{1}{y}\right) = -y^2 \mathcal{H}'(y). \tag{7.20}$$

Hence $\mathcal{H}'(1) = 0$, that is, $y = 1$ is a critical point of $\mathcal{W}_{2,\rho}(yi)$.

By (7.20), we just need to consider the functional $\mathcal{W}_{2,\rho}(yi)$ on $(1, \infty)$. For this, one uses Theorem 7.1 by rewriting $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi)$ as

$$\begin{aligned} \sqrt{2}\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi) &= \frac{\partial}{\partial y}\left(\sqrt{2}\theta\left(1; \frac{yi+1}{2}\right) + \rho\sqrt{2}\theta(2; yi)\right) \\ &= \mathcal{A}'(y) + \mathcal{B}'(y) + \rho\mathcal{A}'(y) \\ &= \mathcal{A}'(y) \cdot \left(1 + \frac{\mathcal{B}'(y)}{\mathcal{A}'(y)} + \rho\right). \end{aligned} \tag{7.21}$$

By Lemma 6.4, we see that

$$\mathcal{A}'(y) > 0 \quad y \in (1, \infty) \quad \text{and} \quad 1 + \frac{\mathcal{B}'(\sqrt{3})}{\mathcal{A}'(\sqrt{3})} = 0. \tag{7.22}$$

By Theorem 7.1, it holds that

$$\frac{\mathrm{d}}{\mathrm{d}y}\Big(1+\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}+\rho\Big)>0,\quad y\in(1,\infty). \tag{7.23}$$

From (7.23), in view of (7.21) and (7.22), we infer that

$$\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi)\ \text{ admits at most one zero point on }\ (1,\infty).$$

By (7.22), we see that

$$\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi)>0\ \text{ if }\ y\in(\sqrt{3},\infty). \tag{7.24}$$

Then one further concludes that the admissible zero point of $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi)$ must lie on $(1,\sqrt{3}]$ (if exists).

Next we consider the function $1+\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}+\rho$ for $\rho>0\in(1,\sqrt{3})$. At the end point $\sqrt{3}$, we have that

$$\left(1+\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}+\rho\right)|_{y=\sqrt{3}}=0+\rho=\rho>0 \tag{7.25}$$

because of (7.22).

Since $\mathcal{A}'(1)=\mathcal{B}'(1)$, at the other end point 1, one evaluates

$$\begin{aligned}\left(1+\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}+\rho\right)|_{y=1}&=1+\rho+\lim_{y\to1}\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}=1+\rho+\lim_{y\to1}\frac{\mathcal{B}''(y)}{\mathcal{A}''(y)}\\&=1+\rho+\frac{\mathcal{B}''(1)}{\mathcal{A}''(1)}\end{aligned} \tag{7.26}$$

by L'Hospital's rule.

In view of (7.25) and (7.26), one deduces from (7.23) that

$$\begin{aligned}&\left(1+\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}+\rho\right)\ \text{ admits one zero point on }\ (1,\sqrt{3})\\&\text{it equivalents to} 1+\rho+\frac{\mathcal{B}''(1)}{\mathcal{A}''(1)}<0,\end{aligned} \tag{7.27}$$

which implies that

$$\rho<\rho_2:=-1-\frac{\mathcal{B}''(1)}{\mathcal{A}''(1)}.$$

It follows that by (7.21) and (7.27), for $\rho\geqq\rho_2$, $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi)$ admits no zero on $(1,\infty)$. Therefore the part 2 of Proposition 7.1 follows from (7.20).

For $\rho\in(0,\rho_2)$, we denote the zero root of $\left(1+\frac{\mathcal{B}'(y)}{\mathcal{A}'(y)}+\rho\right)$ (and hence also of $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi)$) as $y_{2,\rho}$. Then by (7.27) $y_{2,\rho}\in(1,\sqrt{3})$. Thus by (7.20) there is another zero point $\frac{1}{y_{2,\rho}} \in (\frac{\sqrt{3}}{3}, 1)$ of $\frac{\partial}{\partial y}\mathcal{W}_{2,\rho}(yi)$. By (7.24), (7.20), (7.23) and (7.21), the part 1 of Proposition 7.1 is proved.

Finally from (7.23), we have that

$$\frac{\mathrm{d}}{\mathrm{d}\rho} y_{2,\rho} < 0, \forall \rho \in [0, \rho_2].$$

This proves (7.1). (For $\rho = 0$, one has $y_{2,\rho} = \sqrt{3}$ by (7.22)). The proof is thus completed.

□

8. Proofs of Theorems 1.2, 1.3 and 1.4

In this section, we are ready to finish the proof of the main results of Theorems 1.2, 1.3 and 1.4 . To make the presentation clear, we introduce the following notations to denote various geometric sets:

$$\begin{aligned}
\mathbb{H} &:= \{z \mid y > 0\},\\
\Omega_a &:= \{z \mid |z| \geqq 1, 0 \leqq x < 1\},\\
\Omega_b &:= \left\{z \mid |z| \geqq 1, 0 \leqq x \leqq \frac{1}{2}\right\} \cup \left\{z \mid |z| = 1, \frac{1}{2} \leqq x < 1\right\},\\
\Omega_c &:= \left\{z \mid |z| \geqq 1, 0 \leqq x \leqq \frac{1}{2}\right\},\\
\Omega_d &:= \left\{z \mid |z| = 1, 0 \leqq x \leqq \frac{1}{2}\right\} \cup \left\{z \mid \ x = 0, 1 \leqq y < \infty\right\},\\
\Omega_e &:= \left\{z \mid |z| = 1, 0 \leqq x \leqq \frac{1}{2}\right\} \cup \left\{z \mid x = 0, 1 \leqq y \leqq \sqrt{3}\right\},\\
\Omega_{ea} &:= \left\{z \mid x = 0, 1 \leqq y \leqq \sqrt{3}\right\},\\
\Omega_{eb} &:= \left\{z \mid |z| = 1, 0 \leqq x < \frac{1}{2}\right\}.
\end{aligned}$$

We divide the proof into the following steps:

Step 1: Reducing minimization problem from $\mathbb{H}$ to $\rightarrow \Omega_a$.

This is a consequence of Theorem 3.2 and the properties of the fundamental group (3.3) and fundamental domain (3.5):

$$\min_{z\in\mathbb{H}} \mathcal{W}_{1,\rho}(z) \equiv \min_{z\in\Omega_a} \mathcal{W}_{1,\rho}(z), \ \min_{z\in\mathbb{H}} \mathcal{W}_{2,\rho}(z) \equiv \min_{z\in\Omega_a} \mathcal{W}_{2,\rho}(z). \tag{8.1}$$

Step 2: Reducing minimization problem from Ω_a to Ω_b.

This follows from Corollary 4.2:

$$\min_{z\in\Omega_a} \mathcal{W}_{1,\rho}(z) \equiv \min_{z\in\Omega_b} \mathcal{W}_{1,\rho}(z), \ \min_{z\in\Omega_a} \mathcal{W}_{2,\rho}(z) \equiv \min_{z\in\Omega_b} \mathcal{W}_{2,\rho}(z).$$

Step 3: Reducing minimization problem from Ω_b to Ω_c.

We first show that

$$\min_{z\in\{z||z|=1,\frac{1}{2}\leqq x<1\}} \mathcal{W}_{j,\rho}(z) \equiv \mathcal{W}_{1,\rho}\left(\frac{1}{2}+i\frac{\sqrt{3}}{2}\right), \ j=1,2. \tag{8.2}$$

One can further conclude that the minimizer $\frac{1}{2}+i\frac{\sqrt{3}}{2}$ is unique by the monotonicity shown below.

In fact, by Propositions 6.1 and 7.1 , we see that

$$\frac{\partial}{\partial y}\mathcal{W}_{j,\rho}(yi) > 0, \quad y\in[\sqrt{3},\infty), \ j=1,2. \tag{8.3}$$

By the special map $z \mapsto w := \frac{z-1}{z+1}$, the set $\{yi, y\in[\sqrt{3},\infty)\}$ is mapped bijectively to $\{|z|=1, \frac{1}{2}\leqq \mathrm{Re}(z)<1\}$. By Lemmas 3.4 and (8.3) we see that both $\mathcal{W}_{1,\rho}(z)$ and $\mathcal{W}_{2,\rho}(z)$ are monotonically decreasing along the set $\{|z|=1, \frac{1}{2}\leqq x<1\}$. This proves (8.2).

By (8.2), we conclude that

$$\min_{z\in\Omega_b}\mathcal{W}_{1,\rho}(z) \equiv \min_{z\in\Omega_c}\mathcal{W}_{1,\rho}(z), \ \min_{z\in\Omega_b}\mathcal{W}_{2,\rho}(z) \equiv \min_{z\in\Omega_c}\mathcal{W}_{2,\rho}(z).$$

Step 4: Reducing minimization problem from Ω_c to Ω_d.

In this case, let $\rho_* = \frac{1}{20}$ be as in Propositions 5.1. For $\rho\in[0,\rho_*]$, Proposition 5.1 implies that

$$\min_{z\in\Omega_c}\mathcal{W}_{1,\rho}(z) \equiv \min_{z\in\Omega_d}\mathcal{W}_{1,\rho}(z), \ \rho\in[0,\rho_*].$$

For $\rho\in(\rho_*,\infty)$, using Lemmas 3.3, 5.2, and (8.2), we get that

$$\begin{aligned}\min_{z\in\Omega_c}\mathcal{W}_{1,\rho}(z) &\equiv \rho\min_{w\in\Omega_c}\mathcal{W}_{2,1/\rho}(w), \ 1/\rho\in(0,1/\rho_*)\\ &\equiv \rho\min_{w\in\Omega_d}\mathcal{W}_{2,1/\rho}(w), \ 1/\rho\in(0,1/\rho_*)\\ &\equiv \min_{z\in\Omega_d}\mathcal{W}_{1,\rho}(z), \ \rho\in(\rho_*,\infty).\end{aligned}$$

Therefore, we obtain that

$$\min_{z\in\Omega_c}\mathcal{W}_{1,\rho}(z) \equiv \min_{z\in\Omega_d}\mathcal{W}_{1,\rho}(z), \ \rho\in[0,\infty). \tag{8.4}$$

By Theorem 3.3, (8.2) and (8.4), we have that

$$\begin{aligned}\min_{z\in\Omega_c,\rho\in[0,\infty)}\mathcal{W}_{2,\rho}(z), &\equiv \rho\min_{w\in\Omega_c,1/\rho\in[0,\infty)}\mathcal{W}_{1,1/\rho}(w),\\ &\equiv \rho\min_{w\in\Omega_d,1/\rho\in[0,\infty)}\mathcal{W}_{1,1/\rho}(w),\\ &\equiv \min_{z\in\Omega_d,\rho\in[0,\infty)}\mathcal{W}_{2,\rho}(z).\end{aligned} \tag{8.5}$$

Step 5: Reducing minimization problem from Ω_d to Ω_e.

This follows from (8.3).

In summary, from Steps 1–5, we conclude that

$$\min_{z\in\mathbb{H}} \mathcal{W}_{1,\rho}(z) \equiv \min_{z\in\Omega_e} \mathcal{W}_{1,\rho}(z),\ \min_{z\in\mathbb{H}} \mathcal{W}_{2,\rho}(z) \equiv \min_{z\in\Omega_e} \mathcal{W}_{2,\rho}(z). \tag{8.6}$$

From (8.6), we just need to find the minimizer in a much smaller curve Ω_e. But this gives no information about uniqueness or multiplicity of the minimizers. In fact, one can further rule out the possible minimizers of $\mathcal{W}_{j,\rho}(z)$, $j = 1, 2$ in a large set. Namely, for $z \in \Omega_a\backslash\Omega_e$, there is no any possible minimizer for $\min_{z\in\Omega_a} \mathcal{W}_{1,\rho}(z)$, $\min_{z\in\Omega_a} \mathcal{W}_{2,\rho}(z)$. The possible multiplicity of minimizer is admitted only in Step 1, see (8.1). Therefore, one can conclude the reduction in (8.6) is unique up to the group transformation $\mathcal{G}_2$. In the next step we will show that $\min_{z\in\Omega_e} \mathcal{W}_{1,\rho}(z)$, $\min_{z\in\Omega_e} \mathcal{W}_{2,\rho}(z)$ exists , is unique and can be located precisely.

Let w be the map $w(z) = \frac{z-1}{z+1}$ whose inverse is $z(w) = \frac{1+w}{1-w}$. Under this map we have $z = yi \in \Omega_{ea} \mapsto w = \frac{y^2-1}{y^2+1} + i\frac{2y}{y^2+1} \in \Omega_{eb}$, $w = u + iv \in \Omega_{eb} \mapsto z = i\frac{\sqrt{1-u^2}}{1-u} \in \Omega_{ea}$.

We note that

$$\rho_1 < 1/\rho_2 < \rho_2 < 1/\rho_1.$$

See in Propositions 6.1 and 7.1 .

Now we consider the minimizer of $\mathcal{W}_{1,\rho}(z)$ on Ω_e. We divide things into three cases.

Case 1. $\rho \in [\rho_1, 1/\rho_2]$.

In this case, $\rho \geqq \rho_1$, $1/\rho \geqq \rho_2$. Then by Propositions 6.1 and 7.1 , both $\mathcal{W}_{1,\rho}(z)$ and $\mathcal{W}_{2,\rho}(z)$ are monotonically increasing on Ω_{ea} along positive y axis direction. Then it follows that $\mathcal{W}_{1,\rho}(z)$ is monotonically increasing on Ω_{eb} clockwise. Therefore, the minimizer of $\mathcal{W}_{1,\rho}(z)$ on Ω_e is uniquely achieved at $z = i$, that is, in this case the minimizer of $\mathcal{W}_{1,\rho}(z)$ is always i, a fixed point representing the square lattice.

Case 2. $\rho \in (0, \rho_1)$.

In this case, $1/\rho > 1/\rho_1 > \rho_2$. Then by Proposition 7.1, $\mathcal{W}_{2,1/\rho}(z)$ is monotonically increasing on Ω_{ea} along positive y axis direction. It follows from Lemma 3.4 or Theorem 3.3 that $\mathcal{W}_{1,\rho}(z)$ is monotone increasing on Ω_{eb} clockwise. On the other hand, by Proposition 6.1, $\mathcal{W}_{1,\rho}(z)$ admits a unique minimizer at $y = iy_{1,\rho} \in i(1, \sqrt{3})$ on Ω_{ea}. We conclude that $\mathcal{W}_{1,\rho}(z)$ has a unique minimizer at $z_{1,\rho} = iy_{1,\rho}$, where $y_{1,\rho} \in (1, \sqrt{3})$ on Ω_e.

Case 3. $\rho \in (1/\rho_2, \infty)$.

In this case, since $1/\rho < \rho_2$, by Proposition 7.1, $\mathcal{W}_{2,1/\rho}(z)$ has a unique minimizer at $y = y_{2,1/\rho} \in (1, \sqrt{3})$ on Ω_{ea}. Then by Theorem 3.3 or Lemmas 3.4, $\mathcal{W}_{1,\rho}(\cdot)$ has a unique minimizer

$$z_{1,\rho} = \frac{y_{2,1/\rho}^2 - 1}{y_{2,1/\rho}^2 + 1} + i\frac{2y_{2,1/\rho}}{y_{2,1/\rho}^2 + 1} \in \text{inner points of } \Omega_{eb}. \tag{8.7}$$

On the other side, one has $\rho > 1/\rho_2 > \rho_1$. Then by Proposition 6.1, $\mathcal{W}_{1,\rho}(z)$ is monotone increasing on Ω_{ea} along the positive y axis direction. Therefore, (8.7) gives the minimizer of $\mathcal{W}_{1,\rho}(z)$ on Ω_e.

This proves Theorems 1.2 and 1.4 . Theorem 1.3 follows from Theorem 1.2 and Lemma 3.3.

9. Proof of Mueller–Ho Functional and Mueller–Ho Conjecture

Proof of Lemma 2.1. Since the computation is elementary, we omit the details here.

Proof of Lemma 2.3.

$$\begin{aligned}
\mathcal{J}\left(z; \frac{1}{2}, \frac{1}{2}\right) &= \sum_{m,n} e^{-\frac{\pi}{y}|mz-n|^2} \cos((m+n)\pi) \\
&= \sum_{m,n} e^{-\frac{\pi}{y}|mz-n|^2} \big(1+\cos((m+n)\pi)\big) - \sum_{m,n} e^{-\frac{\pi}{y}|mz-n|^2} \\
&= \sum_{m,n} e^{-\frac{\pi}{y}|mz-n|^2} 2\cos^2\left(\frac{(m+n)\pi}{2}\right) - \theta(1;z) \\
&= \sum_{m+n=2k, k\in\mathbb{Z}} 2e^{-\frac{\pi}{y}|mz+n|^2} - \theta(1;z) \\
&= 2\sum_{m,k} e^{-\frac{\pi}{y}|m(z+1)-2k|^2} - \theta(1;z) \\
&= 2\sum_{m,k} e^{-\frac{2\pi}{\operatorname{Im}(\frac{z+1}{2})}|m\frac{z+1}{2}-k|^2} - \theta(1;z) \\
&= 2\theta\left(2; \frac{z+1}{2}\right) - \theta(1;z).
\end{aligned}$$

□

Proof of Theorem 2.1. This follows by Theorems 1.2, 1.3 and 1.4 , by the relation $\rho = \frac{1-\alpha}{2\alpha}$. □

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11. Appendix A: Proof of Lemma 2.2

Recall that

$$\mathcal{J}(z; a, b) = \sum_{(m,n)\in\mathbb{Z}^2} e^{-\frac{\pi}{y}|mz-n|^2} \cos(2\pi(ma+nb)). \tag{10.1}$$

In this appendix we show that when the lattice is square type, then $(\frac{1}{3}, \frac{1}{3})$ is not a critical point while when the lattice is hexagonal (or triangular), it is a critical point. First we show that

Lemma 11.1.

$$\frac{\partial}{\partial a}\mathcal{J}(z; a, b)|_{z=i,(a,b)=(\frac{1}{3},\frac{1}{3})} = \frac{\partial}{\partial b}\mathcal{J}(z; a, b)|_{z=i,(a,b)=(\frac{1}{3},\frac{1}{3})} < 0. \tag{10.2}$$

This implies that $\mathcal{J}(z; a, b)$ is not always critical point for any lattice shape.

Proof.

$$\begin{aligned}\frac{\partial}{\partial a}\mathcal{J}(z; a, b)|_{z=i,(a,b)=(\frac{1}{3},\frac{1}{3})} &= -2\pi\sum_{m,n} me^{-\pi(m^2+n^2)} \sin\left(\frac{2\pi(m+n)}{3}\right)\\ \frac{\partial}{\partial a}\mathcal{J}(z; a, b)|_{z=i,(a,b)=(\frac{1}{3},\frac{1}{3})} &= -2\pi\sum_{m,n} ne^{-\pi(m^2+n^2)} \sin\left(\frac{2\pi(m+n)}{3}\right).\end{aligned} \tag{10.3}$$

It is clear that

$$\frac{\partial}{\partial a}\mathcal{J}(a, b; z)|_{z=i,(a,b)=(\frac{1}{3},\frac{1}{3})} = \frac{\partial}{\partial b}\mathcal{J}(a, b; z)|_{z=i,(a,b)=(\frac{1}{3},\frac{1}{3})}.$$

Let

$$A := \sum_{m,n} e^{-\pi(m^2+n^2)} \sin\left(\frac{2\pi(m+n)}{3}\right) m.$$

Equivalently, we show that

$$A > 0.$$

Grouping by $m+n = 3k+j$, $j = 0, 1, 2$, we have

$$\frac{A}{\sin(\frac{\pi}{3})} = \sum_{m+n\equiv 1(\mod 3)} me^{-\pi(m^2+n^2)} - \sum_{m+n\equiv 2(\mod 3)} me^{-\pi(m^2+n^2)}. \tag{10.4}$$

For the first part in (10.4), splitting the summation by $m > 0$ or $m < 0$, we have (dropping the $\mod 3$)

$$\sum_{m+n\equiv 1} e^{-\pi(m^2+n^2)} m = \sum_{m>0,m+n\equiv 1} me^{-\pi(m^2+n^2)} - \sum_{m>0,m+n\equiv 2} me^{-\pi(m^2+n^2)} \tag{10.5}$$

For the second part in (10.4), similarly, one has

$$\sum_{m+n\equiv 2} e^{-\pi(m^2+n^2)} m = \sum_{m>0,m+n\equiv 2} m e^{-\pi(m^2+n^2)} - \sum_{m>0,m+n\equiv 1} m e^{-\pi(m^2+n^2)} \tag{10.6}$$

By (10.5) and (10.6), we have

$$\sum_{m+n\equiv 2} m e^{-\pi(m^2+n^2)} = -\sum_{m+n\equiv 1} m e^{-\pi(m^2+n^2)} \tag{10.7}$$

and by (10.4)

$$\frac{A}{2\sin(\frac{\pi}{3})} = \sum_{m>0,m+n\equiv 1} m e^{-\pi(m^2+n^2)} - \sum_{m>0,m+n\equiv 2} m e^{-\pi(m^2+n^2)}. \tag{10.8}$$

Notice that $e^{-\pi}$ is one term in the first summation in (10.8), it suffices to prove that

$$\sum_{m>0,m+n\equiv 2} m e^{-\pi(m^2+n^2)} < e^{-\pi}.$$

Now we have

$$\sum_{m>0,m+n\equiv 2} e^{-\pi(m^2+n^2)} m = \sum_{m=1}^{\infty} \sum_{k\in\mathbb{N}} m e^{-\pi(m^2+(3k+2)^2)}$$
$$= \sum_{m=1}^{\infty} m e^{-\pi m^2} \sum_{k\in\mathbb{N}} e^{-\pi(3k+2)^2} < (e^{-\pi}+4e^{-4\pi})(e^{-\pi}+2e^{-4\pi}) < e^{-\pi}.$$

This completes the proof. □

Next we show that $(a,b)=(\frac{1}{3},\frac{1}{3})$ is a critical point when $z=\frac{1}{2}+i\frac{\sqrt{3}}{2}$.

Proof. We first claim that

$$\sum_{(m,n)\in\mathbb{Z}^2} e^{-x(m^2+n^2-mn)} m \sin\left(\frac{2\pi(m+n)}{3}\right) = 0, \quad \text{for } \forall x>0. \tag{10.9}$$

To prove (10.9), it suffices to prove that

$$\sum_{n} e^{-x(m^2+n^2-mn)} \sin\left(\frac{2\pi(m+n)}{3}\right) = 0, \quad \text{for } \forall x>0. \tag{10.10}$$

In fact,

$$\begin{aligned}
&\sum_{n} e^{-x(m^2+n^2-mn)} \sin\left(\frac{2\pi(m+n)}{3}\right)\\
&= -e^{-\frac{3}{4}xm^2} \sum_{n} e^{-\frac{x}{4}(2n-m)^2} \sin\frac{\pi(2n-m)}{3}\\
&= 0.
\end{aligned} \tag{10.11}$$

In the last equality, one uses $2n-m, n \in \mathbb{Z}$ and takes all the even or odd integers when m is even or odd.
By simple calculation, now the second part of Lemma 2.2 is equivalent to

$$\sum_{m,n} e^{-\frac{\pi}{2y}\left((m-n)^2y^2+(m+n)^2\right)} m \sin\frac{2\pi(m+n)}{3} = 0, \quad \text{if} \quad y=\sqrt{3} \tag{10.12}$$

which is of consequence of (10.9). This completes the proof.

□

12. Appendix 2: The Rest of Proof in Theorems 6.1 and 7.1

In this appendix, we finish the technical proofs of Theorems 6.1 and 7.1 .
Throughout this appendix we frequently use the following Lemma whose proof is straightforward calculus and is omitted:

Lemma 12.1. *Let* $f(y)^{(j)}$ *denote* $\frac{d^j}{dy^j}f(y)$. *For* , $j=1,2,3,4$, *there holds*

- *For* $a>0, b>0$,

$$\left(y^be^{-ay}\right)'<0, \quad \textit{if} \quad y>\frac{b}{a}; \quad \left(y^be^{-ay}\right)''>0, \quad \textit{if} \quad y>\frac{b+\sqrt{b}}{a}.$$

- *For* $a>0$,

$$(-1)^j\left(\sqrt{y}e^{-ay}\right)^{(j)}>0, \quad \textit{if} \quad y>f_j(a).$$

Here

$$f_1(a)=\frac{1}{2a},\ f_2(a)=\frac{1+\sqrt{2}}{2a},\ f_3(a)=\frac{1}{a},\ f_4(a)=\frac{1}{2a}.$$

- *For* $y \geqq 1$ *and* $a_n>0$

$$\left|\left(\sum_{n=k}^{\infty}\sqrt{y}e^{-a_ny}\right)^{(j)}\right| \leqq (1+\sigma_{j,k})\sqrt{y}(a_k)^je^{-a_ky},$$

$$\sigma_{j,k}=\sum_{n=k+1}^{\infty}\left(\frac{a_n}{a_k}\right)^je^{-(a_n-a_k)}.$$

In applying Lemma 12.1, we will choose k by the desired estimates.
The structure of this appendix is organized as follows. (6.11)⇔ Lemma 12.2; (6.12)⇔ Lemma 12.3; (6.13)⇔ Lemma 12.4; (6.26)⇔ Lemma 12.5; (6.27)⇔ Lemma 12.6; (6.25)⇔ Lemma 12.7; (7.7)⇔ Lemma 12.8; (7.8)⇔ Lemma 12.9; (7.9)⇔ Lemma 12.10; (7.17)⇔ Lemma 12.11; (7.18)⇔ Lemma 12.12; (7.19)⇔ Lemma 12.13.

12.1. The Rest of Proof in Theorem 6.1

Lemma 12.2. *$y \mapsto \frac{16y}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}_a''\mathcal{X}_a' - \mathcal{X}_a''\mathcal{Y}_a'\Big)(y)$, $y \in [1,\infty)$ is monotonically increasing.*

Proof. Calculating and grouping the terms, we get

$$
\begin{aligned}
&\frac{16y}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}_a''\mathcal{X}_a' - \mathcal{X}_a''\mathcal{Y}_a'\Big)(y)\\
&= \Big(\pi y - 2496e^{-7\pi y}\pi^2y^2 - 144e^{-7\pi y} - 700e^{-6\pi y}\pi y - 1440e^{-5\pi y}\pi^2y^2\\
&\quad - 288e^{-5\pi y} - 2176e^{-4\pi y}\pi y\\
&\quad - 840e^{-3\pi y}\pi^2y^2 - 108e^{-3\pi y} - 243e^{-2\pi y}\pi y - 110e^{-\pi y}\pi y - 6\Big) \qquad (11.12)\\
&\quad + \Big(696e^{-7\pi y}\pi y + 2016e^{-6\pi y}\pi^2y^2 + 168e^{-6\pi y} + 1008e^{-5\pi y}\pi y\\
&\quad + 2208e^{-4\pi y}\pi^2y^2 + 768e^{-4\pi y}\\
&\quad + 234e^{-3\pi y}\pi y + 192e^{-2\pi y}\pi^2y^2 + 162e^{-2\pi y} + 24e^{-\pi y}\pi^2y^2 + 132e^{-\pi y}\Big).
\end{aligned}
$$

Denote the terms in first and second brackets of $\frac{16y}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}_a''\mathcal{X}_a' - \mathcal{X}_a''\mathcal{Y}_a'\Big)(y)$ by $\mathcal{P}^+_{\mathcal{X}\mathcal{Y}}$ and $\mathcal{P}^-_{\mathcal{X}\mathcal{Y}}$ respectively. One has $\frac{16y}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}_a''\mathcal{X}_a' - \mathcal{X}_a''\mathcal{Y}_a'\Big)(y) = \mathcal{P}^+_{\mathcal{X}\mathcal{Y}}(y) + \mathcal{P}^-_{\mathcal{X}\mathcal{Y}}(y)$ by (11.12). It remains to prove that $\Big(\mathcal{P}^+_{\mathcal{X}\mathcal{Y}} + \mathcal{P}^-_{\mathcal{X}\mathcal{Y}}\Big)' > 0, \quad y \in [1,\infty)$.
It is clear that the leading order term is πy, this gives that $\Big(\mathcal{P}^+_{\mathcal{X}\mathcal{Y}} + \mathcal{P}^-_{\mathcal{X}\mathcal{Y}}\Big)' > 0$ when y is large.
By Lemma 12.1, one has

$$\Big(\mathcal{P}^+_{\mathcal{X}\mathcal{Y}}\Big)' > \pi, \quad \Big(\mathcal{P}^-_{\mathcal{X}\mathcal{Y}}\Big)' < 0, \quad \Big(\mathcal{P}^+_{\mathcal{X}\mathcal{Y}}\Big)'' < 0, \quad \Big(\mathcal{P}^-_{\mathcal{X}\mathcal{Y}}\Big)'' > 0 \ \text{ if } \ y \geqq 1. \qquad (11.13)$$

Direct calculation shows that $\Big(\mathcal{P}^-_{\mathcal{X}\mathcal{Y}}\Big)' |_{y=2.2} = -3.012967072\cdots$. Then by (11.13)

$$\Big(\mathcal{P}^+_{\mathcal{X}\mathcal{Y}} + \mathcal{P}^-_{\mathcal{X}\mathcal{Y}}\Big)'(y) > \pi - 3.012967072\cdots > 0, \quad \text{if} \ \ y \geqq 2.2. \qquad (11.14)$$

Next we prove that

$$\Big(\mathcal{P}^+_{\mathcal{X}\mathcal{Y}} + \mathcal{P}^-_{\mathcal{X}\mathcal{Y}}\Big)'(y) > 0, \quad \text{for} \ \ y \in [1, 2.2]. \qquad (11.15)$$

To prove (11.15), we regroup the terms by

$$
\begin{aligned}
&\mathcal{P}^{+}_{\mathcal{X}\mathcal{Y}}(y)+\mathcal{P}^{-}_{\mathcal{X}\mathcal{Y}}(y)\\
&=(\pi y-6)+e^{-\pi y}(-110\pi y+24\pi^2y^2+132)\\
&\quad+e^{-2\pi y}(-243\pi y+192\pi^2y^2+162)\\
&\quad+e^{-3\pi y}(-840\pi^2y^2-108+234\pi y)\\
&\quad+e^{-4\pi y}(-2176\pi y+2208\pi^2y^2+768)\\
&\quad+e^{-5\pi y}(-1440\pi^2y^2-288+1008\pi y)\\
&\quad+e^{-6\pi y}(-700\pi y+2016\pi^2y^2+168)\\
&\quad+e^{-7\pi y}(-2496\pi^2y^2-144+696\pi y).
\end{aligned}
\tag{11.16}
$$

To prove (11.16), one divides the interval $[1, 2.2]$ into, say, ten subintervals, $[1, 2.2) = \cup_{i=0}^{9}[a_i, a_{i+1})$. In each intervals, by careful calculations, we can show that the function is positive on each interval.

□

Lemma 12.3. *The following estimates hold:* $|\Big(\mathcal{Y}_e''\mathcal{X}'-\mathcal{Y}_e'\mathcal{X}''+\mathcal{Y}_a''\mathcal{X}_e'-\mathcal{X}_e''\mathcal{Y}_a'\Big)(y)| \leqq (44\pi^2+18\pi+36\pi y)e^{-\frac{17}{4}\pi y}$.

Remark 12.1. The coefficient of the bound is not sharp, but the exponential term captures the main feature.

Proof. By Lemma 12.1, one infers that

$$
\begin{aligned}
&|\mathcal{Y}_e'(y)| \leqq 18\pi\sqrt{y}e^{-\frac{17}{4}\pi y},\ |\mathcal{Y}_e''(y)| \leqq \frac{290\pi^2}{4}\sqrt{y}e^{-\frac{17}{4}\pi y},\\
&|\mathcal{X}_e'(y)| \leqq 41\pi\sqrt{y}e^{-5\pi y},\ |\mathcal{X}_e''(y)| \leqq 201\pi^2\sqrt{y}e^{-5\pi y}
\end{aligned}
$$

For $\mathcal{X}', \mathcal{X}'', \mathcal{Y}_a', \mathcal{Y}_a''$, by their expressions, one has

$$
\begin{aligned}
&|\mathcal{X}'(y)| \leqq \frac{3}{5\sqrt{y}},\ |\mathcal{X}''(y)| \leqq \left(\frac{1}{4y^{3/2}}+2\sqrt{y}\right),\\
&|\mathcal{Y}_a'(y)| \leqq \left(\frac{1}{\sqrt{y}}+2\sqrt{y}\right),\ |\mathcal{Y}_a'(y)| \leqq \left(\frac{1}{4y^{3/2}}+2\sqrt{y}\right).
\end{aligned}
$$

Thus, one can get the result.

□

Lemma 12.4. *It holds that* $\Big(\mathcal{Y}''\mathcal{X}'-\mathcal{Y}''\mathcal{X}'\Big)(y) > 0, \quad y \in [1.1, \infty)$.

Proof. It remains to prove that $\frac{16y}{\pi}e^{\frac{1}{4}\pi y}\left(\mathcal{Y}''\mathcal{X}'-\mathcal{Y}''\mathcal{X}'\right)(y) > 0, \quad y \in [1.1, \infty)$. By Lemmas 12.2 and 12.3 ,

$$
\begin{aligned}
&\frac{16y}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}''\mathcal{X}'-\mathcal{Y}''\mathcal{X}'\Big)(y)\\
&\quad=\frac{16y}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}_a''\mathcal{X}_a'-\mathcal{X}_a''\mathcal{Y}_a'\Big)(y)\\
&\qquad+\frac{16y}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}_e''\mathcal{X}'-\mathcal{Y}_e'\mathcal{X}''+\mathcal{Y}_a''\mathcal{X}_e'-\mathcal{X}_e''\mathcal{Y}_a'\Big)(y)\\
&\quad\geqq\frac{16y}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}_a''\mathcal{X}_a'-\mathcal{X}_a''\mathcal{Y}_a'\Big)(y)-\frac{16y}{\pi}(44\pi^2+18\pi+36\pi y)e^{-4\pi y}\\
&\quad\geqq\Big(\frac{16y}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}_a''\mathcal{X}_a'-\mathcal{X}_a''\mathcal{Y}_a'\Big)(y)-16y(44\pi+18+36y)e^{-4\pi y}\Big)\;|_{y=1.1}\\
&\quad=0.001671778\cdots,\ y\in[1.1,\infty)\\
&\quad>0,\qquad y\in[1.1,\infty).
\end{aligned}
$$

In the second last step, one uses the fact that $y\mapsto -16y(44\pi+18+36y)e^{-4\pi y}$, $y>1$ is strictly increasing.

□

Lemma 12.5. $y\to\frac{512y^4}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}_a''''\mathcal{X}_a''-\mathcal{Y}_a''\mathcal{X}_a''''\Big)(y)$ *is monotonically decreasing on* $(1,1.2)$.

Proof. By direct calculations, one regroups the terms by

$$
\begin{aligned}
&\frac{512y^4}{\pi}e^{\frac{1}{4}\pi y}\Big(\mathcal{Y}_a''''\mathcal{X}_a''-\mathcal{Y}_a''''\mathcal{X}_a''''\Big)(y)\\
&\quad=-\pi^3y^3+8\pi^2y^2+84\pi y-144\\
&\qquad+e^{-\pi y}\Big(-240\pi^5y^5-9240\pi y-6320\pi^2y^2+1392\pi^4y^4+350\pi^3y^3+3168\Big)\\
&\qquad+e^{-2\pi y}\Big(-11232\pi^5y^5-14877\pi^3y^3-20412\pi y-32856\pi^2y^2+36096\pi^4y^4+3888\Big)\\
&\qquad+e^{-3\pi y}\Big(-348240\pi^4y^4-2592+178854\pi^3y^3+209040\pi^5y^5+19656\pi y+91536\pi^2y^2\Big)\\
&\qquad+e^{-4\pi y}\Big(-804576\pi^5y^5-121856\pi^3y^3-472576\pi^2y^2\\
&\qquad-182784\pi y+1465533\pi^4y^4+18432\Big)\qquad\qquad(11.17)\\
&\qquad+e^{-5\pi y}\Big(-140064\pi 64y^4-6912+160272\pi^3y^3+685440\pi^5y^5\\
&\qquad+84672\pi y+284544\pi^2y^2\Big)\\
&\qquad+e^{-6\pi y}\Big(-570500\pi^3y^3-3628800\pi^5y^5-58800\pi y\\
&\qquad-301280\pi^2y^2+3100608\pi^4y^4+4032\Big)\\
&\qquad+e^{-7\pi y}\Big(-5236608\pi^4y^4-3456+862344\pi^3y^3+7527936\pi^5y^5\\
&\qquad+361152\pi^2y^2+58464\pi y\Big).
\end{aligned}
$$

The rest is found through careful calculations by taking derivatives.

□

Lemma 12.6. *There has* $|\left(\mathcal{Y}_e''''\mathcal{X}''-\mathcal{Y}_e''\mathcal{X}''''+\mathcal{Y}_a''''\mathcal{X}_e''-\mathcal{X}_e''''\mathcal{Y}_a''\right)(y)| \leqq 16(\frac{17}{4}\pi)^4 \sqrt{y}e^{-\frac{17}{4}\pi y}, \quad y \geqq 1.$

Remark 12.2. The coefficient of the bound is rather rough but is enough to get our result. The exponential power captures the main feature.

Proof. By Lemma 12.1, one infers that

$$\begin{aligned} |\mathcal{Y}_e''(y)| &\leqq 4\left(\frac{17}{4}\pi\right)^2 (1+\sigma_{\mathcal{Y}_e,2})\sqrt{y}e^{-\frac{17}{4}\pi y}, |\mathcal{Y}_e''''(y)| \\ &\leqq 4\left(\frac{17}{4}\pi\right)^4 (1+\sigma_{\mathcal{Y}_e,4})\sqrt{y}e^{-\frac{17}{4}\pi y} \end{aligned} \tag{11.18}$$

and

$$\begin{aligned} |\mathcal{X}_e''(y)| &\leqq 8(5\pi)^2(1+\sigma_{\mathcal{X}_e,2})\sqrt{y}e^{-5\pi y}, |\mathcal{X}_e''''(y)| \\ &\leqq 8(5\pi)^4(1+\sigma_{\mathcal{X}_e,4})\sqrt{y}e^{-5\pi y}. \end{aligned} \tag{11.19}$$

Here $\sigma_{\mathcal{X}_e,j}, \sigma_{\mathcal{Y}_e,j}, j=2,4$ are small and can be bounded by $\frac{1}{4}$. For $\mathcal{X}''$, $\mathcal{X}''''$, $\mathcal{Y}_a''$ and $\mathcal{Y}_a''''$, by their explicit expressions, one has

$$|\mathcal{X}''''(y)| \leqq 10, \quad |\mathcal{X}''(y)| \leqq 1.2, |\mathcal{Y}_a''''(y)| \leqq \frac{1}{10}, \quad |\mathcal{Y}_a''''(y)| \leqq 1, \quad y \geqq 1. \tag{11.20}$$

Combining (11.18), (11.19) with (11.20), one gets the estimate.

□

Lemma 12.7. *There holds* $\left(\mathcal{Y}''''\mathcal{X}''-\mathcal{Y}''\mathcal{X}''''\right)(y) > 0, \quad y \in [1, 1.11].$

Proof. It suffices to prove that $\frac{512y^4}{\pi}e^{\frac{1}{4}\pi y}\left(\mathcal{Y}''''\mathcal{X}''-\mathcal{Y}''\mathcal{X}''''\right)(y) > 0, \quad y \in [1, 1.11]$. By the decomposition and Lemmas 12.5 and 12.6 , we obtain that

$$\begin{aligned} &\frac{512y^4}{\pi}e^{\frac{1}{4}\pi y}\left(\mathcal{Y}''''\mathcal{X}''-\mathcal{Y}''\mathcal{X}''''\right)(y) \\ &= \frac{512y^4}{\pi}e^{\frac{1}{4}\pi y}\left(\mathcal{Y}_a''''\mathcal{X}_a''-\mathcal{Y}_a''\mathcal{X}_a''''\right)(y) \\ &\quad + \frac{512y^4}{\pi}e^{\frac{1}{4}\pi y}\left(\mathcal{Y}_e''''\mathcal{X}''-\mathcal{Y}_e''\mathcal{X}''''+\mathcal{Y}_a''''\mathcal{X}_e''-\mathcal{X}_e''''\mathcal{Y}_a''\right)(y) \\ &\geqq \frac{512y^4}{\pi}e^{\frac{1}{4}\pi y}\left(\mathcal{Y}_a''''\mathcal{X}_a''-\mathcal{Y}_a''\mathcal{X}_a''''\right)(y) - \frac{72}{5}\cdot 17^4\pi^3y^{9/2}e^{-4\pi y} \qquad (11.21) \\ &\geqq \frac{512y^4}{\pi}e^{\frac{1}{4}\pi y}\left(\mathcal{Y}_a''''\mathcal{X}_a''-\mathcal{Y}_a''\mathcal{X}_a''''\right)(y)\ |_{y=1.11} \\ &- \frac{72}{5}\cdot 17^4\pi^3y^{9/2}e^{-4\pi y}\ |_{y=1}, y \in [1, 1.11] \\ &= 158.4646175\cdots - 130.0476135\cdots \\ &> 0. \end{aligned}$$

□

12.2. The Rest of Proof in Theorem 7.1

Lemma 12.8. *The function* $y \to \frac{4y}{\pi}e^{\frac{1}{2}\pi y}\Big(\mathcal{B}_a''\mathcal{A}_a' - \mathcal{A}_a''\mathcal{B}_a'\Big)(y)$, $y > 1$ *is monotone increasing.*

Proof. By direct calculations, one regroups the terms by

$$\begin{aligned}
&\frac{4y}{\pi}e^{\frac{1}{2}\pi y}\Big(\mathcal{B}_a''\mathcal{A}_a' - \mathcal{A}_a''\mathcal{B}_a'\Big)(y)\\
&= \Big(\pi y - 3 - 288e^{-8\pi y}\pi^2y^2 - 12e^{-8\pi y} - 144e^{-\frac{9}{2}\pi y} - 72e^{-3\pi y}\\
&\quad - 48e^{-\frac{5}{2}\pi y} - 84e^{-5\pi y} - 12\pi e^{-\pi y}y\\
&\quad - 8\pi e^{-\frac{1}{2}\pi y}y - 768\pi^2e^{-\frac{9}{2}\pi y}y^2 - 128\pi^2e^{-\frac{5}{2}\pi y}y^2 - 240y^2e^{-3\pi y}\pi^2\\
&\quad - 504e^{-5\pi y}\pi^2y^2 - 52e^{-6\pi y}\pi y\\
&\quad - 99e^{-4\pi y}\pi y - 10e^{-2\pi y}\pi y\Big)\\
&\quad + \Big(68e^{-8\pi y}\pi y + 240e^{-6\pi y}\pi^2y^2 + 12e^{-\frac{1}{2}\pi y} + 12e^{-6\pi y} + 33e^{-4\pi y}\\
&\quad + 6e^{-2\pi y} + 12e^{-\pi y} + 96\pi e^{-\frac{5}{2}\pi y}y\\
&\quad + 480\pi e^{-\frac{9}{2}\pi y}y + 8\pi^2e^{-\pi y}y^2 + 168ye^{-3\pi y}\pi + 64e^{-4\pi y}\pi^2y^2\\
&\quad + 48e^{-2\pi y}\pi^2y^2 + 308e^{-5\pi y}\pi y\Big)
\end{aligned} \tag{11.22}$$

Denote the terms in the first and second bracket of (11.22) by $\mathcal{P}^+_{\mathcal{AB}}$ and $\mathcal{P}^-_{\mathcal{AB}}$. Then

$$\frac{4y}{\pi}e^{\frac{1}{2}\pi y}\Big(\mathcal{B}_a''\mathcal{A}_a' - \mathcal{A}_a''\mathcal{B}_a'\Big)(y) = \mathcal{P}^+_{\mathcal{AB}}(y) + \mathcal{P}^-_{\mathcal{AB}}(y). \tag{11.23}$$

It remains to prove that $\mathcal{P}^+_{\mathcal{AB}}(y) + \mathcal{P}^-_{\mathcal{AB}}(y) > 0, \quad y > 1.$
By Lemma 12.1,

$$\begin{aligned}
&\Big(\mathcal{P}^+_{\mathcal{AB}}(y)\Big)'(y) > \pi, \quad \Big(\mathcal{P}^+_{\mathcal{AB}}(y)\Big)''(y) < 0, \; \Big(\mathcal{P}^-_{\mathcal{AB}}(y)\Big)'(y) < 0,\\
&\Big(\mathcal{P}^-_{\mathcal{AB}}(y)\Big)''(y) > 0
\end{aligned} \tag{11.24}$$

Since $\Big(\mathcal{P}^-_{\mathcal{AB}}(y)\Big)'(y)\mid_{y=1.82} = -3.051954266\cdots$, one has

$$\mathcal{P}^+_{\mathcal{AB}}(y) + \mathcal{P}^-_{\mathcal{AB}}(y) \geqq \pi - 3.051954266\cdots, \; y \in [1.82, \infty) > 0. \tag{11.25}$$

It remains to prove that $\mathcal{P}^+_{\mathcal{AB}}(y) + \mathcal{P}^-_{\mathcal{AB}}(y) > 0$ on the bounded interval $(1, 1.82]$. To this end, we divide the interval $(1, 1.82]$ into 10 smaller subintervals, and compute the derivatives on each interval to arrive the result. □

Lemma 12.9. *There holds:* $|\Big(\mathcal{B}_e''\mathcal{A}' - \mathcal{B}_e'\mathcal{A}'' + \mathcal{B}_a''\mathcal{A}_e' - \mathcal{A}_e''\mathcal{B}_a'\Big)(y)| \leqq 8(\frac{13}{8}\pi)^2 \sqrt{y}e^{-\frac{13}{2}\pi y}, \quad y \geqq 1.$

By Lemma 12.1, one has for $j = 1, 2, \ldots$

$$
\begin{aligned}
|\mathcal{A}_e^{(j)}(y)| &\leqq 4(1+\sigma_{\mathcal{A}_e,j})\left(\frac{13}{2}\pi\right)^j \sqrt{y}e^{-\frac{13}{2}\pi y},\\
|\mathcal{B}_e^{(j)}(y)| &\leqq 4(1+\sigma_{\mathcal{B}_e,j})\left(\frac{13}{2}\pi\right)^j \sqrt{y}e^{-\frac{13}{2}\pi y}.
\end{aligned}
\tag{11.26}
$$

Here the $\sigma_{\mathcal{A}_e,j}, \sigma_{\mathcal{B}_e,j}$ are small and can be bounded by $\frac{1}{2}$. For $\mathcal{A}', \mathcal{A}', \mathcal{B}_a', \mathcal{B}_a''$, by their explicit expressions, one deduces that

$$
|\mathcal{A}'(y)| \leqq 0.3, \quad |\mathcal{A}''(y)| \leqq \frac{1}{2}, \quad |\mathcal{B}_a'(y)| \leqq \frac{1}{5}, \quad |\mathcal{B}_a''(y)| \leqq \frac{1}{5}. \tag{11.27}
$$

Combining (11.26) and (11.27), one gets the estimate.

Lemma 12.10. *There holds* $\left(\mathcal{B}''\mathcal{A}' - \mathcal{A}''\mathcal{B}'\right)(y) > 0$ *if* $y \in [1.05, \infty)$.

Proof. Equivalently, it suffice to prove that $\frac{4y}{\pi}e^{\frac{1}{2}\pi y}\left(\mathcal{B}''\mathcal{A}' - \mathcal{A}''\mathcal{B}'\right)(y) > 0$ if $y \in [1.05, \infty)$. By Lemmas 12.8 and 12.9 , we deduce that

$$
\begin{aligned}
&\frac{4y}{\pi}e^{\frac{1}{2}\pi y}\left(\mathcal{B}''\mathcal{A}' - \mathcal{A}''\mathcal{B}'\right)(y)\\
&= \frac{4y}{\pi}e^{\frac{1}{2}\pi y}\left(\mathcal{B}_a''\mathcal{A}_a' - \mathcal{A}_a''\mathcal{B}_a'\right)(y)\\
&+ \frac{4y}{\pi}e^{\frac{1}{2}\pi y}\left(\mathcal{B}_e''\mathcal{A}' - \mathcal{B}_e'\mathcal{A}'' + \mathcal{B}_a''\mathcal{A}_e' - \mathcal{A}_e''\mathcal{B}_a'\right)(y)\\
&\geqq \frac{4y}{\pi}e^{\frac{1}{2}\pi y}\left(\mathcal{B}_a''\mathcal{A}_a' - \mathcal{A}_a''\mathcal{B}_a'\right)(y) - 1352\pi y^{3/2}e^{-6\pi y}\\
&\geqq \left(\frac{4y}{\pi}e^{\frac{1}{2}\pi y}\left(\mathcal{B}_a''\mathcal{A}_a' - \mathcal{A}_a''\mathcal{B}_a'\right)(y) - 1352\pi y^{3/2}e^{-6\pi y}\right)|_{y=1.05}\\
&= 0.001189906301\cdots\\
&> 0.
\end{aligned}
\tag{11.28}
$$

Here we use the fact that $y \mapsto -y^{3/2}e^{-6\pi y}$, $y > 1$ is strictly increasing in the second last inequality.

□

Lemma 12.11. $y \to \frac{32y^4}{\pi}e^{\frac{1}{2}\pi y}\left(\mathcal{B}_a''''\mathcal{A}_a'' - \mathcal{B}_a''\mathcal{A}_a''''\right)(y)$ *is strictly decreasing on* $(1, 1.12)$.

Proof. By Direct calculations, one regroups the terms by

$$\begin{aligned}
&\frac{32y^4}{\pi}e^{\frac{1}{2}\pi y}\Big(\mathcal{B}_a''''\mathcal{A}_a''-\mathcal{B}_a''''\mathcal{A}_a''''\Big)(y)\\
&\quad=-\pi^3y^3+4\pi^2y^2+21\pi y-18\\
&\quad\quad+e^{-\frac{1}{2}\pi y}(32\pi^3y^3+72-64\pi^2y^2-168\pi y)\\
&\quad\quad+e^{-\pi y}(176\pi^4y^4+72-48\pi^5y^5-252\pi y-304\pi^2y^2-132\pi^3y^3)\\
&\quad\quad+e^{-2\pi y}(2784\pi^4y^4+36-960\pi^5y^5-2150\pi^3y^3-1160\pi^2y^2-210\pi y)\\
&\quad\quad+e^{-\frac{5}{2}\pi y}(6144\pi^5y^5+4224\pi^3y^3+2016\pi y+4864\pi^2y^2-11264\pi^4y^4-288)\\
&\quad\quad+e^{-3\pi y}(8568\pi^3y^3+16800\pi^5y^5+9504\pi^2y^2+3528\pi y-28320\pi^4y^4-432)\\
&\quad\quad+e^{-4\pi y}(2007\pi^3y^3+28800\pi^5y^5+8708\pi^2y^2+3213\pi y-32320\pi^4y^4-306)\\
&\quad\quad+e^{-5\pi y}(99792\pi^5y^5+18172\pi^3y^3+23632\pi^2y^2+6468\pi y-140112\pi^4y^4-504)\\
&\quad\quad+e^{-6\pi y}(49660\pi^3y^3+336960\pi^5y^5+27920\pi^2y^2+5460\pi y-295200\pi^4y^4-360).
\end{aligned}\tag{11.29}$$

Using the explicit expression in (11.29) and dividing the interval (1, 1.12) into 10 smaller intervals and calculating the derivatives on each interval, we obtain the result.

□

Lemma 12.12. *The error estimate holds:*

$$\Big|\left(\mathcal{B}_e''''\mathcal{A}''-\mathcal{B}_e''\mathcal{A}''''+\mathcal{B}_a''''\mathcal{A}_e''-\mathcal{A}_e''''\mathcal{B}_a''\right)(y)\Big|\leqq 8\left(\frac{13}{2}\pi\right)^4\sqrt{y}e^{-\frac{13}{2}\pi y}. \tag{11.30}$$

Remark 12.3. The coefficient of the bound is rather rough but is enough to get our result. The exponential power captures the main feature.

Proof. Using the explicit expressions of $\mathcal{A}$ and $\mathcal{B}_a$, after tedious estimates, we arrive at

$$|\mathcal{A}''''(y)|\leqq 8,\quad |\mathcal{B}_a''''(y)|\leqq 5. \tag{11.31}$$

This, combining with (11.26) and (11.27), gives the estimate.

□

Lemma 12.13. *It holds that*

$$\Big(\mathcal{B}''''\mathcal{A}''-\mathcal{B}''\mathcal{A}''''\Big)(y)>0,\ y\in[1,1.12]. \tag{11.32}$$

Proof. It is equivalent to proving that $\frac{32y^4}{\pi}e^{\frac{1}{2}\pi y}\Big(\mathcal{B}''''\mathcal{A}''-\mathcal{B}''\mathcal{A}''''\Big)(y)>0,\ y\in[1,1.12]$. By Lemmas 12.11 and 12.12 , we have that

$$
\begin{aligned}
&\frac{32y^4}{\pi}e^{\frac{1}{2}\pi y}\Big(\mathcal{B}''''\mathcal{A}''-\mathcal{B}''\mathcal{A}''''\Big)(y)\\
&=\frac{32y^4}{\pi}e^{\frac{1}{2}\pi y}\Big(\mathcal{B}_a''''\mathcal{A}_a''-\mathcal{B}_a''\mathcal{A}_a''''\Big)(y)\\
&\quad+\frac{32y^4}{\pi}e^{\frac{1}{2}\pi y}\Big(\mathcal{A}_2''\mathcal{B}''''+\mathcal{B}_2''''\mathcal{A}_a''-\mathcal{A}_2''''\mathcal{B}''-\mathcal{B}_2''\mathcal{A}_a''''\Big)(y)\\
&\geqq\frac{32y^4}{\pi}e^{\frac{1}{2}\pi y}\Big(\mathcal{B}_a''''\mathcal{A}_a''-\mathcal{B}_a''\mathcal{A}_a''''\Big)(y)-26^4\pi^3y^{9/2}e^{-6\pi y}\\
&\geqq\frac{32y^4}{\pi}e^{\frac{1}{2}\pi y}\Big(\mathcal{B}_a''''\mathcal{A}_a''-\mathcal{B}_a''\mathcal{A}_a''''\Big)(y)\mid_{y=1.12}-26^4\pi^3y^{9/2}e^{-6\pi y}\mid_{y=1}\\
&=49.93918473\cdots-0.09227517899\cdots\\
&>0.
\end{aligned}
\tag{11.33}
$$

□

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