On lattice energy minimization problem for non-completely monotone functions and applications

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Abstract

Let $z \in \mathbb{H} := \{z = x + iy \in \mathbb{C} : y > 0\}$, and $\Lambda = \sqrt{\frac{1}{\operatorname{Im}(z)}}(\mathbb{Z} \oplus z\mathbb{Z})$ be the lattice in $\mathbb{R}^2$ with unit area. Let $\theta(\alpha; z) := \sum_{\mathbb{P}\in\Lambda} e^{-\alpha\pi\|\mathbb{P}\|^2}$ be the Theta function, $\zeta(s; z) := \sum_{\mathbb{P}\in\Lambda\setminus\{0\}} \frac{1}{\|\mathbb{P}\|^{2s}}$ be the Epstein-Zeta function, and $\mathcal{Y}(\alpha; z) := \sum_{\mathbb{P}\in\Lambda\setminus\{0\}} \frac{e^{-\alpha\pi\|\mathbb{P}\|^2}}{\|\mathbb{P}\|^{2s}}$ be the Coulomb potential. In this paper, we give complete classification of optimal lattice for the difference of two Theta functions

$$\min_{z\in\mathbb{H}} \Big(\theta(\alpha; z) - b\theta(\beta; z)\Big), \quad \alpha, \beta > 0 \text{ and } b \in \mathbb{R},$$

the difference of two Epstein-Zeta functions

$$\min_{z\in\mathbb{H}} \Big(\zeta(s_1; z) - b\zeta(s_2; z)\Big), \quad s_1 > s_2 > 1 \text{ and } b \in \mathbb{R},$$

and the difference of two Coulomb potentials

$$\min_{z\in\mathbb{H}} \Big(\mathcal{Y}(\alpha; z) - b\mathcal{Y}(\beta; z)\Big), \quad \alpha, \beta > 0 \text{ and } b \in \mathbb{R},$$

Our results reveal that the lowest energy lattice arrangement under the above potentials undergoes a hexagonal-rhombic-square-rectangular transition. These results have natural applications to Born-Mayer, Morse, Lennard-Jones, Buckinglam and Yukawa (Coulomb) potentials. These potentials have strong physical backgrounds and have important applications in chemistry, materials science, molecular dynamics simulations, etc. We give complete results for the lattice energy minimization problem in the above cases, and completely describe optimal lattice arrangements. Furthermore we present

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a novel and unified approach through balancing the attractive and repulsive forces. We obtain two **necessary conditions** for the minimizer: one is that the direction of the energy gradient formed by the attractive force must be opposite to that formed by the repulsive force (see (3.4) below), the other is the duality invariance (see (3.8). For highly symmetric lattices such as hexagonal, rhombic, square and rectangular lattices, this condition is always satisfied. However, for general oblique lattices, this condition is difficult to satisfy and often relies on specific forms of attractive and repulsive forces. In the analysis of the Born-Mayer, Lennard-Jones, and Yukawa potentials, we precisely verify this necessary condition to rule out the possibility of the oblique lattice. Furthermore, by comparing the magnitudes of the attractive and repulsive forces, we discover that the lowest energy state varies monotonically from hexagonal to rhombic to square to rectangular, allowing us to determine the exact form of the minimizer for specific parameters. In physics, the lowest energy state is considered to be the most stable state. We show that the highly symmetric structure ensures that the attractive and repulsive forces are in a balanced and stable relationship, which explains why the lowest energy lattice always tends to be highly symmetric, especially hexagonal and square lattices.

Keywords: Theta and Zeta functions, Lattice minimizations, Crystallization phenomena, Born-Mayer potential, Lennard-Jones potential, Yukawa potential.
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Contents

1 Introduction

Crystals are the result of atoms coming together in a stable environment to form a structure with a periodic arrangement. This structural periodicity is such that the directional indices marking the faces of a crystal are precise integers. This fascinating attribute was first noted by mineralogists and was subsequently verified in 1912 through experiments using X-ray diffraction. The establishment of the atomic model for crystal structures enabled physicists to make significant advances in the field of solid-state physics. The advent and progression of quantum theory have profoundly impacted the development and comprehension of solid-state physics, marking a crucial turning point in the field. This theoretical foundation has not only enhanced our understanding of crystalline materials but has also led to the exploration of amorphous solids and quantum fluids. Today, the scope of solid-state physics has broadened to encompass condensed matter physics, which delves into the properties of both crystalline and non-crystalline materials, along with quantum fluids. This area of study stands as one of the most vibrant and expansive fields within contemporary physics, continually pushing the boundaries of our knowledge and understanding of the physical world.

Crystals are ideally formed by repeating groups of atoms, known as bases, arranged uniformly in space. These groups can be mathematically represented by geometric points, creating a structure called a lattice. A Bravais lattice is a unique, infinite collection of discrete points that looks the same from any vantage point within the arrangement. In three-dimensional space, there are 14 distinct Bravais lattice types, organized into seven crystal systems: cubic, tetragonal, orthorhombic, hexagonal, rhombohedral (or trigonal), monoclinic, and triclinic. Each Bravais lattice type has its specific arrangement and orientation, defined by a unique set of lattice parameters: the lengths of the unit cell edge (a, b, c) and the angles between them (α, β, γ). In the realm of two-dimensional space, five Bravais lattice types are identified: square, rectangular, rhombic, hexagonal, and oblique.

Recent efforts have been focused on establishing the crystallization phenomena rigorously, i.e., the fact that ground states of systems exhibit a periodic order. Understanding why solids form crystals at absolute zero temperature and how atomic interaction dictates the specific crystal shape that a material chooses is a fundamental problem. This phenomenon has been observed numerically and experimentally in a variety of circumstances, but its rigorous mathematical justification appears to be extremely difficult, and the principles at work appear to be far from fully understood (see the reviews [22, 105]). The outcomes of physics-inspired phenomenological models are known for one-dimensional models [13, 20, 26, 54, 74, 109, 128, 129, 130] and for some higher-dimensional cases [44, 46, 53, 61, 88, 89, 104, 126]. Parallel to this, research into the subject using number theory and related combinatorial approaches (see the book [92]) yields significant results in dimensions 2 and 3 (see [11, 12, 14, 16, 18, 28, 43, 48, 49, 57, 59, 67, 73, 79, 82, 83, 84, 85, 86, 96, 102, 106, 122, 123, 124, 131]), as well as in some specific higher dimensions (cf.

[6, 35, 38, 39, 40, 110]), which leads to the recent proof of optimality of optimum packings, which can be viewed as a ground state energy determined by the specific potential, in dimensions 8 and 24, see [37, 132].

The study of the two-dimensional crystal lattice plays a key role in the development of modern science. It can help us better understand the fundamental properties of material substances, provide insight into how different interaction forces affect the crystal structure, and help us design and synthesize new materials with specific properties, which are widely used in the fields of drug discovery, nanotechnology, molecular mechanics, new energy sources and environmental science. For the five lattice types in two dimensions, we most often study hexagonal lattice, followed by square. Classical examples of hexagonal lattices are Graphene, Hexagonal Boron Nitride, and Transition metal disulfides (e.g. MoS2, WS2), and square lattices are Chalcogenide structural materials and two-dimensional magnetic materials. The discovery and application of all these materials have greatly advanced society, but we have done relatively little research on other lattice situations. We also do not know the principle of lattice structure generation. The study of the lowest energy arrangement of two-dimensional lattices is crucial to explaining crystal formation and has a wide range of applications in physics ([11, 12, 14, 15, 16, 17, 31, 34, 50, 62, 78, 92, 98, 112, 115, 117, 136]), especially condensed matter physics ([25, 30, 69, 100, 125, 135]), superconductivity theory ([2, 32, 41, 81, 107, 108, 114, 118]), chemistry ([29, 56]), and number theory ([22, 80, 102, 110]), etc.

In this paper, we aim to study the problem of the minimum lattice energy of potentials in two dimensions. Let $L := \mathbb{Z}\vec{u} \oplus \mathbb{Z}\vec{v}$ be a two-dimensional lattice, where $\vec{u}$ and $\vec{v}$ are two linearly independent two-dimensional vectors. Let $E_f[L] := \sum_{\mathbb{P}\in L} f\left(\|\mathbb{P}\|^2\right)$ or $\sum_{\mathbb{P}\in L\backslash\{0\}} f\left(\|\mathbb{P}\|^2\right)$ be the total energy of the system under the background potential f over a periodical lattice L, where $\|\cdot\|$ is the Euclidean norm on $\mathbb{R}^2$, then the minimization problem on lattices be written as $\min_L E_f[L]$, In fact, without loss of generality, we only need to consider the lattice $\Lambda := \sqrt{\frac{1}{\mathrm{Im}(z)}}\,(\mathbb{Z}\oplus z\mathbb{Z})$ (readers can see the proof in Section 3). For any admissible function f (the definition here is the same as in [12] Definition 2.4), we can define its lattice energy, that is,

$$\mathcal{F}(z) := E_f[\Lambda] = \sum_{\mathbb{P}\in\Lambda} f(\|P\|^2) \quad \text{or} \quad \sum_{\mathbb{P}\in\Lambda\backslash\{0\}} f(\|P\|^2). \tag{1.1}$$

In particular, for the classical physical potential, such as Theta function $\theta(\alpha; z)$, Coulomb potential $\mathcal{Y}(\alpha; z)$, and Epstein-Zeta function $\zeta(s; z)$, we denote them by

$$\begin{aligned}
\theta(\alpha; z) &:= \sum_{\mathbb{P}\in\Lambda} e^{-\pi\alpha\|\mathbb{P}\|^2} = \sum_{(m,n)\in\mathbb{Z}^2} e^{-\frac{\pi\alpha}{\mathrm{Im}(z)}|mz+n|^2} = \sum_{(m,n)\in\mathbb{Z}^2} e^{-\pi\alpha\left(m^2y+\frac{(mx+n)^2}{y}\right)}, \\
\zeta(s; z) &:= \sum_{\mathbb{P}\in\Lambda\backslash\{0\}} \frac{1}{\|\mathbb{P}\|^{2s}} = \sum_{(m,n)\in\mathbb{Z}^2\backslash\{0\}} \frac{(\mathrm{Im}(z))^{2s}}{|mz+n|^{2s}}, \\
\mathcal{Y}(\alpha; z) &:= \sum_{\mathbb{P}\in\Lambda\backslash\{0\}} \frac{e^{-\pi\alpha\|\mathbb{P}\|^2}}{\|\mathbb{P}\|^2} = \sum_{(m,n)\in\mathbb{Z}^2\backslash\{0\}} \frac{e^{-\frac{\pi\alpha}{\mathrm{Im}(z)}|mz+n|^2}(\mathrm{Im}(z))^2}{|mz+n|^2}.
\end{aligned} \tag{1.2}$$

Up to rotation and translation, we only need to work on the problem in the fundamental domain $\overline{\mathcal{D}_{\mathcal{G}}}$ (see Section 3). The minimizer of $\zeta(s; z)$ for a range of s was firstly studied by the number theorist Rankin [106], and then followed by Cassels [28], Diananda [43] and Ennola [48, 49]. They demonstrated that the minimizer of $\zeta(s; z)$ is $z = e^{i\frac{\pi}{3}}$. In 1988, Montgomery [96] demonstrated that the minimizer of $\theta(\alpha; z)$ is always $z = e^{i\frac{\pi}{3}}$ for all $\alpha > 0$, thus regaining the outcomes of [28, 48, 49, 106]. In mathematical physics, Montgomery's Theorem [96] has significant applications in [19, 115]. By using the Hausdor-Bernstein-Widder Theorem, Cohn and Kumar [36] extended Montgomery's result to any completely monotone functions, which are infinitely smooth and satisfy

$$(-1)^j f^{(j)}(x) > 0, \quad j = 0, 1, 2, \cdots \infty.$$

Besides, Sandier and Serfaty [108] studied the Coulomb potential $f(\cdot) = -\log|\cdot|$, and proved that its minimizer is still $z = e^{i\frac{\pi}{3}}$. Coulombian renormalized energy via a regularized procedure, which was extended to a two-component Coulombian competing system by Luo, Ren and the second author [81].

However, in many physical models, the potential function f, which can be found in [68], may not be completely monotone. For instance, we mention that

a. The sums of Born-Mayer potential $U(r) = \sum_{i=1}^{n} B_i e^{-\frac{r}{\rho_i}}$. This potential was proposed by Born and Mayer [24] firstly in their study of the properties of ionic crystals to model the repulsive part of the interaction between neutral atoms or molecules, where B_i is a parameter that determines the strength of the repulsion, ρ_i is a parameter related to the range of the potential, and n denotes the number of atomic molecules in the system. In particular, the potential $e^{-a_1\pi r} - be^{-a_2\pi r}$ ($a_1 > 0$, $a_2 > 0$, $b \in \mathbb{R}$) has received a lot of attention in [12, 82, 84, 86] as a derivation of the Theta function. Particularly, Luo and the second author [84, 86] considered the minimization problem of $\theta(\alpha; z) - b\theta(\beta; z)$ for $\alpha \leq \beta$, and observed that the minimizer is always $z = e^{i\frac{\pi}{3}}$. We will completely solve the minimization problem of $\theta(\alpha; z) - b\theta(\beta; z)$ in this paper, and show that for $\alpha > \beta$, the hexagonal-rhombic-square-rectangular transition appears as b goes from $-\infty$ to $+\infty$.

b. The Morse potential $U(r) = D_e(1 - e^{-a(r-r_e)})^2$. It's named after physicist P. M. Morse [97] and is a convenient interatomic interaction model for the potential energy of a diatomic molecule. Here r is the distance between the atoms, r_e is the equilibrium bond distance, D_e is the well depth, and a controls the width of the potential. We will solve the case where r_e is at the origin.

c. The Lennard-Jones-type potential $U(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$, also called the (12-6) Lennard-Jones potential. It was initially proposed by Lennard-Jones [66] to study the thermodynamic properties of rare gases. Here, ε is the depth of the potential well, σ is the finite distance at which the inter-particle potential is zero, and r is the distance between the particles. It's worth mentioning that the attractive term corresponds to the dispersion dipole-dipole interaction. Its generalization $U(r) = \frac{a_2}{r^{s_2}} - \frac{a_1}{r^{s_1}}$ ($s_2 > s_1 > 0$, $a_1, a_2 > 0$), also called the Mie potential [95], now are commonly used in molecular dynamics simulations and statistical mechanics to describe the interaction between pairs of neutral atoms or molecules and to represent the intermolecular forces. Lots of researchers have done much valuable works (see [7, 11, 14, 16, 18, 59, 67, 85, 131]). A numerical simulation suggests the hexagonal-rhombic-square-rectangular lattice phase transitions, but a complete rigorous mathematical proof needs to be provided. Therefore, this is a long-standing question. Luo and the second author [85] only solved the case of (12-6) Lennard-Jones potential. In this paper we will solve all cases completely.

d. The Buckingham potential $U(r) = Ae^{-\frac{r}{\rho}} - \frac{C}{r^6}$. It was proposed by Buckingham [27], where A is a parameter related to the depth of the potential well, ρ is the range of the potential, and C is a parameter related to the strength of the long-range attractive dispersion forces. It is another mathematical model used to describe the interaction between neutral atoms or molecules. Like the Lennard-Jones potential, it is often employed to represent van der Waals interactions, but this potential is a more sophisticated model and is characterized by an exponential term that accounts for the short-range repulsion between particles. There are many very important physical aspects of this potential (cf. [9, 65, 71, 90, 93, 121, 127]), but some require more rigorous mathematical proof. The first and third author [122] gave results for this potential.

e. The sums of screened Coulomb potential $U(r) = \sum_{i=1}^{n} \frac{Z_{i1}Z_{i2}e^2}{r} e^{-\frac{r}{\lambda_i}}$. It is also known as the Yukawa potential, proposed by Bohr [23] for short atom-atom distances, where Z_{i1} and Z_{i2} are the charges of the two particles, e is the elementary charge, r is the separation distance between the particles, and λ_i is the screening length, which determines the range of the interaction. Now it's used widely for describing the interaction between charged particles, typically in the context of plasma physics, fusion research, colloidal suspensions, dusty plasmas, the Thomas-Fermi model for solids, or other situations where charged particles are present, see [11, 21]. We will also give an important result for this potential.

Through the above introduction, we find that many research work (see [4, 14, 16, 18, 36, 81, 82, 83, 84, 85, 86, 87]) are concerning the energy minimization problem for non-monotone functions. However, these problems have not been proven rigorously in mathematics, except some numerical simulations or experimental findings. Furthermore, these approaches fall short of capturing the underlying mechanisms of lattice arrangement. Previous research has predominantly aimed at computing the potential for specific parameters, with the proof process heavily dependent on sophisticated numerical techniques, making the outcomes somewhat contingent. In this paper, we will propose a new method that first yields necessary conditions (see (3.4) and (3.8)) for the minimizer through some interesting observations, which reduces the problem considerably, and finally we can determine the exact location of the minimizer. This method has strong applicability and can address a range of issues, specifically the potentials arising from the difference between two completely monotone functions, including well-known potentials like the Lennard-Jones and Yukawa potentials. Notably, our work is the first to give comprehensive outcomes for the difference of two Theta functions as well as the Lennard-Jones potential. Our methodology, to some extent, unravels why crystals adopt specific arrangements, highlighting a crucial interplay between the attractive and repulsive forces among molecules.

Let

$$\begin{aligned}\Gamma_a &:= \{z \in \mathbb{H} : \mathrm{Re}(z) = 0,\ \mathrm{Im}(z) \geq 1\},\\ \Gamma_b &:= \left\{z \in \mathbb{H} : |z| = 1,\ \mathrm{Im}(z) \in \left[\tfrac{\sqrt{3}}{2}, 1\right]\right\},\\ \Gamma_c &:= \left\{z \in \mathbb{H} : \mathrm{Re}(z) = \tfrac{1}{2},\ \mathrm{Im}(z) \geq \tfrac{\sqrt{3}}{2}\right\}.\end{aligned}$$

Our first main result concerns the difference of two Theta functions:

Theorem 1.1. *For any $\alpha > 1$, $\frac{1}{\alpha} \leq \lambda < 1$, we consider the minimization problem:*

$$\min_{z\in\mathbb{H}} \left(\theta(\alpha; z) - b\theta(\lambda\alpha; z)\right). \tag{1.3}$$

Then

1. *for any $b \in (-\infty, \sqrt{\lambda})$, the minimizer of (1.3) only occurs on the curve $\Gamma_a \cup \Gamma_b$. Moreover, the minimizer monotonically follows on this curve from $e^{i\frac{\pi}{3}}$ to i and then from i to infinity, as b goes from $-\infty$ to $\sqrt{\lambda}$.*

2. *for any $b \in [\sqrt{\lambda}, +\infty)$, (1.3) doesn't have any minimizer.*

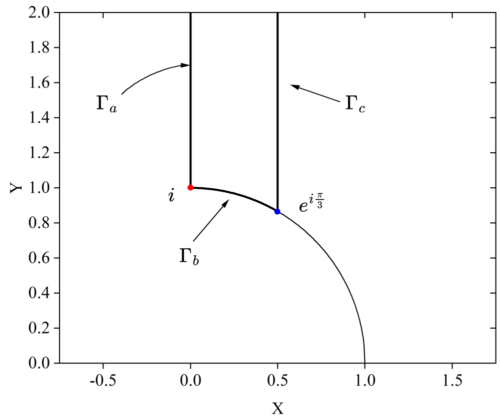

Figure 1: Schematic diagram of Γ_a, Γ_b and Γ_c.

Corollary 1.2. *For any $\alpha > 0$, $\beta > 0$, we denote $b_{\alpha,\beta} = \sqrt{\frac{\beta}{\alpha}}$. Then the minimization problem:*

$$\min_{z\in\mathbb{H}} \left(\theta(\alpha; z) - b\theta(\beta; z)\right) \tag{1.4}$$

has the following solutions:

1. *if $|\ln \alpha| \le |\ln \beta|$, when $b \in (-\infty, b_{\alpha,\beta}]$, the minimizer is $e^{i\frac{\pi}{3}}$; when $b \in (b_{\alpha,\beta}, +\infty)$, the (1.4) doesn't have any minimizer.*

2. *if $|\ln \alpha| > |\ln \beta|$, when $b \in (-\infty, b_{\alpha,\beta})$, the minimizer only occurs on the curve $\Gamma_a \cup \Gamma_b$. Moreover, the minimizer is monotonically moving along this curve from $e^{i\frac{\pi}{3}}$ to i and then from i to infinity, as b goes from $-\infty$ to $b_{\alpha,\beta}$; when $b \in [b_{\alpha,\beta}, +\infty)$, (1.4) doesn't have any minimizer.*

Corollary 1.3. *For any $\alpha_i, \beta_j, c_i, d_j > 0$, where $i = 1, 2, \cdots, n$ and $j = 1, 2, \cdots, m$, we consider the minimization problem:*

$$\min_{z\in\mathbb{H}} \left(\sum_{i=1}^{n} c_i\theta(\alpha_i; z) - \sum_{j=1}^{m} d_j\theta(\beta_j; z) \right). \tag{1.5}$$

Denote by

$$a = \min\{|\ln \alpha_1|, |\ln \alpha_2|, \cdots, |\ln \alpha_n|\}, \quad A = \max\{|\ln \alpha_1|, |\ln \alpha_2|, \cdots, |\ln \alpha_n|\},$$

$$b = \min\{|\ln \beta_1|, |\ln \beta_2|, \cdots, |\ln \beta_m|\}, \quad B = \max\{|\ln \beta_1|, |\ln \beta_2|, \cdots, |\ln \beta_m|\}.$$

The followings hold:

1. *When $\sum_{i=1}^{n} \frac{c_i}{\sqrt{\alpha_i}} - \sum_{j=1}^{m} \frac{d_j}{\sqrt{\beta_j}} < 0$, (1.5) doesn't have the minimizer.*

2. *When* $\sum_{i=1}^{n}\frac{c_i}{\sqrt{\alpha_i}}-\sum_{j=1}^{m}\frac{d_j}{\sqrt{\beta_j}}>0$*, if* $A\leq b$*, the minimizer of (1.5) is* $e^{i\frac{\pi}{3}}$*.*

3. *When* $\sum_{i=1}^{n}\frac{c_i}{\sqrt{\alpha_i}}-\sum_{j=1}^{m}\frac{d_j}{\sqrt{\beta_j}}>0$*, if* $a\geq B$*, the minimizer of (1.5) only occurs on the curve* $\Gamma_a\cup\Gamma_b$*.*

Remark 1.4. Luo and the second author [84, 86] only solved the lattice energy minimization problem of the Born-Mayer potential (1.4) for $\alpha\leq\beta$. In the present paper, we give a complete result, which can also be seen as the answer to Morse potential when r_e is at the origin. Moreover, Corollary 1.3 discusses the case of multiple Born-Mayer potential composites, offering insights into conclusions for more complex and generalized cases.

Next, we present the relevant conclusions of the well-known Lennard-Jones potential.

Theorem 1.5. *For any* $s_1>s_2>1$*, and any* $b\in\mathbb{R}$*, the minimizer of*

$$\min_{z\in\mathbb{H}}\left(\zeta(s_1;z)-b\zeta(s_2;z)\right) \tag{1.6}$$

only occurs on the curve $\Gamma_a\cup\Gamma_b$*. Moreover, the minimizer monotonically follows on this curve from* $e^{i\frac{\pi}{3}}$ *to* i *and then from* i *to infinity, as* b *goes from* $-\infty$ *to* $+\infty$*.*

Corollary 1.6. *For any* $s_1>s_2>\cdots>s_n>t_1>t_2>\cdots>t_m>1$*, and* $a_i,b_j>0$*, the minimizer of*

$$\min_{z\in\mathbb{H}}\left(\sum_{i=1}^{n}a_j\zeta(s_i,z)-\sum_{j=1}^{m}b_j\zeta(t_j,z)\right) \tag{1.7}$$

only occurs on the curve $\Gamma_a\cup\Gamma_b$*.*

Remark 1.7. Luo and the second author [85] solved the minimization problem of Lennard-Jones potential (1.6) for the specific case $s_1=6$ and $s_2=3$. Bétermin [16] solved the case when $\pi^{-s_1}\Gamma(s_1)s_1\leq\pi^{-s_2}\Gamma(s_2)s_2$. Here we give a complete classification, which can also be seen as an answer to the question raised by Bétermin ([17], Remark 4.3). Moreover, Corollary 1.6 examined the case of multiple Leonard-Jones potential complexes, providing potential conclusions for a broader and more intricate scenario. This conclusion is interesting and readers can go to Section 2 for a detailed explanation.

Next, we state the main results in the case of the Yukawa potential.

Theorem 1.8. *For any* $\alpha\geq1$*,* $0<\beta<\alpha$*, the minimization problem:*

$$\min_{z\in\mathbb{H}}\left(\mathcal{Y}(\alpha;z)-b\mathcal{Y}(\beta;z)\right) \tag{1.8}$$

has the following conclusions:

1. *for any* $b \in (-\infty, 1)$*, the minimizer only occurs on the curve* $\Gamma_a \cup \Gamma_b$*. Moreover, the minimizer monotonically follows on this curve from* $e^{i\frac{\pi}{3}}$ *to* i *and then from* i *to infinity, as* b *goes from* $-\infty$ *to* 1*;*

2. *for any* $b \in [1, +\infty)$*, (1.8) doesn't have any minimizer.*

Corollary 1.9. *For any* $\alpha > 0$*,* $\beta > \alpha$*, we consider the minimization problem:*

$$\min_{z\in\mathbb{H}} \left(\mathcal{Y}(\alpha; z) - b\mathcal{Y}(\beta; z)\right). \tag{1.9}$$

Then

1. *for any* $b \in (-\infty, 1]$*, the minimizer is* $e^{i\frac{\pi}{3}}$*.*

2. *for any* $b \in (1, +\infty)$*, (1.9) doesn't have any minimizer.*

Remark 1.10. The first and third author [79] solved the problem for the Yukawa potential when $\alpha \leq \beta$. Bétermin [16] solved the case when $\frac{b(b\alpha+\beta(1-b)\pi)}{\alpha(b+(1-b)\pi)} e^{(1-\frac{\beta}{\alpha})(\frac{1}{b}-1)\pi} \geq 1$. Here, we consider the Yukawa potential when $\alpha > \beta$. Moreover, by numerical calculation, there exists $\gamma = 0.6894\cdots$, when $\beta < \alpha < \gamma$, the function $\frac{\partial}{\partial\alpha}\left(\frac{\frac{\partial}{\partial y}\mathcal{Y}(\alpha;z)}{\frac{\partial}{\partial x}\mathcal{Y}(\alpha;z)}\right)$ is always positive, then the minimizer only occurs on Γ_c. For example, the minimizer of $\mathcal{Y}(0.6; z) - 0.91\mathcal{Y}(0.4; z)$ is $0.5 + i4.2363\cdots$. We conjecture that for any α, β, b, the minimizer only occurs on $\Gamma_a \cup \Gamma_b \cup \Gamma_c$.

Indeed, by Hausdorff-Bernstein-Widder Theorem [10], for any adimissible and completely monotonic function f, we have $f(r) = \int_0^{+\infty} e^{-rt}\mu_f(t)\,dt$, where $\mu_f(t)$ is the inverse Laplace transform of f with $\mu_f(t) \geq 0$. To simplify writing, we denote $\hat{\mu}_f(t) := \pi \cdot \mu_f(\pi t)$. Therefore, our conclusions can be generalized to more general situations below.

Theorem 1.11. *For any completely monotonic function* $f_1 = \int_0^{+\infty} e^{-\pi rt}\hat{\mu}_{f_1}(t)\,dt$*,* $f_2 = \int_0^{+\infty} e^{-\pi rt}\hat{\mu}_{f_2}(t)\,dt$*, if* $\frac{\hat{\mu}_{f_1}(t)+\frac{1}{t}\hat{\mu}_{f_1}(\frac{1}{t})}{\hat{\mu}_{f_2}(t)+\frac{1}{t}\hat{\mu}_{f_2}(\frac{1}{t})}$ *is strictly monotonically increasing/decreasing for* $t \in (1, +\infty)$*, then the minimizer of*

$$\min_{z\in\mathbb{H}} \left(\mathcal{F}_1(z) - b\mathcal{F}_2(z)\right)$$

only occurs on the curve $(\Gamma_a \cup \Gamma_b)/\,\Gamma_c$*. Moreover, the minimizer monotonically follows on this curve from* $e^{i\frac{\pi}{3}}$ *to infinity, as* b *changes from* $-\infty$ *to* $+\infty$*.*

Remark 1.12. It is a new approach to get the result of the minimization problem by proving the formula (4.5). Excluding the possibility of the minimizer being in the interior of $\mathcal{D}_{\mathcal{G}}$ by comparing the difference between attraction and repulsion. Besides, this method is highly flexible, and on the basis of the formula (4.5), related results for Lennard-Jones potential and Yukawa potential can be easily proved.

The remaining part of this paper is organized as follows: In Section 2, we will present some applications and implications of our conclusions. In Section 3, we show some preliminaries and construct two necessary conditions, which are crucial for the proof of the main theorems. In Section 4, we prove the Theorem 1.1, which is the core proof of the paper. In section 5, we use Theorem 1.1 to prove Corollaries 1.2-1.3. In Section 6, we use Chebyshev's inequality and establish the relationship between general completely monotone functions and the Theta function to prove the Theorems 1.5-1.11. First-time readers can skip the tedious computational proofs in Section 4 and focus on seeing how Sections 5 and 6 use the conclusions of Section 4 to complete the proofs of other potentials.

2 Remarks and Applications

This section consists of two main parts. We first present the role of the complete solution of the Lennard-Jones potential problem in probing the results of neutral atomic and molecular materials. Secondly, we give possible physical explanations for specific crystal arrangements based on the new methods used.

2.1 Lennard-Jones (Mie) potential

The Lennard-Jones potential has a wide range of applications in theoretical chemistry, physics, and materials science. It is primarily used to characterize non-bonded interactions between neutral atoms and molecules. It is commonly used to model interactions between atoms of noble gases, to perform molecular dynamics simulations of proteins, peptides, and other biological macromolecules, to study the properties of carbon-based nanomaterials (e.g. carbon nanotubes, fullerenes, and graphene), and to perform equation-of-state calculations on simple molecular liquids (e.g. methane) and gases [42, 52, 55, 75, 101, 137].

The Mie potential was initially proposed by the German physicist Gustav Mie [95], which is the generalized case of the Lennard-Jones potential (yet the history of intermolecular potentials is more complicated [51]), and can be written as

$$V(r) = \frac{n}{n-m}\left(\frac{n}{m}\right)^{\frac{m}{n-m}} \varepsilon\left[\left(\frac{\sigma}{r}\right)^{n} - \left(\frac{\sigma}{r}\right)^{m}\right].$$

The (12-6) Lennard-Jones potential is the most widely used. However, many cases do not fulfill the (12-6) form. In high-pressure physics and complex fluids, the Mie potential can better simulate molecular behavior in these environments by adjusting the values of n and m. Therefore, many scientific experiments have been conducted to study the Mie potential [3, 63, 64, 72, 99, 103, 111, 120, 133], and experimental measurements have led to the conclusion that for many cases the most accurate form is not (12-6). For example, the results could be accurately reproduced by (n-6) Mie potentials with $n = 8$ for H2 [1], $n = 11$ for Ne [116], $n = 12.085$ for Ar [45], $n = 13$ for Xe [116], and $n = 14$ for Kr

[94], etc. The article [119] emphasized that the general applicability of classical nucleation theory has been repeatedly called into question, and conjectured that improvement of the existing interatomic potentials will enable the precise study of real systems of practical significance. This article [8] emphasized several times that Lennard-Jones parameters need to be reparametrized for different scenarios. Determining the Lennard-Jones parameters for different cases is still an open problem.

Molecular interactions vary significantly across different materials and environments, necessitating the use of distinct m and n values in the Lennard-Jones potential to accurately capture the real interactions. It is worth noting that, because of the inherent errors in experimental measurements, the actual values of both m and n may not be integers, and any perturbation will cause a change in the coefficients. Therefore, an exclusive focus on the traditional (12-6) Lennard-Jones potential falls short of offering a comprehensive understanding of these physical phenomena. Compared with the result in [16, 85], our Theorem 1.5 gives a complete result for all $s_1 > s_2 > 1$, which can deal with all cases and overcome the bias caused by errors. This is a complete and rigorous proof that the crystal arrangement under Lennard-Jones potential shows a hexagonal-rhombic-square-rectangular lattice phase transition as the lattice parameter changes. Our results are consistent with Landau's theory. When a phase transition occurs, the symmetry is broken. If we take the length and angle of the lattice as the order parameters, we can see that the order parameters increase when the symmetry decreases. Moreover, based on our conclusions, it is easy to find the exact location of the minimizer for any particular bit potential.

For many more complex cases, we need to use a mixed Lennard-Jones potential to characterize the interactions between particles. For instance, to describe the interaction between a carbon atom in the polyatomic ion and a buffer gas helium atom in fullerene C_{60}, Mason and Schamp [91] defined the (12-6-4) potential by

$$V(r) = \frac{a_1}{r^{12}} - \frac{a_2}{r^6} - \frac{a_3}{r^4}. \tag{2.1}$$

To describe the interactions of metal ions in highly charged systems, and to reproduce the hydration free energies and the ion-oxygen distance, Li, Song, and Merz [76, 77] also used the (12-6-4) potential (2.1). To describe rare gases, Klein and Hanley [58, 70] proposed the (m-6-8) potential, that is

$$V(r) = \frac{a_1}{r^m} - \frac{a_2}{r^6} - \frac{a_3}{r^8},$$

where $m > 8$. Our Corollary 1.6 gives a complete result for all these cases.

2.2 Explanations

The specific form of the crystal arrangement is due to a variety of factors, such as chemical bonding, non-bonding interactions, ambient temperature, etc. Among them there are also many differences in non-bonding interactions between different particles, van der Waals forces, electrostatic interactions, hydrogen bonding, $\pi - \pi$ interactions, and hydrophobic interactions are all common forms of non-bonding interactions.

Without considering the effects of chemical bonding, we can generalize these forces into attractive and repulsive forces. This arrangement of crystals is a natural consequence of a substance reaching a state of minimum energy and maximum stability under given conditions. We conjecture that the specific form of the lattice arrangement is determined by the relationship between attractive and repulsive forces. Once the lattice arrangement reaches a steady state, the gradient of the potential energy with respect to the position should be 0. This implies that the gradient of the potential energy posed by the attractive force and the repulsive force, respectively, should be in exactly the opposite direction (that is $F(z) = 0$, see (3.4)). However, due to the different forms of attractive and repulsive forces, the above conditions are very difficult to satisfy for most lattice arrangements, which explains why the oblique lattice is a very rare form. The proof in this paper focuses on the interrelationship between attractive and repulsive forces, and finds that the direction of the gradient of both of them is always opposite when the lattice arrangement is hexagonal, rhombic, square or rectangular, and the possibility of any other arrangement is very low. This is also in line with our intuitive idea that the structures with high symmetry are more stable.

It is also important to note here that even if the potential energy gradients of the repulsive and attractive forces are opposite, the point is not necessarily a local energy minimum, which also depends on the lattice parameter, which is represented in this paper by the parameter b. Especially, in Lennard-Jones potential, b is related to effective particle diameter. When b is not too large, the crystal always remains hexagonal, and when b is within a certain range, the crystal remains square. However, only when b is a specific value, does the crystal exhibit a specific rhombic or rectangular lattice. This also explains why hexagonal lattices are the most common case and square lattices the second most common. The rhombic and rectangular are highly unstable for perturbations of b and exist for a relatively short period.

Our research points the way to the discovery of new two-dimensional materials. In addition to the common hexagonal lattice, the new two-dimensional materials may be square, rectangular, or rhombic in structure. Our research also provides new directions for material synthesis, as the hexagonal lattice is recognized as the most stable lattice, and scientists can synthesize more stable materials by adjusting the attractive and repulsive forces.

3 Preliminaries

In this section, we present the relation between minimizers and lattice shapes, and some group invariance of $E_f[L]$, followed by its corresponding fundamental domain.

Firstly, we fix the parametrization of a lattice in $\mathbb{R}^2$ (cf. [11]). Let the lattice $L = \mathbb{Z}\vec{u} \oplus \mathbb{Z}\vec{v}$ be spanned by two linearly independent two-dimensional vectors $\vec{u}$, $\vec{v}$. Without losing generality, we can fix the cell area of the lattice to be 1, namely, $|\vec{u} \wedge \vec{v}| = 1$. Up to rotations and translations, one can set $\vec{u} = \frac{1}{\sqrt{y}}(1,0)$, and $\vec{v} = \frac{1}{\sqrt{y}}(x,y)$, where $y > 0$. In this way, $|\vec{u} \wedge \vec{v}| = 1$, $\vec{v} = z\vec{u}$ where $z = x + iy \in \mathbb{H}$, and we denote $\Lambda = \sqrt{\frac{1}{y}}(\mathbb{Z} \oplus z\mathbb{Z})$.

In particular, $z = e^{i\frac{\pi}{3}}$ corresponds to hexagonal lattice, $z = i$ corresponds to square lattice, $z = e^{i\theta}$, $\theta \in \left(0, \frac{\pi}{2}\right)$ corresponds to rhombic lattice, and $z = iy$, $y > 1$ corresponds to (strict) rectangular lattice.

Let $\mathcal{S}$ denote the modular group

$$\mathcal{S} := SL_2(\mathbb{Z}) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix}, ad - bc = 1,\ a, b, c, d \in \mathbb{Z} \right\}.$$

We use the following definition of the fundamental domain which is slightly different from the classical definition (see [96]):

Definition 3.1. (page 108, [47]). The fundamental domain associated to group G is a connected domain $\mathcal{D}$ satisfying

1. for any $z \in \mathbb{H}$, there exists an element $\pi \in G$ such that $\pi(z) \in \overline{\mathcal{D}}$;
2. 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 the modular group $\mathcal{S}$ is

$$\mathcal{D}_{\mathcal{S}} := \left\{ z \in \mathbb{H} : |z| > 1, -\tfrac{1}{2} < x < \tfrac{1}{2} \right\},$$

which is open. Note that the fundamental domain can be an open set, see [5] for instance. Next, we introduce another group $\mathcal{G}$ related to the functional $\mathcal{F}(z)$. The generators of the group $\mathcal{G}$ are given by

$$\tau \mapsto -\frac{1}{\tau}, \tau \mapsto \tau + 1, \tau \mapsto -\bar{\tau}.$$

It is easy to see that the fundamental domain associated with group $\mathcal{G}$, denoted by $\mathcal{D}_{\mathcal{G}}$, is

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

Therefore, we have the following lemma.

Lemma 3.2. *For any admissible function f, $\gamma \in \mathcal{G}$, and $z \in \mathbb{H}$, we have*

$$\mathcal{F}(z) = \mathcal{F}(\gamma(z)).$$

By this lemma, we can reduce the problem from $z \in \mathbb{H}$ to $\overline{\mathcal{D}_{\mathcal{G}}}$.

When f is a compeletly monotonic function, by a result in [36], the minimizer of $\mathcal{F}(z)$ is $e^{i\frac{\pi}{3}}$. This paper will focus on the situation about the potential being the difference of two completely monotonic functions. To this end, we will first study the properties of Theta function

$$\theta(\alpha; z) = \sum_{\mathbb{P}\in\Lambda} e^{-\pi\alpha|\mathbb{P}|^2} = \sum_{(m,n)\in\mathbb{Z}^2} e^{-\frac{\pi\alpha}{\mathrm{Im}(z)}|mz+n|^2} = \sum_{(m,n)\in\mathbb{Z}^2} e^{-\pi\alpha\left(m^2y+\frac{(mx+n)^2}{y}\right)}. \tag{3.1}$$

By the Chowla-Selberg formula [33, 113], we have the following lemma.

Lemma 3.3. *The Theta function can be rewritten to the following form:*

$$\begin{aligned}\theta(\alpha; z) &= \sqrt{\frac{y}{\alpha}}\left(2\sum_{n=1}^{\infty} e^{-\alpha\pi n^2 y} + 2\sum_{n=1}^{\infty} e^{-\frac{1}{\alpha}\pi n^2 y} + 1 + 4\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} e^{-\alpha\pi m^2 y} e^{-\frac{1}{\alpha}\pi n^2 y}\cos(2\pi mnx)\right)\\ &= \sqrt{\frac{y}{\alpha}}\left(2\sum_{n=1}^{\infty} e^{-\alpha\pi n^2 y} + 2\sum_{n=1}^{\infty} e^{-\frac{1}{\alpha}\pi n^2 y} + 1 + 4\sum_{n=1}^{\infty}\sum_{d|n} e^{-\pi y\left(\alpha d^2+\frac{n^2}{\alpha d^2}\right)}\cos(2\pi nx)\right)\\ &= 2\sqrt{\frac{y}{\alpha}}\sum_{n=1}^{\infty} e^{-\alpha\pi n^2 y} + 2\sum_{n=1}^{\infty} e^{-\frac{\alpha\pi n^2}{y}} + 4\sqrt{\frac{y}{\alpha}}\sum_{n=1}^{\infty}\sum_{d|n} e^{-\pi y\left(\alpha d^2+\frac{n^2}{\alpha d^2}\right)}\cos(2\pi nx) + 1.\end{aligned} \tag{3.2}$$

Remark 3.4. We give an alternative form of Theta function, which is crucial for our computations. The two different forms describe the effect of the parameters α and y on the Theta function respectively. The original form (3.1) shows that the higher order power terms decay exponentially as α becomes larger. The new form (3.2) clearly shows that the higher order terms decay exponentially as y gets larger. Notice that $\frac{\partial}{\partial y}\theta(\alpha; i) = 0$ and hence we have the following interesting identity:

$$\sum_{m\in\mathbb{Z}}\sum_{n\in\mathbb{Z}} e^{-\pi(\alpha m^2+\frac{n^2}{\alpha})} = 2\pi\sum_{m\in\mathbb{Z}}\sum_{n\in\mathbb{Z}}(\alpha m^2 + \frac{n^2}{\alpha})e^{-\pi(\alpha m^2+\frac{n^2}{\alpha})}.$$

Proof. Note that the convergence of the function, the various orders of summation and transformation that we perform on m and n, as well as the derivative operation on the parameters x and y, are all valid. So we have

$$
\begin{aligned}
\theta(\alpha;z) =& \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty} e^{-\alpha\pi\left(\frac{(mx+n)^2}{y}+m^2y\right)}\\
=& \sum_{m\in\mathbb{Z}} e^{-\alpha\pi m^2 y}\sum_{n\in\mathbb{Z}} e^{-\alpha\pi\frac{(mx+n)^2}{y}}\\
=& \sum_{m\in\mathbb{Z}} e^{-\alpha\pi m^2 y}\cdot\sqrt{\frac{y}{\alpha}}\sum_{n\in\mathbb{Z}} e^{-\frac{1}{\alpha}\pi n^2 y}\cos(2\pi mnx)\\
=& \sqrt{\frac{y}{\alpha}}\left(2\sum_{n=1}^{\infty} e^{-\alpha\pi n^2 y} + 2\sum_{n=1}^{\infty} e^{-\frac{1}{\alpha}\pi n^2 y} + 1 + 4\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} e^{-\alpha\pi m^2 y} e^{-\frac{1}{\alpha}\pi n^2 y}\cos(2\pi mnx)\right)\\
=& \sqrt{\frac{y}{\alpha}}\left(2\sum_{n=1}^{\infty} e^{-\alpha\pi n^2 y} + 2\sum_{n=1}^{\infty} e^{-\frac{1}{\alpha}\pi n^2 y} + 1 + 4\sum_{n=1}^{\infty}\sum_{d|n} e^{-\pi y\left(\alpha d^2+\frac{n^2}{\alpha d^2}\right)}\cos(2\pi nx)\right)\\
=& 2\sqrt{\frac{y}{\alpha}}\sum_{n=1}^{\infty} e^{-\alpha\pi n^2 y} + 2\sum_{n=1}^{\infty} e^{-\frac{\alpha\pi n^2}{y}} + 4\sqrt{\frac{y}{\alpha}}\sum_{n=1}^{\infty}\sum_{d|n} e^{-\pi y\left(\alpha d^2+\frac{n^2}{\alpha d^2}\right)}\cos(2\pi nx) + 1,
\end{aligned}
$$

where the third and the last equality are derived from the Poisson summation formula. (We refer to the book [134]). □

Next, we present some properties of completely monotone functions and some properties of the potential formed by the difference of two completely monotone functions.

Lemma 3.5. *For any completely monotone functions f_1 and f_2, let $\mathcal{F}_i(z) = E_{f_i}[\Lambda]$ be the lattice energy, where $i = 1, 2$. Then for any $z \in \mathcal{D}_{\mathcal{G}}$, we have*

$$
\frac{\partial}{\partial y}\mathcal{F}_i(z) > 0 \quad \textit{and} \quad \frac{\partial}{\partial x}\mathcal{F}_i(z) < 0. \tag{3.3}
$$

Moreover, if the minimizer of $\mathcal{F}_1(z) - b\mathcal{F}_2(z)$ only occurs on the curve $\Gamma_a \cup \Gamma_b$, then the minimizer monotonically follows on this curve from $e^{i\frac{\pi}{3}}$ to i and then from i to infinity, as b becomes larger. We call this the hexagonal-rhombic-square-rectangular lattice phase transition.

Proof. By [36] and [96] , (3.3) holds. For any $b_2 > b_1$, let the minimizer be z_1 and z_2 respectively. We have

$$
\begin{aligned}
&\mathcal{F}_1(z_1) - b_1\mathcal{F}_2(z_1) - (b_2-b_1)\mathcal{F}_2(z_2)\\
\le&\, \mathcal{F}_1(z_2) - b_1\mathcal{F}_2(z_2) - (b_2-b_1)\mathcal{F}_2(z_2)\\
=&\, \mathcal{F}_1(z_2) - b_2\mathcal{F}_2(z_2)\\
\le&\, \mathcal{F}_1(z_1) - b_2\mathcal{F}_2(z_1)\\
=&\, \mathcal{F}_1(z_1) - b_1\mathcal{F}_2(z_1) - (b_2-b_1)\mathcal{F}_2(z_1).
\end{aligned}
$$

Then we have

$$\mathcal{F}_2(z_1) \le \mathcal{F}_2(z_2).$$

This with (3.3) proves the lemma. □

Considering any admissible functions f_1 and f_2, let $f = f_1 - bf_2$, and $\mathcal{F}(z) = \mathcal{F}_1(z) - b\mathcal{F}_2(z)$ be the formula used to express the energy. In fact, for such a potential, the conditions for the existence of its minimizer are very demanding. We will obtain the necessary conditions for $z \in \overline{\mathcal{D}_{\mathcal{G}}}$ to be a minimizer from two different perspectives (see (3.4) and (3.8) below). An important consequence of these conditions is to exclude the interior minimizers.

Let

$$F(z) \coloneqq \frac{\partial}{\partial y}\mathcal{F}_1(z) \cdot \frac{\partial}{\partial x}\mathcal{F}_2(z) - \frac{\partial}{\partial x}\mathcal{F}_1(z) \cdot \frac{\partial}{\partial y}\mathcal{F}_2(z). \tag{3.4}$$

We will show that $F(z) = 0$ is a necessary condition. The physical meaning of this equation is that the gradient directions of attraction and repulsion are exactly opposite. To simplify the exposition, we introduce the following notation,

$$\Gamma_f \coloneqq \{z \in \overline{\mathcal{D}_{\mathcal{G}}} : F(z) = 0\},$$

$$\Gamma_{\mathcal{T}} \coloneqq \Gamma_a \cup \Gamma_b \cup \Gamma_c, \quad \text{and} \quad \Gamma_{\mathcal{F}} \coloneqq \{z \in \mathcal{D}_{\mathcal{G}} : F(z) = 0\}.$$

Lemma 3.6. *For any $b \in \mathbb{R}$, the minimizer of the energy $\mathcal{F}(z) = \mathcal{F}_1(z) - b\mathcal{F}_2(z)$ only occurs on the curve Γ_f.*

Proof. It is easy to see that for any $z \in \Gamma_a \cup \Gamma_c$, $\frac{\partial}{\partial x}\mathcal{F}_1(z) = \frac{\partial}{\partial x}\mathcal{F}_2(z) = 0$, which implies that $F = 0$. When $z \in \Gamma_b$, notice that $\frac{\partial}{\partial r}\mathcal{F}_1(z) = \frac{\partial}{\partial r}\mathcal{F}_2(z) = 0$, it's easy to check that $F = 0$. Therefore, we call $\Gamma_{\mathcal{T}}$ the set of trivial zero points, which is independent of f.

On the other hand, if $z \in \mathcal{D}_{\mathcal{G}}$ is the minimizer, then

$$\frac{\partial}{\partial x}\mathcal{F}(z) = \frac{\partial}{\partial x}\mathcal{F}_1(z) - b\frac{\partial}{\partial x}\mathcal{F}_2(z) = 0,$$
$$\frac{\partial}{\partial y}\mathcal{F}(z) = \frac{\partial}{\partial y}\mathcal{F}_1(z) - b\frac{\partial}{\partial y}\mathcal{F}_2(z) = 0,$$

this implies that $z \in \Gamma_{\mathcal{F}}$. □

More properties related to this function are given in the following proposition.

Proposition 3.7. *Here are some conditions to exclude minimizers.*

1. *For any $z_0 \in \Gamma_a \backslash \{i\}$, if $\frac{F(z)}{\sin(2\pi x)}\Big|_{z=z_0} > 0$, then z_0 can not be the minimizer;*

2. *For any $z_0 \in \Gamma_b \backslash \{e^{i\frac{\pi}{3}}, i\}$, if $\frac{F(z)}{r^2-1}\Big|_{z=z_0} > 0$, then z_0 can not be the minimizer;*

3. *For any* $z_0 \in \Gamma_c \backslash \{e^{i\frac{\pi}{3}}\}$, *if* $\frac{F(z)}{\sin(2\pi x)}\Big|_{z=z_0} < 0$, *then* z_0 *can not be the minimizer;*

4. *For any* $z_0 \in \Gamma_{\mathcal{F}}$, *if* z_0 *is an isolated zero, and* $\frac{\partial}{\partial x}\mathcal{F}_1(z_0) \cdot \frac{\partial}{\partial x}\mathcal{F}_2(z_0) \cdot \frac{\partial}{\partial y}\mathcal{F}_1(z_0) \cdot \frac{\partial}{\partial y}\mathcal{F}_2(z_0) \neq 0$, *then* z_0 *can not be the minimizer.*

Proof. If $z_0 \in \Gamma_a$ is the minimizer for some b_0, then

$$\left(\frac{\partial}{\partial y}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial y}\mathcal{F}_2(z)\right)\Bigg|_{z=z_0} = 0.$$

It is easy to see that $\frac{\frac{\partial}{\partial x}\mathcal{F}_1(z)}{\sin(2\pi x)}$ and $\frac{\frac{\partial}{\partial x}\mathcal{F}_2(z)}{\sin(2\pi x)}$ are both well-defined in $\overline{\mathcal{D}_{\mathcal{G}}}$. Then

$$\frac{b_0\frac{\partial}{\partial x}\mathcal{F}_2(z) - \frac{\partial}{\partial x}\mathcal{F}_1(z)}{\sin(2\pi x)}\Bigg|_{z=z_0} > 0.$$

By the continuity of the above function, there exists a neighborhood $U = B(z_0, r_0) \cap \mathcal{D}_{\mathcal{G}}$ such that

$$\frac{\partial}{\partial x}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial x}\mathcal{F}_2(z) < 0,$$

which is a contradiction.

If $z_0 \in \Gamma_b$ is the minimizer for some b_0, then

$$\left(\frac{\partial}{\partial \theta}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial \theta}\mathcal{F}_2(z)\right)\Bigg|_{z=z_0} = 0.$$

Notice that

$$\begin{aligned} F &= \frac{\partial}{\partial y}\mathcal{F}_1(z) \cdot \frac{\partial}{\partial x}\mathcal{F}_2(z) - \frac{\partial}{\partial x}\mathcal{F}_1(z) \cdot \frac{\partial}{\partial y}\mathcal{F}_2(z) \\ &= \frac{\partial}{\partial \theta}\mathcal{F}_1(z) \cdot \frac{\partial}{\partial r}\mathcal{F}_2(z) - \frac{\partial}{\partial r}\mathcal{F}_1(z) \cdot \frac{\partial}{\partial \theta}\mathcal{F}_2(z). \end{aligned}$$

Using the same method, we can deduce that

$$\frac{\frac{\partial}{\partial r}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial r}\mathcal{F}_2(z)}{r^2 - 1}\Bigg|_{z=z_0} < 0$$

By the continuity of the above function, then there exists a neighborhood $U = B(z_0, r_0) \cap \mathcal{D}_{\mathcal{G}}$ such that

$$\frac{\partial}{\partial r}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial r}\mathcal{F}_2(z) < 0,$$

which is a contradiction.

If $z_0 \in \Gamma_c$ is the minimizer for some b_0, using the same method, we can prove that there exists a neighborhood $U = B(z_0, r_0) \cap \mathcal{D}_\mathcal{G}$ such that

$$\frac{\partial}{\partial x}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial x}\mathcal{F}_2(z) > 0,$$

which is also a contradiction.

If $z_0 \in \Gamma_\mathcal{F}$ and it is an isolated zero, without losing generality, we can assume that there exists a deleted neighborhood $U_1 \subset \mathcal{D}_\mathcal{G}$, such that $F(z) > 0$ for any $z \in U$. That is

$$F(z) = \left(\tfrac{\partial}{\partial y}\mathcal{F}_1(z) - b_0\tfrac{\partial}{\partial y}\mathcal{F}_2(z)\right)\tfrac{\partial}{\partial x}\mathcal{F}_2(z) - \left(\tfrac{\partial}{\partial x}\mathcal{F}_1(z) - b_0\tfrac{\partial}{\partial x}\mathcal{F}_2(z)\right)\tfrac{\partial}{\partial y}\mathcal{F}_2(z) > 0. \quad (3.5)$$

On the other hand, z_0 is the minimizer of $\mathcal{F}_1(z) - b_0\mathcal{F}_2$, by Taylor's expansion, we know that there exists a neighborhood U_2 such that

$$\left(\tfrac{\partial}{\partial y}\mathcal{F}_1(z) - b_0\tfrac{\partial}{\partial y}\mathcal{F}_2(z)\right)(y - y_0) + \left(\tfrac{\partial}{\partial x}\mathcal{F}_1(z) - b_0\tfrac{\partial}{\partial x}\mathcal{F}_2(z)\right)(x - x_0) \geq 0 \quad (3.6)$$

holds for any $z \in U_2$. It's not hard to find a deleted neighborhood U_3 such that both of the above inequalities are satisfied at the same time. If $\frac{\partial}{\partial x}\mathcal{F}_2(z_0) \neq 0$, and $\frac{\partial}{\partial y}\mathcal{F}_2(z_0) \neq 0$, without lossing generality, assume $\frac{\partial}{\partial x}\mathcal{F}_2(z_0) < 0$, and $\frac{\partial}{\partial y}\mathcal{F}_2(z_0) > 0$ we can find a deleted negihberhood U_4 such that

$$\frac{\partial}{\partial x}\mathcal{F}_2(z) < 0 \quad \text{and} \quad \frac{\partial}{\partial y}\mathcal{F}_2(z) > 0.$$

Then for any $z \in U_5 = U_4 \cap \{(x, y) \in \mathcal{D}_\mathcal{G} : (x - x_0) > 0, \text{ and } (y - y_0) > 0\}$

$$\begin{aligned}
&\frac{\partial}{\partial x}\mathcal{F}_2(z)(y - y_0) < 0 \quad \text{and} \quad \frac{\partial}{\partial x}\mathcal{F}_2(z)(x - x_0) < 0.\\
&\frac{\partial}{\partial y}\mathcal{F}_2(z)(x - x_0) > 0 \quad \text{and} \quad \frac{\partial}{\partial y}\mathcal{F}_2(z)(y - y_0) > 0.
\end{aligned}$$

Multiplying (3.5) and (3.6) gives

$$\begin{aligned}
I := &\left(\frac{\partial}{\partial y}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial y}\mathcal{F}_2(z)\right)^2\frac{\partial}{\partial x}\mathcal{F}_2(z)(y - y_0)\\
&- \left(\frac{\partial}{\partial x}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial x}\mathcal{F}_2(z)\right)^2\frac{\partial}{\partial y}\mathcal{F}_2(z)\,(x - x_0)\\
&+ \left(\frac{\partial}{\partial y}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial y}\mathcal{F}_2(z)\right)\left(\frac{\partial}{\partial x}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial x}\mathcal{F}_2(z)\right)\frac{\partial}{\partial x}\mathcal{F}_2(z)(x - x_0)\\
&- \left(\frac{\partial}{\partial y}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial y}\mathcal{F}_2(z)\right)\left(\frac{\partial}{\partial x}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial x}\mathcal{F}_2(z)\right)\frac{\partial}{\partial y}\mathcal{F}_2(z)(y - y_0) \geq 0.
\end{aligned} \quad (3.7)$$

Let

$$X := \left(\frac{\partial}{\partial x}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial x}\mathcal{F}_2(z)\right) \quad \text{and} \quad Y := \left(\frac{\partial}{\partial y}\mathcal{F}_1(z) - b_0\frac{\partial}{\partial y}\mathcal{F}_2(z)\right).$$

If $XY < 0$ holds for all $z \in U_5$, then $X > 0$, $Y < 0$, or $X < 0$, $Y > 0$. However, by (3.5) and (3.6), when $z \in \partial U_5 \cap \{(x,y) \in \mathcal{D}_{\mathcal{G}} : x = x_0\}$, $X < 0$, meanwhile, when $z \in \partial U_5 \cap \{(x,y) \in \mathcal{D}_{\mathcal{G}} : y = y_0\}$, $Y < 0$. This implies that $XY < 0$ can not hold for all $z \in U_5$. If $XY \geq 0$, by (3.5), we get $X^2 + Y^2 \neq 0$, then $I < 0$, which contradicts with (3.7). □

Proposition 3.8. *If f_1 and f_2 are two completely monotonic functions, the above properties can be simplified as follows.*

1. *For any $z_0 \in \Gamma_a \backslash \{i\}$, if there exists a deleted neighberhood U such that $\frac{F(z)}{\sin(2\pi x)} > 0$ holds for all $z \in U \cap \overline{\mathcal{D}_{\mathcal{G}}}$, then z_0 can not be the minimizer;*
2. *For any $z_0 \in \Gamma_b \backslash \{e^{i\frac{\pi}{3}}, i\}$, if there exists a deleted neighberhood U such that $F(z) > 0$ holds for all $z \in U \cap \mathcal{D}_{\mathcal{G}}$, then z_0 can not be the minimizer;*
3. *For $z_0 = i$, if there exists a deleted neighberhood U such that $\frac{F(z)}{(y^2-1)\sin(2\pi x)} > 0$ holds for all $z \in U \cap \overline{\mathcal{D}_{\mathcal{G}}}$, then z_0 can not be the minimizer;*
4. *For any $z_0 \in \Gamma_c \backslash \{e^{i\frac{\pi}{3}}\}$, if there exists a deleted neighberhood U such that $\frac{F(z)}{\sin(2\pi x)} < 0$ holds for all $z \in U \cap \overline{\mathcal{D}_{\mathcal{G}}}$, then z_0 can not be the minimizer;*
5. *For any $z_0 \in \Gamma_{\mathcal{F}}$, if z_0 is an isolated zero, then z_0 can not be the minimizer.*

Proof. By Lemma 3.3, we know that

$$\theta(\alpha; z) = 2\sqrt{\frac{y}{\alpha}}\sum_{n=1}^{\infty} e^{-\alpha\pi n^2 y} + 2\sum_{n=1}^{\infty} e^{-\frac{\alpha\pi n^2}{y}} + 4\sqrt{\frac{y}{\alpha}}\sum_{n=1}^{\infty}\sum_{d|n} e^{-\pi y\left(\alpha d^2 + \frac{n^2}{\alpha d^2}\right)}\cos(2\pi n x) + 1.$$

Simultaneous partial derivatives for both sides of the above equation give

$$\frac{\partial}{\partial x}\theta(\alpha; z) = -8\pi\sqrt{\frac{y}{\alpha}}\sum_{n=1}^{\infty}\sum_{d|n} e^{-\pi y\left(\alpha d^2 + \frac{n^2}{\alpha d^2}\right)} n\sin(2\pi n x).$$

Consider the polar coordinate form,

$$\theta(\alpha; z) = \sum_{m=-\infty}^{+\infty}\sum_{n=-\infty}^{+\infty} e^{-\alpha\pi\left(m^2 r\frac{1}{\sin\theta} + n^2\frac{1}{r}\frac{1}{\sin\theta} + 2mn\frac{\cos\theta}{\sin\theta}\right)}.$$

Taking the partial derivative on both sides of the above equation, we have

$$\frac{\partial}{\partial r}\theta(\alpha;z) = -\alpha\pi\left(\frac{m^2}{\sin\theta} - \frac{n^2}{r^2\sin\theta}\right)\sum_{m=-\infty}^{+\infty}\sum_{n=-\infty}^{+\infty} e^{-\alpha\pi\left(m^2 r\frac{1}{\sin\theta}+n^2\frac{1}{r}\frac{1}{\sin\theta}+2mn\frac{\cos\theta}{\sin\theta}\right)}.$$

By a simple observation and calculation, we can get

$$\frac{\frac{\partial}{\partial x}\theta(\alpha;z)}{\sin(2\pi x)} \quad \text{and} \quad \frac{\frac{\partial}{\partial r}\theta(\alpha;z)}{r^2-1}$$

are well-defined in $\overline{\mathcal{D}_{\mathcal{G}}}$. By Lemma 3.5, if f is completely monotonic function, we have $\frac{\partial}{\partial x}\mathcal{F}(z) < 0$ and $\frac{\partial}{\partial y}\mathcal{F}(z) > 0$ for any $z \in \mathcal{D}_{\mathcal{G}}$. Using the same method as in the proof of Proposition 3.7, we can get a similar solution. □

Up to this point, we have obtained a very important conclusion, a necessary condition for determining whether z is the minimizer or not. Next, we will introduce another new perspective and give another important observation.

Remark 3.9. If $z \in \overline{\mathcal{D}_{\mathcal{G}}}$ is the minimizer, by the group action $\mathcal{G}$, we know that $\frac{z}{|z|^2}$ must be the minimizer too.

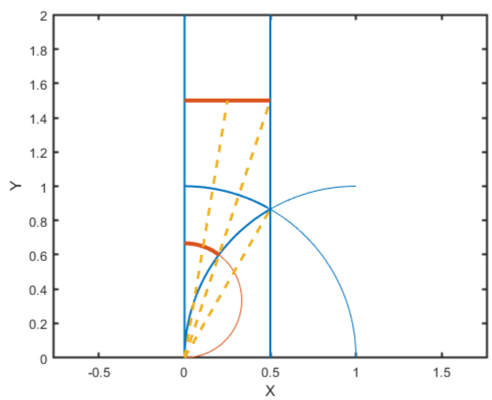

Figure 2: Schematic diagram of the relationship between z and $\frac{z}{|z|^2}$.

Let

$$F_x(z) := \frac{\partial}{\partial x}\mathcal{F}_1(z)\cdot\frac{\partial}{\partial x}\mathcal{F}_2(\frac{z}{|z|^2}) - \frac{\partial}{\partial x}\mathcal{F}_2(z)\cdot\frac{\partial}{\partial x}\mathcal{F}_1(\frac{z}{|z|^2}). \tag{3.8}$$

We will show that $F_x(z) = 0$ is an another necessary condition, which implies the symmetric geometric relationship of the lattice. We call this the duality invariance.

Lemma 3.10. *If z is the minimizer of $\mathcal{F}(z) = \mathcal{F}_1(z) - b\mathcal{F}_2(z)$, then we have $F_x(z) = 0$. Moreover, if f_1 and f_2 are two completely monotonic functions, for any $z_0 \in \Gamma_c \backslash \{e^{i\frac{\pi}{3}}\}$, if there exists a deleted neighberhood U such that $\frac{F_x(z)}{\sin^2(2\pi x)} < 0$ holds for all $z \in U \cap \overline{\mathcal{D}_{\mathcal{G}}}$, then z_0 can not be the minimizer.*

Proof. For any $\mathcal{F}(z) = \mathcal{F}_1(z) - b\mathcal{F}_2(z)$, it's obvious that if z it the minimizer, there exists

$$\frac{\partial}{\partial x}\mathcal{F}(z) = \frac{\partial}{\partial x}\mathcal{F}_1(z) - b\frac{\partial}{\partial x}\mathcal{F}_2(z) = 0,$$

meanwhile,

$$\frac{\partial}{\partial x}\mathcal{F}(\frac{z}{|z|^2}) = \frac{\partial}{\partial x}\mathcal{F}_1(\frac{z}{|z|^2}) - b\frac{\partial}{\partial x}\mathcal{F}_2(\frac{z}{|z|^2}) = 0,$$

which shows $F_x(z) = 0$. Moreover, if $z_0 \in \Gamma_c \backslash \{e^{i\frac{\pi}{3}}\}$ with $\frac{F_x(z)}{\sin^2(2\pi x)} < 0$ is the minimizer of $\mathcal{F}_1(z) - b_0\mathcal{F}_2(z)$, we have

$$\frac{\frac{\partial}{\partial x}\mathcal{F}(z)}{\sin(2\pi x)} = \frac{\frac{\partial}{\partial x}\mathcal{F}_1(z)}{\sin(2\pi x)} - b_0\frac{\frac{\partial}{\partial x}\mathcal{F}_2(z)}{\sin(2\pi x)} > \frac{\frac{\partial}{\partial x}\mathcal{F}_1(\frac{z}{|z|^2})}{\sin(2\pi x)} - b_0\frac{\frac{\partial}{\partial x}\mathcal{F}_2(\frac{z}{|z|^2})}{\sin(2\pi x)} = 0,$$

which contradicts the minimizer. □

4 Proof of Theorem 1.1

In this section, we will prove Theorem 1.1, which is also the main theorem of this article. By Proposition 3.8 and Lemma 3.10, if we can prove that for any $\alpha > 1$, $\frac{1}{\alpha} \le \lambda < 1$ and $z \in \mathcal{D}_{\mathcal{G}}$, the following inequalities either

$$\frac{\partial}{\partial y}\theta(\alpha; z) \cdot \frac{\partial}{\partial x}\theta(\lambda\alpha; z) - \frac{\partial}{\partial x}\theta(\alpha; z) \cdot \frac{\partial}{\partial y}\theta(\lambda\alpha; z) < 0 \tag{4.1}$$

or

$$\frac{\partial}{\partial x}\theta(\alpha; z) \cdot \frac{\partial}{\partial x}\theta(\lambda\alpha; \frac{z}{|z|^2}) - \frac{\partial}{\partial x}\theta(\alpha; \frac{z}{|z|^2}) \cdot \frac{\partial}{\partial x}\theta(\lambda\alpha; z) < 0, \tag{4.2}$$

holds, then the Theorem 1.1 follows naturally. By [96], we have $\frac{\partial}{\partial y}\theta(\alpha; z) > 0$ holds for any $\alpha > 0$ and $z \in \mathcal{D}_{\mathcal{G}}$, and $\frac{\partial}{\partial x}\theta(\alpha; z) < 0$ holds for any $\alpha > 0$ and $z \in \{0 \le x \le 0.5, y \ge 0.5\}$.

When $z \in \mathcal{D}_{\mathcal{G}}$, the inequality (4.1) can be equal to

$$\frac{\frac{\partial}{\partial y}\theta(\alpha; z)}{\frac{\partial}{\partial x}\theta(\alpha; z)} - \frac{\frac{\partial}{\partial y}\theta(\lambda\alpha; z)}{\frac{\partial}{\partial x}\theta(\lambda\alpha; z)} < 0.$$

Then we only need to prove for any $\alpha \ge 1$,

$$\frac{\partial}{\partial\alpha}\left(\frac{\frac{\partial}{\partial y}\theta(\alpha; z)}{\frac{\partial}{\partial x}\theta(\alpha; z)}\right) < 0.$$

When $z \in \mathcal{D}_{\mathcal{G}} \cap \{y \leq 1.5\}$, the inequality (4.2) can be equal to

$$\frac{\frac{\partial}{\partial x}\theta(\alpha; z)}{\frac{\partial}{\partial x}\theta(\alpha; \frac{z}{|z|^2})} - \frac{\frac{\partial}{\partial x}\theta(\lambda\alpha; z)}{\frac{\partial}{\partial x}\theta(\lambda\alpha; \frac{z}{|z|^2})} < 0.$$

Then we only need to prove for any $\alpha \geq 1$,

$$\frac{\partial}{\partial \alpha}\left(\frac{\frac{\partial}{\partial x}\theta(\alpha; z)}{\frac{\partial}{\partial x}\theta(\alpha; \frac{z}{|z|^2})}\right) < 0.$$

For the convenience of the following proof, we introduce the following notation.

$$\mathcal{F}_{\alpha,z} := \frac{\frac{\partial^2}{\partial \alpha \partial y}\theta(\alpha; z)}{\frac{\partial}{\partial y}\theta(\alpha; z)} - \frac{\frac{\partial^2}{\partial \alpha \partial x}\theta(\alpha; z)}{\frac{\partial}{\partial x}\theta(\alpha; z)}, \tag{4.3}$$

$$\mathcal{F}_{\alpha,z,y} := \frac{\frac{\partial^2}{\partial \alpha \partial y}\theta(\alpha; z)}{\frac{\partial}{\partial y}\theta(\alpha; z)} \quad \text{and} \quad \mathcal{F}_{\alpha,z,x} := -\frac{\frac{\partial^2}{\partial \alpha \partial x}\theta(\alpha; z)}{\frac{\partial}{\partial x}\theta(\alpha; z)}. \tag{4.4}$$

With the above analysis, we only need to prove that

Lemma 4.1. *For any $\alpha \geq 1$, when $z \in \mathcal{D}_{\mathcal{G}} \cap \{y \geq 1.5\}$, we have*

$$\frac{\partial}{\partial \alpha}\left(\frac{\frac{\partial}{\partial y}\theta(\alpha; z)}{\frac{\partial}{\partial x}\theta(\alpha; z)}\right) < 0. \tag{4.5}$$

When $z \in \mathcal{D}_{\mathcal{G}} \cap \{y \leq 1.5\}$, we have

$$\frac{\partial}{\partial \alpha}\left(\frac{\frac{\partial}{\partial x}\theta(\alpha; z)}{\frac{\partial}{\partial x}\theta(\alpha; \frac{z}{|z|^2})}\right) < 0. \tag{4.6}$$

Remark 4.2. In fact, through numerical simulations we know that (4.5) and (4.6) hold for any $z \in \mathcal{D}_{\mathcal{G}}$. Notice that when $z \in \overline{\mathcal{D}_{\mathcal{G}}} \cap \{r = 1\}$, the function $\mathcal{F}_{\alpha,z} = 0$, and when $r \to \infty$, $\frac{z}{|z|^2} \to 0$, which create difficulties in estimating around that point. Therefore, in the pursuit of a rigorous and concise mathematical proof, we divide the region into two parts. The proof of Lemma 4.1 is contained in the following two subsections 4.1 and 4.2.

4.1 $z \in \mathcal{D}_{\mathcal{G}} \cap \{y \geq 1.5\}$

Lemma 4.3. *For any $\alpha \geq 1$, $z \in \mathcal{D}_{\mathcal{G}} \cap \{y \geq 1.5\}$, we have $\mathcal{F}_{\alpha,z} > 0$.*

Remark 4.4. Notice that $\frac{\partial}{\partial y}\theta(\alpha; z) > 0$ and $\frac{\partial}{\partial x}\theta(\alpha; z) < 0$, it's easy to see that (4.5) is equivalent to $\mathcal{F}_{\alpha,z} > 0$. We will estimate these $\mathcal{F}_{\alpha,z,x}$ and $\mathcal{F}_{\alpha,z,y}$ separately.

Proof. We divide the proof into three cases, each using different expressions and different computations. In Case 1, we consider the situation when $\frac{y}{\alpha} \geq \frac{1}{2}$ and $\alpha \geq 3$. In Case 2, we consider the situation when $\alpha \leq 3$. In Case 3, we consider the situation when $\frac{y}{\alpha} \leq \frac{1}{2}$, i.e., $\frac{\alpha}{y} \geq 2$.

Case 1. $\frac{y}{\alpha} \geq \frac{1}{2}$ and $\alpha \geq 3$.

The constraint $\frac{y}{\alpha} \geq \frac{1}{2}$ is designed to handle the case where y is relatively large. We utilize a suitable expression (3.2) to ensure that when y is larger, the higher-order power terms that follow are smaller. In this case, we will show that the function $\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z} > 0$. Dividing $\mathcal{F}_{\alpha,z}$ by $1-\frac{1}{\alpha^2}$ is partly for the convenience of the computational process, and partly to make the connection with Case 2. By Lemma 3.3, we have

$$\theta(\alpha; z) = \sqrt{\frac{y}{\alpha}}\left(2\sum_{n=1}^{\infty} e^{-\alpha\pi n^2 y} + 2\sum_{n=1}^{\infty} e^{-\frac{1}{\alpha}\pi n^2 y} + 1 + 4\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} e^{-\alpha\pi m^2 y} e^{-\frac{1}{\alpha}\pi n^2 y}\cos(2\pi mnx)\right).$$

We will estimate $\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z,x}$, $\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z,y}$ separately. First, by direct calculation, we obtain that

$$\begin{aligned}
&\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z,x} - \frac{1}{1-\frac{1}{\alpha^2}}\frac{1}{2\alpha}\\
&= \pi y \cdot \frac{\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn(n^2 - \frac{1}{\alpha^2}m^2)e^{-\pi y(\alpha n^2 + \frac{1}{\alpha}m^2)}\sin(2\pi mnx)}{\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mne^{-\pi y(\alpha n^2 + \frac{1}{\alpha}m^2)}\sin(2\pi mnx)}\frac{1}{1-\frac{1}{\alpha^2}}\\
&= \pi y \cdot \left(1 + \frac{1}{1-\frac{1}{\alpha^2}}\frac{\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn((n^2-1) - \frac{1}{\alpha^2}(m^2-1))e^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}}{\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mne^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}}\right).
\end{aligned} \tag{4.7}$$

Next, we estimate the second part of the above function to verify that it's relatively small. Indeed, we have

$$\begin{aligned}
&\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mne^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}\\
&\geq 1 - \sum_{mn\geq 2} mne^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\left|\frac{\sin(2\pi mnx)}{\sin(2\pi x)}\right|\\
&\geq 1 - \sum_{mn\geq 2} m^2n^2e^{-\pi(\frac{9}{2}(n^2-1)+\frac{1}{2}(m^2-1))},
\end{aligned} \tag{4.8}$$

and

$$\left|\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn((n^2-1)-\frac{1}{\alpha^2}(m^2-1))e^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}\right|$$

$$\leq \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^2n^2((n^2-1)+\frac{1}{\alpha^2}(m^2-1))e^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))} \tag{4.9}$$

$$\leq \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^2n^2((n^2-1)+\frac{1}{9}(m^2-1))e^{-\pi(\frac{9}{2}(n^2-1)+\frac{1}{2}(m^2-1))}.$$

We deduce $\frac{1}{1-\frac{1}{\alpha^2}} \leq \frac{1}{1-\frac{1}{9}}$ by $\alpha \geq 3$. This with (4.8) and (4.9) yields

$$\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z,x} - \frac{1}{1-\frac{1}{\alpha^2}}\frac{1}{2\alpha} \geq \pi y\cdot(1-0.015) = 0.985\pi y. \tag{4.10}$$

Applying a similar method to $\mathcal{F}_{\alpha,z,y}$, since this equation is complex, we introduce a new symbolic notation to estimate the numerator and denominator separately. By direct calculation, we get

$$\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z,y} + \frac{1}{1-\frac{1}{\alpha^2}}\frac{1}{2\alpha} = \pi y\cdot\frac{N}{D}\cdot\frac{1}{1-\frac{1}{\alpha^2}}, \tag{4.11}$$

where

$$\begin{aligned} N =& -3\sum_{n=1}^{+\infty} n^2 e^{-\alpha\pi n^2 y} + \frac{3}{\alpha^2}\sum_{n=1}^{+\infty} n^2 e^{-\frac{1}{\alpha}\pi n^2 y} + 2\alpha\pi y\sum_{n=1}^{+\infty} n^4 e^{-\alpha\pi n^2 y} - \frac{2}{\alpha^3}\pi y\sum_{n=1}^{+\infty} n^4 e^{-\frac{1}{\alpha}\pi n^2 y} \\ &-6\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(n^2-\frac{1}{\alpha^2}m^2)e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\cos(2\pi mnx) \\ &+4\pi y\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(n^2-\frac{1}{\alpha^2}m^2)(\alpha n^2+\frac{1}{\alpha}m^2)e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\cos(2\pi mnx), \end{aligned} \tag{4.12}$$

and

$$\begin{aligned} D =& \frac{1}{2} + \sum_{n=1}^{+\infty} e^{-\alpha\pi n^2 y} + \sum_{n=1}^{+\infty} e^{-\frac{1}{\alpha}\pi n^2 y} - 2\alpha\pi y\sum_{n=1}^{+\infty} n^2 e^{-\alpha\pi n^2 y} - \frac{2}{\alpha}\pi y\sum_{n=1}^{+\infty} n^2 e^{-\frac{1}{\alpha}\pi n^2 y} \\ &+2\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\cos(2\pi mnx) \\ &-4\pi y\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(\alpha n^2+\frac{1}{\alpha}m^2)e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\cos(2\pi mnx). \end{aligned} \tag{4.13}$$

A simple monotonicity analysis, with an appropriate estimate of each part, yields

$$
\begin{aligned}
D \geq & \frac{1}{2}+\sum_{n=1}^{+\infty}(1-\frac{2}{\alpha}\pi n^2 y)e^{-\frac{1}{\alpha}\pi n^2 y}-2\alpha\pi y\sum_{n=1}^{+\infty}n^2 e^{-\alpha\pi n^2 y}\\
& -2\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}-4\pi y\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(\alpha n^2+\frac{1}{\alpha}m^2)e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\\
\geq & \frac{1}{2}+\sum_{n=1}^{+\infty}(1-\pi n^2)e^{-\frac{1}{2}\pi n^2}-9\pi\sum_{n=1}^{+\infty}n^2 e^{-\frac{9}{2}\pi n^2}\\
& -2\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}e^{-\pi(\frac{9}{2}n^2+\frac{1}{2}m^2)}-4\pi\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(\frac{9}{2}n^2+\frac{1}{2}m^2)e^{-\pi(\frac{9}{2}n^2+\frac{1}{2}m^2)}\\
\geq & 0.0331,
\end{aligned}
\tag{4.14}
$$

and

$$
\begin{aligned}
N \geq & \frac{1}{\alpha^2}(3-2\pi\frac{y}{\alpha})e^{-\pi\frac{y}{\alpha}}+\frac{1}{\alpha^2}\sum_{n=2}^{+\infty}(3-2\pi\frac{y}{\alpha}n^2)n^2 e^{-\frac{y}{\alpha}\pi n^2}-3\sum_{n=1}^{+\infty}n^2 e^{-\alpha\pi n^2 y}\\
& -6\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(n^2+\frac{1}{\alpha^2}m^2)e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\\
& -4\pi y\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(n^2+\frac{1}{\alpha^2}m^2)(\alpha n^2+\frac{1}{\alpha}m^2)e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\\
\geq & \frac{1}{9}(3-5)e^{-\pi\frac{5}{2\pi}}+\frac{1}{9}\sum_{n=2}^{+\infty}(3-2\pi\frac{1}{2}n^2)n^2 e^{-\frac{1}{2}\pi n^2}-3\sum_{n=1}^{+\infty}n^2 e^{-\frac{9}{2}\pi n^2}\\
& -6\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(n^2+\frac{1}{9}m^2)e^{-\pi(\frac{9}{2}n^2+\frac{1}{2}m^2)}\\
& -4\pi\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(n^2+\frac{1}{9}m^2)(\frac{9}{2}n^2+\frac{1}{2}m^2)e^{-\pi(\frac{9}{2}n^2+\frac{1}{2}m^2)}\\
\geq & -0.0263.
\end{aligned}
\tag{4.15}
$$

Together with (4.11), (4.14) and (4.15), we have

$$
\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z,y}+\frac{1}{1-\frac{1}{\alpha^2}}\frac{1}{2\alpha}\geq -0.7946\pi y. \tag{4.16}
$$

Therefore, conbining (4.10) and (4.16), we have $\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z}>0$.

Case 2. $1\leq\alpha<3$.

It is not difficult to see that $\mathcal{F}_{\alpha,z,x} = \mathcal{F}_{\alpha,z,y} = 0$ for $\alpha = 1$. So the term $\frac{1}{1-\frac{1}{\alpha^2}}$ becomes very important to our estimate. By calculation, we can obtain the same expression as in the above case, but this time we have to estimate the numerator and denominator separately, especially the numerator, in more detail,

$$\begin{aligned}
&\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z,x} - \frac{1}{1-\frac{1}{\alpha^2}}\frac{1}{2\alpha} \\
&= \pi y \cdot \frac{\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn(n^2 - \frac{1}{\alpha^2}m^2)e^{-\pi y(\alpha n^2 + \frac{1}{\alpha}m^2)}\sin(2\pi mnx)}{\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mne^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\sin(2\pi mnx)}\frac{1}{1-\frac{1}{\alpha^2}} \\
&= \pi y \cdot \left(1 + \frac{1}{1-\frac{1}{\alpha^2}}\frac{\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn((n^2-1) - \frac{1}{\alpha^2}(m^2-1))e^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}}{\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mne^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}}\right).
\end{aligned} \tag{4.17}$$

The part of the denominator is relatively simple. By using $\left|\frac{\sin(2\pi mnx)}{\sin(2\pi x)}\right| \leq mn$, we have

$$\begin{aligned}
&\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mne^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\frac{\sin(2\pi mnx)}{\sin(2\pi x)} \\
&\geq 1 - \sum_{mn\geq 2} mne^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\left|\frac{\sin(2\pi mnx)}{\sin(2\pi x)}\right| \\
&\geq 1 - \sum_{mn\geq 2} m^2n^2e^{-\pi(\frac{3}{2}(n^2-1)+\frac{1}{2}(m^2-1))} \\
&\geq 0.9640.
\end{aligned} \tag{4.18}$$

We carefully estimate the numerator and divide it into two parts of which the smaller part can be roughly estimated. First, we have the following two estimates.

$$12 \cdot \frac{e^{-3\alpha\pi y} - \frac{1}{\alpha^2}e^{-\frac{3}{\alpha}\pi y}}{1-\frac{1}{\alpha^2}} \geq 12 \cdot \frac{e^{-3\alpha\pi y} - \frac{1}{\alpha^2}e^{-\frac{3}{\alpha}\pi y}}{1-\frac{1}{\alpha^2}}\Bigg|_{y=1.5,\alpha=3} \geq -0.01348, \tag{4.19}$$

and

$$\left|\frac{e^{-\alpha\pi y} - e^{-\frac{1}{\alpha}\pi y}}{1-\frac{1}{\alpha^2}}\right| \leq 0.234. \tag{4.20}$$

Then we have

$$\frac{\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn((n^2-1)-\frac{1}{\alpha^2}(m^2-1))e^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}}{1-\frac{1}{\alpha^2}}$$

$$\begin{aligned}
=&6\cdot\frac{e^{-3\alpha\pi y}-\frac{1}{\alpha^2}e^{-\frac{3}{\alpha}\pi y}}{1-\frac{1}{\alpha^2}}\frac{\sin(4\pi x)}{\sin(2\pi x)}\\
&+\sum_{mn\geq 3} mn(m^2-1)e^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}\\
&-\sum_{mn\geq 3} mn(m^2-1)\frac{-e^{\pi y(\alpha(m^2-1)+\frac{1}{\alpha}(n^2-1))}-e^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}}{1-\frac{1}{\alpha^2}}\frac{\sin(2\pi mnx)}{\sin(2\pi x)} \qquad (4.21)\\
\geq&12\cdot\frac{e^{-3\alpha\pi y}-\frac{1}{\alpha^2}e^{-\frac{3}{\alpha}\pi y}}{1-\frac{1}{\alpha^2}}\\
&-\sum_{m\cdot n\geq 3} m^2n^2(m^2-1)e^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}\\
&-\sum_{mn\geq 3} m^2n^2(m^2-1)\left|\frac{-e^{\pi y(\alpha(m^2-1)+\frac{1}{\alpha}(n^2-1))}-e^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1))}}{1-\frac{1}{\alpha^2}}\right|.
\end{aligned}$$

By using $x^n-y^n=(x-y)(x^{n-1}+x^{n-2}y+\cdots+y^{n-1})$, we have

$$\begin{aligned}
&\frac{\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn((n^2-1)-\frac{1}{\alpha^2}(m^2-1))e^{-\pi y(\alpha(n^2-1)+\frac{1}{\alpha}(m^2-1)}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}}{1-\frac{1}{\alpha^2}}\\
&\geq -0.013475-5.4684\times 10^{-4}.
\end{aligned} \qquad (4.22)$$

(4.22) together with (4.17), (4.18), yields

$$\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z,x}-\frac{1}{1-\frac{1}{\alpha^2}}\frac{1}{2\alpha}\geq \pi y\cdot(1-0.015)=0.985\pi y. \qquad (4.23)$$

Next, we begin to estimate $\mathcal{F}_{\alpha,z,y}$. Dividing the numerator and denominator into two pieces each according to the major and minor components. By direct calculation, we have

$$\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z,y}+\frac{1}{1-\frac{1}{\alpha^2}}\frac{1}{2\alpha}=\pi y\cdot\frac{N_1+N_2}{D_1+D_2}, \qquad (4.24)$$

where

$$N_1=-3\sum_{n=1}^{2} n^2\frac{e^{-\alpha\pi n^2 y}-\frac{1}{\alpha^2}e^{-\frac{1}{\alpha}\pi n^2 y}}{1-\frac{1}{\alpha^2}}+2\alpha\pi y\sum_{n=1}^{2} n^4\frac{e^{-\alpha\pi n^2 y}-\frac{1}{\alpha^4}e^{-\frac{1}{\alpha}\pi n^2 y}}{1-\frac{1}{\alpha^2}}, \qquad (4.25)$$

$$
\begin{aligned}
N_2 =& -3\sum_{n=3}^{+\infty} n^2 \frac{e^{-\alpha\pi n^2 y} - \frac{1}{\alpha^2} e^{-\frac{1}{\alpha}\pi n^2 y}}{1-\frac{1}{\alpha^2}} + 2\alpha\pi y \sum_{n=3}^{+\infty} n^4 \frac{e^{-\alpha\pi n^2 y} - \frac{1}{\alpha^4} e^{-\frac{1}{\alpha}\pi n^2 y}}{1-\frac{1}{\alpha^2}} \\
& - 6\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^2 e^{-\pi y(\alpha n^2 + \frac{1}{\alpha} m^2)} \cos(2\pi mnx) \\
& - 6\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^2 \frac{e^{-\pi y(\alpha m^2 + \frac{1}{\alpha} n^2)} - e^{-\pi y(\alpha n^2 + \frac{1}{\alpha} m^2)}}{1-\frac{1}{\alpha^2}} \cos(2\pi mnx) \\
& + 4\alpha(1+\frac{1}{\alpha^2})\pi y \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^4 e^{-\pi y(\alpha n^2 + \frac{1}{\alpha} m^2)} \cos(2\pi mnx) \\
& + 4\alpha\pi y \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^4 \frac{e^{-\pi y(\alpha m^2 + \frac{1}{\alpha} n^2)} - e^{-\pi y(\alpha n^2 + \frac{1}{\alpha} m^2)}}{1-\frac{1}{\alpha^2}} \cos(2\pi mnx),
\end{aligned} \tag{4.26}
$$

and

$$
D_1 = \frac{1}{2} + \sum_{n=1}^{2} e^{-\alpha\pi n^2 y} + \sum_{n=1}^{2} e^{-\frac{1}{\alpha}\pi n^2 y} - 2\alpha\pi y \sum_{n=1}^{2} n^2 e^{-\alpha\pi n^2 y} - \frac{2}{\alpha}\pi y \sum_{n=1}^{2} n^2 e^{-\frac{1}{\alpha}\pi n^2 y}. \tag{4.27}
$$

$$
\begin{aligned}
D_2 =& \sum_{n=3}^{+\infty} e^{-\alpha\pi n^2 y} + \sum_{n=3}^{+\infty} e^{-\frac{1}{\alpha}\pi n^2 y} - 2\alpha\pi y \sum_{n=3}^{+\infty} n^2 e^{-\alpha\pi n^2 y} - \frac{2}{\alpha}\pi y \sum_{n=3}^{+\infty} n^2 e^{-\frac{1}{\alpha}\pi n^2 y} \\
& + 2\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} e^{-\pi y(\alpha n^2 + \frac{1}{\alpha} m^2)} \cos(2\pi mnx) \\
& - 4\pi y \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} (\alpha n^2 + \frac{1}{\alpha} m^2) e^{-\pi y(\alpha n^2 + \frac{1}{\alpha} m^2)} \cos(2\pi mnx).
\end{aligned} \tag{4.28}
$$

By direct calculation, we obtain

$$
\begin{aligned}
&\frac{N_1}{D_1} \\
=& \frac{-3\sum_{n=1}^{2} n^2 \frac{e^{-\alpha\pi n^2 y} - \frac{1}{\alpha^2} e^{-\frac{1}{\alpha}\pi n^2 y}}{1-\frac{1}{\alpha^2}} + 2\alpha\pi y \sum_{n=1}^{2} n^4 \frac{e^{-\alpha\pi n^2 y} - \frac{1}{\alpha^4} e^{-\frac{1}{\alpha}\pi n^2 y}}{1-\frac{1}{\alpha^2}}}{\frac{1}{2} + \sum_{n=1}^{2} e^{-\alpha\pi n^2 y} + \sum_{n=1}^{2} e^{-\frac{1}{\alpha}\pi n^2 y} - 2\alpha\pi y \sum_{n=1}^{2} n^2 e^{-\alpha\pi n^2 y} - \frac{2}{\alpha}\pi y \sum_{n=1}^{2} n^2 e^{-\frac{1}{\alpha}\pi n^2 y}} \\
\geq& \left.\frac{-3\sum_{n=1}^{2} n^2 \frac{e^{-\alpha\pi n^2 y} - \frac{1}{\alpha^2} e^{-\frac{1}{\alpha}\pi n^2 y}}{1-\frac{1}{\alpha^2}} + 2\alpha\pi y \sum_{n=1}^{2} n^4 \frac{e^{-\alpha\pi n^2 y} - \frac{1}{\alpha^4} e^{-\frac{1}{\alpha}\pi n^2 y}}{1-\frac{1}{\alpha^2}}}{\frac{1}{2} + \sum_{n=1}^{2} e^{-\alpha\pi n^2 y} + \sum_{n=1}^{2} e^{-\frac{1}{\alpha}\pi n^2 y} - 2\alpha\pi y \sum_{n=1}^{2} n^2 e^{-\alpha\pi n^2 y} - \frac{2}{\alpha}\pi y \sum_{n=1}^{2} n^2 e^{-\frac{1}{\alpha}\pi n^2 y}}\right|_{y=1.5,\alpha=3} \\
\geq& -0.3794.
\end{aligned} \tag{4.29}
$$

We estimate the remaining terms as follows

$$
\begin{aligned}
D_2 \geq & -2\alpha\pi y \sum_{n=3}^{+\infty} n^2 e^{-\alpha\pi n^2 y} - \frac{2}{\alpha}\pi y \sum_{n=3}^{+\infty} n^2 e^{-\frac{1}{\alpha}\pi n^2 y} \\
& -2 \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} e^{-\pi y(\alpha n^2 + \frac{1}{\alpha}m^2)} \\
& -4\pi y \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} (\alpha n^2 + \frac{1}{\alpha}m^2) e^{-\pi y(\alpha n^2 + \frac{1}{\alpha}m^2)}.
\end{aligned}
\tag{4.30}
$$

Furthermore, observe that

$$
\left| \frac{e^{-\alpha\pi y} - e^{-\frac{1}{\alpha}\pi y}}{1 - \frac{1}{\alpha^2}} \right| \leq 0.234. \tag{4.31}
$$

We have

$$
\begin{aligned}
N_2 \geq & 2\alpha\pi y \sum_{n=3}^{+\infty} n^4 \frac{e^{-\alpha\pi n^2 y} - \frac{1}{\alpha^4} e^{-\frac{1}{\alpha}\pi n^2 y}}{1 - \frac{1}{\alpha^2}} \\
& -6 \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^2 e^{-\pi y(\alpha n^2 + \frac{1}{\alpha}m^2)} \\
& -6 \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^2 \left| \frac{e^{-\pi y(\alpha m^2 + \frac{1}{\alpha}n^2)} - e^{-\pi y(\alpha n^2 + \frac{1}{\alpha}m^2)}}{1 - \frac{1}{\alpha^2}} \right| \\
& -4(\alpha + \frac{1}{\alpha})\pi y \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^4 e^{-\pi y(\alpha n^2 + \frac{1}{\alpha}m^2)} \\
& -4\alpha\pi y \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^4 \left| \frac{e^{-\pi y(\alpha m^2 + \frac{1}{\alpha}n^2)} - e^{-\pi y(\alpha n^2 + \frac{1}{\alpha}m^2)}}{1 - \frac{1}{\alpha^2}} \right|.
\end{aligned}
\tag{4.32}
$$

By the monotonicity of D_1, D_2, N_1, N_2 with $\alpha y \geq 1.5$ and $\frac{y}{\alpha} \geq 0.5$, we can get

$$
\left| \frac{N_2}{N_1} \right| \leq 0.0424 \quad \text{and} \quad \left| \frac{D_2}{D_1} \right| \leq 0.0092.
$$

This together with (4.24) and (4.29) shows

$$
\frac{1}{1 - \frac{1}{\alpha^2}} \mathcal{F}_{\alpha,z,y} + \frac{1}{1 - \frac{1}{\alpha^2}} \frac{1}{2\alpha} \geq -\pi y \cdot \frac{0.3794 \cdot (1 + 0.0424)}{1 - 0.0092} \geq -0.3992\pi y. \tag{4.33}
$$

Therefore, (4.23) and (4.33) yield

$$
\frac{1}{1 - \frac{1}{\alpha^2}} \mathcal{F}_{\alpha,z} > 0. \tag{4.34}
$$

Case 3. $\frac{y}{\alpha} < \frac{1}{2}$.

In this case, the constraint $\frac{\alpha}{y} > 2$ is designed to handle the case where α is relatively large. We make use of a suitable expression (1.2) to ensure that when α is larger, the higher-order power terms that follow are smaller. Recall that

$$\theta(\alpha; z) = \sum_{(m,n)\in\mathbb{Z}^2} e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}.$$

By direct calculation, we have

$$\begin{aligned}
&\mathcal{F}_{\alpha,z,y} - \frac{1}{\alpha}\\
=& -\frac{\pi\sum_{(m,n)\in\mathbb{Z}^2}(m^2y - \frac{(mx+n)^2}{y})(m^2y + \frac{(mx+n)^2}{y})e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}}{\sum_{(m,n)\in\mathbb{Z}^2}(m^2y - \frac{(mx+n)^2}{y})e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}}\\
=& -\frac{\pi}{y}\frac{2+\sum_{(m,n)\in\mathbb{Z}^2\backslash\{(0,\pm1)\}}(m^2y^2-(mx+n)^2)(m^2y^2+(mx+n)^2)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2-1}{y})}}{2+\sum_{(m,n)\in\mathbb{Z}^2\backslash\{(0,\pm1)\}}(m^2y^2-(mx+n)^2)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2-1}{y})}}.
\end{aligned} \tag{4.35}$$

Notice that

$$\begin{aligned}
&\sum_{(m,n)\in\mathbb{Z}^2\backslash\{(0,\pm1)\}}(m^2y^2-(mx+n)^2)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2-1}{y})}\\
\geq& -2\sum_{n=2}^{+\infty}n^2e^{-\pi\alpha(\frac{n^2-1}{y})} - 2\sum_{m=1}^{+\infty}(m^2x^2)e^{-\pi\alpha(m^2y+\frac{m^2x^2-1}{y})}\\
&-4\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(m^2x^2+n^2)e^{-\pi\alpha(m^2y+\frac{m^2x^2+n^2-1}{y})}\cosh(2\pi mn\frac{\alpha}{y}x)\\
&+4\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}(2mnx)e^{-\pi\alpha(m^2y+\frac{m^2x^2+n^2-1}{y})}\sinh(2\pi mn\frac{\alpha}{y}x)\\
\geq& -2\sum_{n=2}^{+\infty}n^2e^{-\pi\alpha(\frac{n^2-1}{y})} - 2\sum_{m=1}^{+\infty}\frac{y}{\alpha\pi}e^{-\pi\alpha(m^2y-\frac{1}{y})-1}\\
&-4\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}n^2e^{-\pi\alpha(m^2y+\frac{n^2-1}{y})}\cosh(\pi mn\frac{\alpha}{y})\\
\geq& -9\times10^{-4},
\end{aligned} \tag{4.36}$$

and

$$\begin{aligned}&\sum_{(m,n)\in\mathbb{Z}^2\setminus\{(0,\pm1)\}}(m^2y^2-(mx+n)^2)(m^2y^2+(mx+n)^2)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2-1}{y})}\\&\leq 2\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty}m^4y^4e^{-\pi\alpha m^2y}e^{-\pi\alpha\frac{n^2-1}{y}}\leq 0.004.\end{aligned}\tag{4.37}$$

We have

$$\mathcal{F}_{\alpha,z,y}-\frac{1}{\alpha}\geq-\frac{\pi}{y}\frac{2+0.004}{2-9\times10^{-4}}\geq-1.0025\cdot\frac{\pi}{y}.\tag{4.38}$$

On the other hand, we have

$$\begin{aligned}&\mathcal{F}_{\alpha,z,x}+\frac{1}{\alpha}\\&=\frac{\pi\sum_{(m,n)\in\mathbb{Z}^2}m(mx+n)(m^2y+\frac{(mx+n)^2}{y})e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}}{\sum_{(m,n)\in\mathbb{Z}^2}m(mx+n)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}}\\&=\pi y+\frac{\pi\sum_{(m,n)\in\mathbb{Z}^2}m(mx+n)((m^2-1)y+\frac{(mx+n)^2}{y})e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}}{\sum_{(m,n)\in\mathbb{Z}^2}m(mx+n)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}}.\end{aligned}\tag{4.39}$$

We find that the denominator tends to 0 as x tends to 0 and 0.5, which causes a lot of difficulties in our estimate. The previous expression (3.2) can be solved by dividing by $\sin(2\pi x)$, but this one doesn't seem to have good properties, so we need to consider it in two parts and analyze the parts closer to 0 and closer to 0.5 separately.

a. $x\in[0,0.3]$.

Notice that as x tends to 0 the function also tends to 0, which is very bad for our estimate. So we have to transform the function appropriately, dividing the numerator and denominator by x to remove this effect. After that, we can achieve our goal by roughly estimating the higher-order power terms. We have

$$
\begin{aligned}
&\frac{1}{2x}\sum_{(m,n)\in\mathbb{Z}^2} m(mx+n)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}\\
&=\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty} m^2e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)}\\
&\quad-\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mne^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x} \qquad (4.40)\\
&\geq \sum_{n=-1}^{1} e^{-\pi\frac{\alpha}{y}(y^2+x^2+n^2+2nx)}-e^{-\pi\frac{\alpha}{y}(y^2+x^2+1-2x)}\frac{1-e^{-4\pi\frac{\alpha}{y}x}}{x}\\
&\quad-\sum_{mn\geq 2} mne^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}.
\end{aligned}
$$

For ease of writing, we introduce the following notation

$$
\begin{aligned}
D_1 &:= \sum_{n=-1}^{1} e^{-\pi\frac{\alpha}{y}(y^2+x^2+n^2+2nx)}-e^{-\pi\frac{\alpha}{y}(y^2+x^2+1-2x)}\frac{1-e^{-4\pi\frac{\alpha}{y}x}}{x},\\
D_2 &:= -\sum_{mn\geq 2} mne^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}.
\end{aligned} \qquad (4.41)
$$

Notice that

$$
\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\leq 4\pi\frac{\alpha}{y}mn,
$$

and

$$
m^2x^2+n^2-2mnx\geq n^2-mn.
$$

By direct calculation, it's easy to get

$$
\left|\frac{D_2}{D_1}\right|\leq 5\times 10^{-4}. \qquad (4.42)
$$

Using the same method to the numerator, we have

$$\frac{1}{2x}\sum_{(m,n)\in\mathbb{Z}^2} m(mx+n)((m^2-1)y^2+(mx+n)^2)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}$$

$$\begin{aligned}
&=\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty} m^2((m^2-1)y^2+m^2x^2+n^2+2mnx)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)}\\
&\quad-\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn((m^2-1)y^2+m^2x^2+n^2-2mnx)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\\
&\quad+\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} 4m^2n^2e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)}\\
&\geq\sum_{n=-1}^{1}(x^2+n^2+2nx)e^{-\pi\frac{\alpha}{y}(y^2+x^2+n^2+2nx)}-(x^2+1-2x)e^{-\pi\frac{\alpha}{y}(y^2+x^2+1-2x)}\frac{1-e^{-4\pi\frac{\alpha}{y}x}}{x}\\
&\quad+4e^{-\pi\frac{\alpha}{y}(y^2+x^2+1+2x)}\\
&\quad-\sum_{mn\geq 2} mn((m^2-1)y^2+m^2x^2+n^2-2mnx)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}.
\end{aligned} \tag{4.43}$$

Denote

$$\begin{aligned}
N_1 &:= \sum_{n=-1}^{1}(x^2+n^2+2nx)e^{-\pi\frac{\alpha}{y}(y^2+x^2+n^2+2nx)}-(x^2+1-2x)e^{-\pi\frac{\alpha}{y}(y^2+x^2+1-2x)}\frac{1-e^{-4\pi\frac{\alpha}{y}x}}{x}\\
&\quad+4e^{-\pi\frac{\alpha}{y}(y^2+x^2+1+2x)},\\
N_2 &:= -\sum_{mn\geq 2} mn((m^2-1)y^2+m^2x^2+n^2-2mnx)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}.
\end{aligned} \tag{4.44}$$

It is easy to get

$$\left|\frac{N_2}{N_1}\right| \leq 5\times 10^{-4}. \tag{4.45}$$

Since U_1 and N_1 are both simple functions, it's easy to see the monotonicity and estimate upper and lower bounds. We have

$$\frac{N_1}{D_1}=\frac{x^3+(x-1)^3e^{-\pi\alpha\frac{1-2x}{y}}+(x+1)^3e^{-\pi\alpha\frac{1+2x}{y}}}{x+(x-1)e^{-\pi\alpha\frac{1-2x}{y}}+(x+1)e^{-\pi\alpha\frac{1+2x}{y}}}\geq -0.0373. \tag{4.46}$$

Combining (4.39), (4.42), (4.45) and (4.46), we get

$$\mathcal{F}_{\alpha,z,x}+\frac{1}{\alpha}\geq\pi y+\frac{\pi}{y}\frac{N_1+N_2}{D_1+D_2}\geq\pi y+\frac{\pi}{y}\frac{N_1}{D_1}\frac{1+\left|\frac{N_2}{N_1}\right|}{1-\left|\frac{D_2}{D_1}\right|}\geq 0.98\pi y. \tag{4.47}$$

b. $x\in[0.3,0.5]$.

This situation is similar to the previous one. We need to eliminate the effect of the function tending to 0 as x tends to 0.5, which can be accomplished by dividing the numerator and denominator by $1-2x$.

$$\begin{aligned}
&\frac{1}{2(1-2x)}\sum_{(m,n)\in\mathbb{Z}^2}m(mx+n)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}\\
=&\frac{1}{1-2x}\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty}m(mx+n)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}\\
=&\sum_{m\equiv 1 \bmod 2}\sum_{n=0}^{+\infty}m(n+\frac{1}{2}+\frac{m}{2}-mx)e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+\frac{1}{2}+n)^2)}\frac{1-e^{-\pi\frac{\alpha}{y}m(2n+1)(1-2x)}}{1-2x}\\
&+\sum_{m\equiv 0 \bmod 2}\sum_{n=1}^{+\infty}m(n+\frac{m}{2}-mx)e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+n)^2)}\frac{1-e^{-\pi\frac{\alpha}{y}2mn(1-2x)}}{1-2x}\\
&-\sum_{m\equiv 1 \bmod 2}\sum_{n=0}^{+\infty}m^2e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+\frac{1}{2}+n)^2)}\\
&-\frac{1}{2}\sum_{m\equiv 0 \bmod 2}m^2e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2(x-\frac{1}{2})^2)}\\
&-\sum_{m\equiv 0 \bmod 2}\sum_{n=1}^{+\infty}m^2e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+n)^2)}\\
\geq&\sum_{n=0}^{1}(n+1-x)e^{-\pi\frac{\alpha}{y}(y^2+(x+n)^2)}\frac{1-e^{-\pi\frac{\alpha}{y}(2n+1)(1-2x)}}{1-2x}-\sum_{n=0}^{1}e^{-\pi\frac{\alpha}{y}(y^2+(x+n)^2)}\\
&-\sum_{n=2}^{+\infty}e^{-\pi\frac{\alpha}{y}(y^2+(x+n)^2)}-\frac{1}{2}\sum_{m=2}^{+\infty}m^2e^{-\pi\frac{\alpha}{y}m^2y^2}\sum_{n=-\infty}^{+\infty}e^{-\pi\frac{\alpha}{y}n^2}.
\end{aligned} \tag{4.48}$$

Using the same method to the numerator, we have

$$
\begin{aligned}
&\frac{1}{2(1-2x)}\sum_{(m,n)\in\mathbb{Z}^2} m(mx+n)\big((m^2-1)y^2+(mx+n)^2\big)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}\\
=&\sum_{m\equiv 1 \bmod 2}\sum_{n=0}^{+\infty} m(n+\frac{1}{2}+\frac{m}{2}-mx)\big((m^2-1)y^2+(mx-\frac{m}{2}+\frac{1}{2}+n)^2\big)e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+\frac{1}{2}+n)^2)}\\
&\cdot\frac{1-e^{-\pi\frac{\alpha}{y}m(2n+1)(1-2x)}}{1-2x}\\
&-\sum_{m\equiv 1 \bmod 2}\sum_{n=0}^{+\infty} m^2(2n+1)(n+\frac{1}{2}+\frac{m}{2}-mx)e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}-\frac{1}{2}-n)^2)}\\
&+\sum_{m\equiv 0 \bmod 2}\sum_{n=1}^{+\infty} m(n+\frac{m}{2}-mx)\big((m^2-1)y^2+(mx-\frac{m}{2}+n)^2\big)e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+n)^2)}\\
&\cdot\frac{1-e^{-\pi\frac{\alpha}{y}2mn(1-2x)}}{1-2x}\\
&-\sum_{m\equiv 0 \bmod 2}\sum_{n=1}^{+\infty} 2m^2n(n+\frac{m}{2}-mx)e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}-n)^2)}\\
&-\sum_{m\equiv 1 \bmod 2}\sum_{n=0}^{+\infty} m^2\big((m^2-1)y^2+(mx-\frac{m}{2}+\frac{1}{2}+n)^2\big)e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+\frac{1}{2}+n)^2)}\\
&-\frac{1}{2}\sum_{m\equiv 0 \bmod 2} m^2((m^2-1)y^2+m^2(x-\frac{1}{2})^2)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2(x-\frac{1}{2})^2)}\\
&-\sum_{m\equiv 0 \bmod 2}\sum_{n=1}^{+\infty} m^2\big((m^2-1)y^2+(mx-\frac{m}{2}+n)^2\big)e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+n)^2)}\\
\geq&(1-x)x^2e^{-\pi\frac{\alpha}{y}(y^2+x^2)}\frac{1-e^{-\pi\frac{\alpha}{y}(1-2x)}}{1-2x}-(1-x)e^{-\pi\frac{\alpha}{y}(y^2+(x-1)^2)}-x^2e^{-\pi\frac{\alpha}{y}(y^2+x^2)}\\
&-\sum_{n=1}^{+\infty}(2n+1)(n+1-x)e^{-\pi\frac{\alpha}{y}(m^2y^2+(x+n-1)^2)}-\sum_{n=1}^{+\infty}(x+n)^2e^{-\pi\frac{\alpha}{y}(y^2+(x+n)^2)}\\
&-\sum_{m=2}^{+\infty} m^2(m^2-1)y^2e^{-\pi\frac{\alpha}{y}m^2y^2}\sum_{n=-\infty}^{+\infty}(n^2+1)e^{-\pi\frac{\alpha}{y}n^2}.
\end{aligned}
\tag{4.49}
$$

Let

$$
\begin{aligned}
D_1 :=& \sum_{n=0}^{1}(n+1-x)e^{-\pi\frac{\alpha}{y}(y^2+(x+n)^2)}\frac{1-e^{-\pi\frac{\alpha}{y}(2n+1)(1-2x)}}{1-2x} - \sum_{n=0}^{1} e^{-\pi\frac{\alpha}{y}(y^2+(x+n)^2)},\\
D_2 :=& -\sum_{n=2}^{+\infty} e^{-\pi\frac{\alpha}{y}(y^2+(x+n)^2)} - \frac{1}{2}\sum_{m=2}^{+\infty} m^2 e^{-\pi\frac{\alpha}{y}m^2y^2}\sum_{n=-\infty}^{+\infty} e^{-\pi\frac{\alpha}{y}n^2},\\
N_1 :=& (1-x)x^2e^{-\pi\frac{\alpha}{y}(y^2+x^2)}\frac{1-e^{-\pi\frac{\alpha}{y}(1-2x)}}{1-2x} - (1-x)e^{-\pi\frac{\alpha}{y}(y^2+(x-1)^2)} - x^2e^{-\pi\frac{\alpha}{y}(y^2+x^2)},\\
N_2 :=& -\sum_{n=1}^{+\infty}(2n+1)(n+1-x)e^{-\pi\frac{\alpha}{y}(m^2y^2+(x+n-1)^2)} - \sum_{n=1}^{+\infty}(x+n)^2e^{-\pi\frac{\alpha}{y}(y^2+(x+n)^2)}\\
&-\sum_{m=2}^{+\infty} m^2(m^2-1)y^2e^{-\pi\frac{\alpha}{y}m^2y^2}\sum_{n=-\infty}^{+\infty}(n^2+1)e^{-\pi\frac{\alpha}{y}n^2}.
\end{aligned} \tag{4.50}
$$

It's easy to see that

$$\frac{N_1}{D_1} = \frac{x^3+(x-1)^3e^{-\pi\alpha\frac{1-2x}{y}}}{x+(x-1)e^{-\pi\alpha\frac{1-2x}{y}}} \geq -0.0032. \tag{4.51}$$

By direct calculation, we have

$$\left|\frac{N_2}{N_1}\right| \leq 5\times 10^{-4}, \quad \text{and} \left|\frac{D_2}{D_1}\right| \leq 5\times 10^{-4}. \tag{4.52}$$

Above all, we get

$$\mathcal{F}_{\alpha,z,x} + \frac{1}{\alpha} \geq \pi y + \frac{\pi}{y}\frac{N_1+N_2}{D_1+D_2} \geq \pi y + \frac{\pi}{y}\frac{N_1}{D_1}\frac{1+\left|\frac{N_2}{N_1}\right|}{1-\left|\frac{D_2}{D_1}\right|} \geq 0.98\pi y. \tag{4.53}$$

Therefore, (4.38), (4.47) and (4.53) yield

$$\mathcal{F}_{\alpha,z} > 0. \tag{4.54}$$

For now, we have finished the Lemma 4.3 □

4.2 $z \in \mathcal{D}_{\mathcal{G}} \cap \{y < 1.5\}$

Lemma 4.5. *For any $\alpha > 1$ and $z \in \{0 < x < 0.5,\, 0.6 \leq y < 1.5\}$, we have*

$$\frac{\partial}{\partial y}\mathcal{F}_{\alpha,z,x} > 0 \quad \text{and} \quad \frac{\partial}{\partial y}\mathcal{F}_{\alpha,z,x} + \frac{1}{\sqrt{3}}\frac{\partial}{\partial x}\mathcal{F}_{\alpha,z,x} > 0. \tag{4.55}$$

Remark 4.6. Notice that $\frac{\partial}{\partial x}\theta(\alpha;z) < 0$ for any $z \in \{0 \le x \le 0.5,\, y \ge 0.5\}$, (4.6) is equivalent to

$$\frac{\frac{\partial^2}{\partial\alpha\partial x}\theta(\alpha;z)}{\frac{\partial}{\partial x}\theta(\alpha;z)} - \frac{\frac{\partial^2}{\partial\alpha\partial x}\theta(\alpha;\frac{z}{|z|^2})}{\frac{\partial}{\partial x}\theta(\alpha;\frac{z}{|z|^2})} < 0. \tag{4.56}$$

Equation (4.55) leads to

$$\frac{\partial}{\partial r}\mathcal{F}_{\alpha,z,x} > 0, \tag{4.57}$$

which leads to (4.56) holding true. Indeed, by numerical calculation, we can get $\frac{\partial}{\partial x}\mathcal{F}_{\alpha,z,x} > 0$. Since $\frac{\partial}{\partial x}\mathcal{F}_{\alpha,z,x} = 0$ for $x = 0$ and $x = 0.5$, which causes difficulties in our calculations, so we retreat to the next best thing and get the result we want by proving (4.55).

Proof. Notice that when $\alpha = 1$, we have $\frac{\partial}{\partial x}\mathcal{F}_{\alpha,z,x} = \frac{\partial}{\partial y}\mathcal{F}_{\alpha,z,x} = \mathcal{F}_{\alpha,z,x} = 0$. To eliminate this effect, we need to split the proof into two parts.

Case 1. $\alpha \ge 2$.

In this situation, we must use form (1.2) to estimate the function. We still split it into two parts as before.

Case 1.1. $x \in [0, 0.3]$.

To eliminate the effect of the function tending to 0 as x tends to 0, we have

$$\mathcal{F}_{\alpha,z,x} = -\frac{1}{\alpha} - \frac{\partial}{\partial\alpha}\log g, \tag{4.58}$$

where g can be written as follows

$$\begin{aligned} g :=& \frac{1}{2x}\sum_{(m,n)\in\mathbb{Z}^2} m(mx+n)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})} \\ =& \frac{1}{x}\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty} m(mx+n)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})} \\ =& \sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty} m^2 e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)} \\ &- \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mne^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}. \end{aligned} \tag{4.59}$$

It is easy to see that

$$\frac{\partial}{\partial y}\mathcal{F}_{\alpha,z,x} = \frac{\frac{\partial}{\partial y}g\cdot\frac{\partial}{\partial\alpha}g - \frac{\partial^2}{\partial\alpha\partial y}g\cdot g}{g^2}, \tag{4.60}$$

and

$$\frac{\partial}{\partial x}\mathcal{F}_{\alpha,z,x} = \frac{\frac{\partial}{\partial x}g \cdot \frac{\partial}{\partial \alpha}g - \frac{\partial^2}{\partial \alpha \partial x}g \cdot g}{g^2}. \tag{4.61}$$

By direct calculation, we have

$$\begin{aligned}
&-\frac{y}{\pi}\frac{\partial g}{\partial \alpha} \\
=&\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty} m^2(m^2y^2+m^2x^2+n^2+2mnx)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)} \\
&+\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} 4m^2n^2e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)} \\
&-\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn(m^2y^2+m^2x^2+n^2-2mnx)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x},
\end{aligned} \tag{4.62}$$

and

$$\begin{aligned}
&-\frac{1}{\pi\alpha}\frac{\partial g}{\partial y} \\
=&\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty} 2m^4e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)} \\
&+\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn(m^2y^2+m^2x^2+n^2-2mnx)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\cdot\frac{1}{y^2} \\
&-\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty} m^2(m^2y^2+m^2x^2+n^2+2mnx)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)}\cdot\frac{1}{y^2} \\
&-\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} 2m^3ne^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x} \\
&-\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} 4m^2n^2e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)}\cdot\frac{1}{y^2},
\end{aligned} \tag{4.63}$$

and

$$
\begin{aligned}
&\frac{y}{\pi^2\alpha}(\frac{\partial^2 g}{\partial y\partial\alpha}-\frac{1}{\alpha}\frac{\partial g}{\partial y})\\
=&\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty}2m^4(m^2y^2+m^2x^2+n^2+2mnx)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)}\\
&+\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}mn(m^2y^2+m^2x^2+n^2-2mnx)^2e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\cdot\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\cdot\frac{1}{y^2}\\
&+\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}8m^4n^2e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)}\\
&-\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty}m^2(m^2y^2+m^2x^2+n^2+2mnx)^2e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)}\cdot\frac{1}{y^2}\\
&-\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}2m^3n(m^2y^2+m^2x^2+n^2-2mnx)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\\
&-\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}8m^2n^2(m^2y^2+m^2x^2+n^2)e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2x^2+n^2+2mnx)}\cdot\frac{1}{y^2}.
\end{aligned}
\tag{4.64}
$$

Similarly, we get

$$
\begin{aligned}
&-\frac{y}{\pi\alpha}\frac{\partial}{\partial x}g\\
=&\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty}m^2(2m^2x+2mn)e^{-\pi\frac{\alpha}{y}(m^2y+m^2x+n^2+2mnx)}\\
&-\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}mn(2m^2x-2mn)e^{-\pi\frac{\alpha}{y}(m^2y+m^2x+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\\
&+\frac{y}{\pi\alpha}\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}mne^{-\pi\frac{\alpha}{y}(m^2y+m^2x+n^2-2mnx)}\left(\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\right)'_x,
\end{aligned}
\tag{4.65}
$$

and

$$
\begin{aligned}
&\frac{y^2}{\pi^2\alpha}(\frac{\partial^2}{\partial\alpha\partial x}g-\frac{1}{\alpha}\frac{\partial}{\partial x}g)\\
=&\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty}m^2(2m^2x+2mn)(m^2y+m^2x+n^2+2mnx)e^{-\pi\frac{\alpha}{y}(m^2y+m^2x+n^2+2mnx)}\\
&-\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}m^2(2m^2x-2mn)(m^2y+m^2x+n^2-2mnx)e^{-\pi\frac{\alpha}{y}(m^2y+m^2x+n^2-2mnx)}\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\\
&+\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}4m^2n^2(2m^2x-2mn)e^{-\pi\frac{\alpha}{y}(m^2y+m^2x+n^2+2mnx)}\\
&+\frac{y^2}{\pi^2\alpha^2}\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}mne^{-\pi\frac{\alpha}{y}(m^2y+m^2x+n^2-2mnx)}\left(\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\right)'_x\\
&+\frac{y}{\pi\alpha}\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}mn(m^2y+m^2x+n^2-2mnx)e^{-\pi\frac{\alpha}{y}(m^2y+m^2x+n^2-2mnx)}\left(\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\right)'_x\\
&+\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}16m^3n^3e^{-\pi\frac{\alpha}{y}(m^2y+m^2x+n^2+2mnx)}.
\end{aligned}
\tag{4.66}
$$

Notice that

$$
\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\leq 4\pi\frac{\alpha}{y}mn \quad \text{and} \quad \left(\frac{1-e^{-4\pi\frac{\alpha}{y}mnx}}{x}\right)'_x\geq -8\pi^2\frac{\alpha^2}{y^2}m^2n^2. \tag{4.67}
$$

It can be seen that when m, n is relatively large, the items have exponential decay, so we can divide them into major and minor parts, the value of the major part is carefully calculated, and the remaining part can be roughly estimated. Indeed we only need to analyze the item satisfying $m^2+n^2\leq 2$ carefully. Let

$$
g=g_1+g_2, \tag{4.68}
$$

where

$$
g_1\coloneqq\sum_{n=-1}^{+1}e^{-\pi\frac{\alpha}{y}(y^2+x^2+n^2+2nx)}-e^{-\pi\frac{\alpha}{y}(y^2+x^2+1-2x)}\frac{1-e^{-4\pi\frac{\alpha}{y}x}}{x}, \tag{4.69}
$$

and g_2 is the remaining term. Similarly, we denote

$$
\frac{\partial}{\partial\alpha}g=g_{\alpha,1}+g_{\alpha,2} \quad \text{and} \quad \frac{\partial}{\partial y}g=g_{y,1}+g_{y,2} \quad \text{and} \quad \frac{\partial}{\partial x}g=g_{x,1}+g_{x,2}.
$$

$$
\frac{\partial^2}{\partial\alpha\partial x}g=g_{\alpha x,1}+g_{\alpha x,2} \quad \text{and} \quad \frac{\partial^2}{\partial\alpha\partial y}g=g_{\alpha y,1}+g_{\alpha y,2}.
$$

Therefore, we have

$$\frac{\partial}{\partial y}g \cdot \frac{\partial}{\partial \alpha}g - \frac{\partial^2}{\partial \alpha \partial y}g \cdot g = g_{y,1} \cdot g_{\alpha,1} - g_{\alpha y,1} \cdot g_1 + R_y, \tag{4.70}$$

and

$$\frac{\partial}{\partial x}g \cdot \frac{\partial}{\partial \alpha}g - \frac{\partial^2}{\partial \alpha \partial x}g \cdot g = g_{x,1} \cdot g_{\alpha,1} - g_{\alpha x,1} \cdot g_1 + R_x, \tag{4.71}$$

where R_y and R_x are the remaining items which are relatively small. Since g_1 is a combination of simple functions, we can compute it directly by analyzing the monotonicity,

$$-\frac{\partial^2}{\partial \alpha \partial y}\log g_1 = \frac{g_{y,1} \cdot g_{\alpha,1} - g_{\alpha y,1} \cdot g_1}{g_1^2} \geq \left.\frac{g_{y,1} \cdot g_{\alpha,1} - g_{\alpha y,1} \cdot g_1}{g_1^2}\right|_{0.3,0.6,2} \geq 0.6138\pi, \tag{4.72}$$

and

$$g_{x,1} \cdot g_{\alpha,1} - g_{\alpha x,1} \cdot g_1 \geq 0. \tag{4.73}$$

By direct calculation, we get

$$\left|\frac{g_2}{g_1}\right| \leq 5 \times 10^{-5} \quad \text{and} \quad \left|\frac{R_y}{g_1^2}\right| \leq 0.002\pi \quad \text{and} \quad \left|\frac{R_x}{g_1^2}\right| \leq 0.001\pi. \tag{4.74}$$

Therefore,

$$\frac{\partial}{\partial y}\mathcal{F}_{\alpha,z,x} \geq \left(\frac{g_{y,1} \cdot g_{\alpha,1} - g_{\alpha y,1} \cdot g_1}{g_1^2} - \left|\frac{R_y}{g_1^2}\right|\right)\frac{1}{1 + \left|\frac{g_2}{g_1}\right|} \geq 0.6\pi, \tag{4.75}$$

and

$$\frac{\partial}{\partial x}\mathcal{F}_{\alpha,z,x} \geq \left(\frac{g_{x,1} \cdot g_{\alpha,1} - g_{\alpha x,1} \cdot g_1}{g_1^2} - \left|\frac{R_x}{g_1^2}\right|\right)\frac{1}{1 - \left|\frac{g_2}{g_1}\right|} \geq -0.01\pi. \tag{4.76}$$

Case 1.2. $x \in [0.3, 0.5]$.

In this case, the method is the same as before. We replace g by h. Because the methods are similar, we omit the detailed steps and only show the main results. We have

$$\mathcal{F}_{\alpha,z,x} = -\frac{1}{\alpha} - \frac{\partial}{\partial \alpha}\log h, \tag{4.77}$$

where

$$
\begin{aligned}
h &:= \frac{1}{2(1-2x)} \sum_{(m,n)\in\mathbb{Z}^2} m(mx+n)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}\\
&= \frac{1}{1-2x}\sum_{m=1}^{+\infty}\sum_{n=-\infty}^{+\infty} m(mx+n)e^{-\pi\alpha(m^2y+\frac{(mx+n)^2}{y})}\\
&= \sum_{m\equiv 1 \bmod 2}\sum_{n=0}^{+\infty} m(n+\frac{1}{2}+\frac{m}{2}-mx)e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+\frac{1}{2}+n)^2)}\frac{1-e^{-\pi\frac{\alpha}{y}m(2n+1)(1-2x)}}{1-2x}\\
&\quad+\sum_{m\equiv 0 \bmod 2}\sum_{n=1}^{+\infty} m(n+\frac{m}{2}-mx)e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+n)^2)}\frac{1-e^{-\pi\frac{\alpha}{y}2mn(1-2x)}}{1-2x}\\
&\quad-\sum_{m\equiv 1 \bmod 2}\sum_{n=0}^{+\infty} m^2e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+\frac{1}{2}+n)^2)}\\
&\quad-\frac{1}{2}\sum_{m\equiv 0 \bmod 2}\sum_{n=0}^{+\infty} m^2e^{-\pi\frac{\alpha}{y}(m^2y^2+m^2(x-\frac{1}{2})^2)}\\
&\quad-\sum_{m\equiv 0 \bmod 2}\sum_{n=1}^{+\infty} m^2e^{-\pi\frac{\alpha}{y}(m^2y^2+(mx-\frac{m}{2}+n)^2)}.
\end{aligned}
\tag{4.78}
$$

We choose $m=1$ and $n=0$ to be the major part, that is

$$
h = h_1 + h_2, \tag{4.79}
$$

where

$$
h_1 := (1-x)x^2e^{-\pi\frac{\alpha}{y}(y^2+x^2)}\frac{1-e^{-\pi\frac{\alpha}{y}(1-2x)}}{1-2x} - (1-x)e^{-\pi\frac{\alpha}{y}(y^2+x^2)}, \tag{4.80}
$$

and h_2 is the remaining term. Similarly, we have

$$
-\frac{\partial^2}{\partial\alpha\partial y}\log h_1 = \frac{h_{y,1}\cdot h_{\alpha,1} - h_{\alpha y,1}\cdot h_1}{h_1^2} \geq \frac{h_{y,1}\cdot h_{\alpha,1} - h_{\alpha y,1}\cdot h_1}{h_1^2}\bigg|_{0.5,0.6,2} \geq 0.2282\pi, \tag{4.81}
$$

and

$$
h_{x,1}\cdot h_{\alpha,1} - h_{\alpha x,1}\cdot h_1 \geq 0. \tag{4.82}
$$

By direct calculation, we have

$$
\left|\frac{h_2}{h_1}\right| \leq 8\times 10^{-5} \quad \text{and} \quad \left|\frac{R_y}{h_1^2}\right| \leq 0.003\pi \quad \text{and} \quad \left|\frac{R_x}{h_1^2}\right| \leq 0.001\pi \tag{4.83}
$$

Therefore, we have

$$\frac{\partial}{\partial y}\mathcal{F}_{\alpha,z,x} \geq \left(\frac{h_{y,1}\cdot h_{\alpha,1} - h_{\alpha y,1}\cdot h_1}{h_1^2} - \left|\frac{R_y}{h_1^2}\right|\right)\frac{1}{1+\left|\frac{h_2}{h_1}\right|} \geq 0.2\pi, \tag{4.84}$$

and

$$\frac{\partial}{\partial x}\mathcal{F}_{\alpha,z,x} \geq \left(\frac{h_{x,1}\cdot h_{\alpha,1} - h_{\alpha x,1}\cdot h_1}{h_1^2} - \left|\frac{R_x}{h_1^2}\right|\right)\frac{1}{1-\left|\frac{h_2}{h_1}\right|} \geq -0.01\pi. \tag{4.85}$$

Case 2. $1 < \alpha \leq 2$.

In this case, we need to using form (3.2), and divide it by $1-\frac{1}{\alpha^2}$ to remove the effect of $\alpha = 1$. We write that

$$\frac{1}{1-\frac{1}{\alpha^2}}\mathcal{F}_{\alpha,z,x} = \frac{1}{1-\frac{1}{\alpha^2}}\frac{1}{2\alpha} - \frac{1}{1-\frac{1}{\alpha^2}}\frac{\partial}{\partial\alpha}\log k, \tag{4.86}$$

where

$$k := \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn e^{-\pi y(\alpha n^2 + \frac{1}{\alpha}m^2)}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}. \tag{4.87}$$

By direct calculation, it is easy to find that

$$\begin{aligned} -\frac{1}{\pi y}\frac{1}{1-\frac{1}{\alpha^2}}\frac{\partial}{\partial\alpha}k = &\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^3 n e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\frac{\sin(2\pi mnx)}{\sin(2\pi x)} \\ &+ \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^3 n \frac{e^{-\pi y(\alpha m^2+\frac{1}{\alpha}n^2)} - e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}}{1-\frac{1}{\alpha^2}}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}, \end{aligned} \tag{4.88}$$

and

$$\frac{\partial}{\partial y}k = -\pi\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn(\alpha n^2 + \frac{1}{\alpha}m^2)e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}, \tag{4.89}$$

and

$$\frac{\partial}{\partial x}k = \sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} mn e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\left(\frac{\sin(2\pi mnx)}{\sin(2\pi x)}\right)'_x, \tag{4.90}$$

and

$$\begin{aligned} &\frac{1}{\pi^2 y}\frac{1}{1-\frac{1}{\alpha^2}}\left(\frac{\partial^2}{\partial\alpha\partial y}k - \frac{1}{y}\frac{\partial}{\partial\alpha}k\right) \\ =&\,\alpha(1+\frac{1}{\alpha^2})\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^5 n e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\frac{\sin(2\pi mnx)}{\sin(2\pi x)} \\ &+ \alpha\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty} m^5 n\frac{e^{-\pi y(\alpha m^2+\frac{1}{\alpha}n^2)} - e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}}{1-\frac{1}{\alpha^2}}\frac{\sin(2\pi mnx)}{\sin(2\pi x)}, \end{aligned} \tag{4.91}$$

and

$$
\begin{aligned}
&-\frac{1}{\pi y}\frac{1}{1-\frac{1}{\alpha^2}}\frac{\partial^2}{\partial\alpha\partial x}k\\
&=\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}m^3ne^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}\left(\frac{\sin(2\pi mnx)}{\sin(2\pi x)}\right)'_x\\
&\quad+\sum_{m=1}^{+\infty}\sum_{n=1}^{+\infty}m^3n\frac{e^{-\pi y(\alpha m^2+\frac{1}{\alpha}n^2)}-e^{-\pi y(\alpha n^2+\frac{1}{\alpha}m^2)}}{1-\frac{1}{\alpha^2}}\left(\frac{\sin(2\pi mnx)}{\sin(2\pi x)}\right)'_x.
\end{aligned}
\tag{4.92}
$$

Notice that

$$\left|\left(\frac{\sin(2\pi mnx)}{\sin(2\pi x)}\right)'_x\right|\leq\pi mn. \tag{4.93}$$

We take the terms satisfying $mn\leq 3$ be the major part, that is

$$k=k_1+k_2, \tag{4.94}$$

where

$$k_1:=e^{-\pi y(\alpha+\frac{1}{\alpha})}+2(e^{-\pi y(4\alpha+\frac{1}{\alpha})}+e^{-\pi y(\alpha+\frac{4}{\alpha})})\frac{\sin(4\pi x)}{\sin(2\pi x)}+3(e^{-\pi y(9\alpha+\frac{1}{\alpha})}+e^{-\pi y(\alpha+\frac{9}{\alpha})})\frac{\sin(6\pi x)}{\sin(2\pi x)}, \tag{4.95}$$

and k_2 is the remaining term. Similarly, we have

$$-\frac{\partial^2}{\partial\alpha\partial y}\log k_1=\frac{k_{y,1}\cdot k_{\alpha,1}-k_{\alpha y,1}\cdot k_1}{k_1^2}\geq\frac{k_{y,1}\cdot k_{\alpha,1}-k_{\alpha y,1}\cdot k_1}{k_1^2}\Big|_{0.5,0.6,1}\geq 0.2791\pi, \tag{4.96}$$

and

$$k_{x,1}\cdot k_{\alpha,1}-k_{\alpha x,1}\cdot k_1\geq 0. \tag{4.97}$$

By direct calculation, we obtain

$$\left|\frac{k_2}{k_1}\right|\leq 3\times 10^{-4}\quad\text{and}\quad\left|\frac{R_y}{k_1^2}\right|\leq 0.006\pi\quad\text{and}\quad\left|\frac{R_x}{k_1^2}\right|\leq 0.004\pi. \tag{4.98}$$

Therefore, we have

$$\frac{\partial}{\partial y}\mathcal{F}_{\alpha,z,x}\geq\left(\frac{k_{y,1}\cdot k_{\alpha,1}-k_{\alpha y,1}\cdot k_1}{k_1^2}-\left|\frac{R_y}{k_1^2}\right|\right)\frac{1}{1+\left|\frac{k_2}{k_1}\right|}\geq 0.2\pi, \tag{4.99}$$

and

$$\frac{\partial}{\partial x}\mathcal{F}_{\alpha,z,x}\geq\left(\frac{k_{x,1}\cdot k_{\alpha,1}-k_{\alpha x,1}\cdot k_1}{k_1^2}-\left|\frac{R_x}{k_1^2}\right|\right)\frac{1}{1-\left|\frac{k_2}{k_1}\right|}\geq -0.01\pi. \tag{4.100}$$

Now, we have completed the proof of Lemma 4.5. □

5 Proof of Corollaries 1.2-1.3

We will use (4.5) and (4.6) several times in this section and in subsequent proofs. Without loss of generality, we may assume that (4.5) holds for any $z \in \mathcal{D}_{\mathcal{G}}$, since it is a very simple operation to replace (4.5) with (4.6), when $z \in \mathcal{D}_{\mathcal{G}} \cap \{y \le 1.5\}$.

5.1 Proof of Corollary 1.2

Lemma 5.1. *When $|\ln \alpha| \le |\ln \beta|$, $b \in (b_{\alpha,\beta}, +\infty)$, or $|\ln \alpha| > |\ln \beta|$, $b \in [b_{\alpha,\beta}, +\infty)$, the (1.4) doesn't have any minimizer.*

Proof. Note that

$$\theta(\alpha; z) = \sqrt{\frac{y}{\alpha}} \left(2\sum_{n=1}^{\infty} e^{-\alpha\pi n^2 y} + 2\sum_{n=1}^{\infty} e^{-\frac{1}{\alpha}\pi n^2 y} + 1 + 4\sum_{n=1}^{\infty}\sum_{d|n} e^{-\pi y\left(\alpha d^2 + \frac{n^2}{\alpha d^2}\right)} \cos(2\pi n x) \right). \tag{5.1}$$

When $y \to +\infty$

$$\theta(\alpha; iy) - b\theta(\beta; iy) \to \sqrt{\frac{y}{\alpha}}(1 + 2e^{-\alpha\pi y} + 2e^{-\frac{1}{\alpha}\pi y}) - b\sqrt{\frac{y}{\beta}}(1 + 2e^{-\beta\pi y} + 2e^{-\frac{1}{\beta}\pi y}). \tag{5.2}$$

When $|\ln \alpha| \le |\ln \beta|$, $b \in (b_{\alpha,\beta}, +\infty)$, or $|\ln \alpha| > |\ln \beta|$, $b \in [b_{\alpha,\beta}, +\infty)$, the above equation tends to $-\infty$, then (1.4) doesn't have any minimizer.

□

Lemma 5.2. *If $|\ln \alpha| > |\ln \beta|$, $b \in (-\infty, b_{\alpha,\beta})$, the minimizer of (1.4) only occurs on the curve $\Gamma_a \cup \Gamma_b$.*

Proof. When $\alpha > \beta \ge 1$, by Theorem 1.1, we know that the minimizer only occurs on the curve $\Gamma_a \cup \Gamma_b$. Since $\theta(\frac{1}{\alpha}; z) = \alpha\theta(\alpha; z)$, the cases $0 < \alpha < \beta \le 1$, $0 < \beta \le 1 \le \frac{1}{\beta} < \alpha$, $0 < \alpha < 1 \le \beta < \frac{1}{\alpha}$ can be easily changed to the first case. □

Lemma 5.3. *If $|\ln \alpha| \le |\ln \beta|$, $b \in (-\infty, b_{\alpha,\beta}]$, the minimizer of (1.4) is $e^{i\frac{\pi}{3}}$.*

Proof. We only need to discuss the case $1 \le \alpha < \beta$. By (4.5), we can get the minimizer only on the curve Γ_c. Moreover, in the course of the proof in the previous section we can easily obtain that $\mathcal{F}_{\alpha,z,y} < -\frac{1}{2\alpha}$, then we have

$$\frac{\partial}{\partial \alpha}\left(\ln\left(\frac{\partial}{\partial y}\theta(\alpha; z)\right)\right) = \frac{\frac{\partial^2}{\partial\alpha\partial y}\theta(\alpha; z)}{\frac{\partial}{\partial y}\theta(\alpha; z)} < -\frac{1}{2\alpha}. \tag{5.3}$$

Integrating from α to β on both sides gives

$$\frac{\frac{\partial}{\partial y}\theta(\beta; z)}{\frac{\partial}{\partial y}\theta(\alpha; z)} < \sqrt{\frac{\alpha}{\beta}}, \tag{5.4}$$

which implies for any $b \in (-\infty, b_{\alpha,\beta}]$, there exists

$$\frac{\partial}{\partial y}\left(\theta(\alpha; z) - b\theta(\beta; z)\right) > 0. \tag{5.5}$$

Therefore, the minimizer is $e^{i\frac{\pi}{3}}$. □

5.2 Proof of Corollary 1.3

Proof of Coroally 1.3. Observe that when $y \to +\infty$, $\theta(\alpha; z) \to \sqrt{\frac{y}{\alpha}}$, so if $\sum_{i=1}^{n} \frac{c_i}{\sqrt{\alpha_i}} - \sum_{j=1}^{m} \frac{d_j}{\sqrt{\beta_j}} < 0$,

$$\sum_{i=1}^{n} c_i\theta(\alpha_i; z) - \sum_{j=1}^{m} d_j\theta(\beta_j; z) \to -\infty,$$

which implies that (1.5) does not have any minimizer. By (4.5), we have

$$\frac{\frac{\partial}{\partial y}\theta(A; z)}{\frac{\partial}{\partial x}\theta(A; z)} < \frac{\frac{\partial}{\partial y}\sum_{i=1}^{n} c_i\theta(\alpha_i; z)}{\frac{\partial}{\partial x}\sum_{i=1}^{n} c_i\theta(\alpha_i; z)} < \frac{\frac{\partial}{\partial y}\theta(a; z)}{\frac{\partial}{\partial x}\theta(a; z)}, \tag{5.6}$$

and

$$\frac{\frac{\partial}{\partial y}\theta(B; z)}{\frac{\partial}{\partial x}\theta(B; z)} < \frac{\frac{\partial}{\partial y}\sum_{i=1}^{n} c_i\theta(\alpha_i; z)}{\frac{\partial}{\partial x}\sum_{i=1}^{n} c_i\theta(\alpha_i; z)} < \frac{\frac{\partial}{\partial y}\theta(b; z)}{\frac{\partial}{\partial x}\theta(b; z)}. \tag{5.7}$$

Then by Proposition 3.8 if $a \geq B$, the minimizer only occurs on $\Gamma_a \cup \Gamma_b$. If $A \leq b$, the minimizer only occurs on Γ_c. Moreover, since for any $\alpha > 1$,

$$\frac{\partial}{\partial \alpha}\log\frac{\partial}{\partial y}\theta(\alpha; z) < -\frac{1}{2\alpha}, \tag{5.8}$$

we have

$$\frac{\partial}{\partial y}\theta(\alpha_i; z) > \sqrt{\frac{b}{\alpha_i}}\frac{\partial}{\partial y}\theta(b; z), \tag{5.9}$$

and

$$\frac{\partial}{\partial y}\theta(\beta_j; z) < \sqrt{\frac{b}{\beta_j}}\frac{\partial}{\partial y}\theta(b; z). \tag{5.10}$$

Therefore, we have

$$\frac{\partial}{\partial y}\left(\sum_{i=1}^{n} c_i\theta(\alpha_i; z) - \sum_{j=1}^{m} d_j\theta(\beta_j; z)\right) \geq \left(\sum_{i=1}^{n} c_i\sqrt{\frac{b}{\alpha_i}} - \sum_{j=1}^{m} d_j\sqrt{\frac{b}{\beta_j}}\right)\frac{\partial}{\partial y}\theta(b; z) > 0. \tag{5.11}$$

In this case, the minimizer is $e^{i\frac{\pi}{3}}$. □

6 Proof of Theorems 1.5-1.11

We begin this section with an important lemma. By using the continuous version of Chebyshev's sum inequality [60], we have the following lemma.

Lemma 6.1. *For any non-negative function $g(x)$, and any non-decreasing, non-negative functions $w_1(x)$, $w_2(x)$, we have*

$$\int_a^b w_1 \cdot w_2 \cdot g \, dx \cdot \int_a^b g \, dx \geq \int_a^b w_1 \cdot g \, dx \cdot \int_a^b w_2 \cdot g \, dx. \tag{6.1}$$

Remark 6.2. Indeed, the above lemma also holds when g is non-negative and w_1, w_2 are both non-increasing or both non-decreasing.

6.1 Lennard Jones potential

In this section, we prove the results of Lennard-Jones potential. By using the Laplace transform, we have

$$\begin{aligned}\zeta(s;z) &= \frac{\pi^s}{\Gamma(s)} \int_0^\infty (\theta(\alpha;z) - 1)\alpha^{s-1} \, d\alpha \\ &= \frac{\pi^s}{\Gamma(s)} \left(\int_1^\infty (\theta(\alpha;z) - 1)(\alpha^{s-1} + \alpha^{-s}) \, d\alpha + \frac{1}{s-1} - \frac{1}{s} \right).\end{aligned} \tag{6.2}$$

It is easy to see that

$$\frac{\frac{\partial}{\partial y}\zeta(s;z)}{\frac{\partial}{\partial x}\zeta(s;z)} = \frac{\frac{\partial}{\partial y}\int_0^{+\infty} \theta(\alpha;z)\alpha^{s-1} \, d\alpha}{\frac{\partial}{\partial x}\int_0^{\infty} \theta(\alpha;z)\alpha^{s-1} \, d\alpha} = \frac{\int_1^{+\infty} \frac{\partial}{\partial y}\theta(\alpha;z)(\alpha^{s-1} + \alpha^{-s}) \, d\alpha}{\int_1^{\infty} \frac{\partial}{\partial x}\theta(\alpha;z)(\alpha^{s-1} + \alpha^{-s}) \, d\alpha}. \tag{6.3}$$

Lemma 6.3. *For any $\alpha > 1$ and $s > 1$, we have*

$$\frac{\partial^2}{\partial\alpha\partial s} \log(\alpha^{s-1} + \alpha^{-s}) > 0.$$

Proof. By direct calculation, we have

$$\alpha^2(\alpha^{s-1} + \alpha^{-s})^2 \frac{\partial^2}{\partial\alpha\partial s} \log(\alpha^{s-1} + \alpha^{-s}) = 2(2s-1)\log\alpha + \alpha^{2s-1} - \alpha^{-2s+1}. \tag{6.4}$$

It is easy to see that the above function is increasing for s and α respectively. Therefore,

$$2(2s-1)\log\alpha + \alpha^{2s-1} - \alpha^{-2s+1} \geq 2(2s-1)\log\alpha + \alpha^{2s-1} - \alpha^{-2s+1}|_{s=1,\alpha=1} = 0. \tag{6.5}$$

□

By using Lemma 6.3, we immediately obtain the following fact.

Lemma 6.4. *For any $s_1 > s_2 > 1$, the function*

$$\frac{\alpha^{s_1-1}+\alpha^{-s_1}}{\alpha^{s_2-1}+\alpha^{-s_2}} \tag{6.6}$$

is increasing for $\alpha \in (1,+\infty)$.

Based on this fact, we will prove the following lemma, which is the key to prove Theorem 1.5.

Lemma 6.5. *For any $s_1 > s_2 > 1$, we have*

$$\frac{\frac{\partial}{\partial y}\int_1^{+\infty}\theta(\alpha;z)(\alpha^{s_1-1}+\alpha^{-s_1})\,d\alpha}{\frac{\partial}{\partial x}\int_1^{\infty}\theta(\alpha;z)(\alpha^{s_1-1}+\alpha^{-s_1})\,d\alpha} < \frac{\frac{\partial}{\partial y}\int_1^{+\infty}\theta(\alpha;z)(\alpha^{s_2-1}+\alpha^{-s_2})\,d\alpha}{\frac{\partial}{\partial x}\int_1^{\infty}\theta(\alpha;z)(\alpha^{s_2-1}+\alpha^{-s_2})\,d\alpha}. \tag{6.7}$$

Proof. This is equivalent to proving

$$\begin{aligned}
&\int_1^{+\infty}\frac{\alpha^{s_1-1}+\alpha^{-s_1}}{\alpha^{s_2-1}+\alpha^{-s_2}}\cdot\frac{\frac{\partial}{\partial y}\theta(\alpha;z)}{-\frac{\partial}{\partial x}\theta(\alpha;z)}\cdot\left(-\frac{\partial}{\partial x}\theta(\alpha;z)(\alpha^{s_2-1}+\alpha^{-s_2})\right)d\alpha\\
&\cdot\int_1^{+\infty}\left(-\frac{\partial}{\partial x}\theta(\alpha;z)(\alpha^{s_2-1}+\alpha^{-s_2})\right)d\alpha\\
>&\int_1^{+\infty}\frac{\alpha^{s_1-1}+\alpha^{-s_1}}{\alpha^{s_2-1}+\alpha^{-s_2}}\cdot\left(-\frac{\partial}{\partial x}\theta(\alpha;z)(\alpha^{s_2-1}+\alpha^{-s_2})\right)d\alpha\\
&\cdot\int_1^{+\infty}\frac{\frac{\partial}{\partial y}\theta(\alpha;z)}{-\frac{\partial}{\partial x}\theta(\alpha;z)}\cdot\left(-\frac{\partial}{\partial x}\theta(\alpha;z)(\alpha^{s_2-1}+\alpha^{-s_2})\right)d\alpha.
\end{aligned} \tag{6.8}$$

By Lemma 6.1 and (4.5), the proof is complete. □

This also means that (6.3) is decreasing for s. By Proposition 3.8, Corollary 1.6 then follows.

6.2 Yukawa potential

In this section, we prove the theorems about the Yukawa potential. By Laplace transform, we have

$$\frac{e^{-\pi\alpha r}}{r} = \int_{\pi\alpha}^{+\infty} e^{-sr}\,ds = \pi\int_{\alpha}^{+\infty} e^{-\pi sr}\,ds. \tag{6.9}$$

Therefore, for any $\alpha > 0$,

$$\mathcal{Y}(\alpha;z) = \pi\int_{\alpha}^{+\infty}\theta(s;z)-1\,ds. \tag{6.10}$$

Furthermore, if $\alpha < 1$, it can be rewritten by

$$\mathcal{Y}(\alpha;z) = \pi\left(\int_1^{+\infty}\theta(s;z)-1\,ds + \int_1^{\frac{1}{\alpha}}\Big(\theta(s;z)-1\Big)\frac{1}{s}\,ds + \alpha - \log\alpha - 1\right). \tag{6.11}$$

Lemma 6.6. *For $\beta > \alpha$ and $b > 1$, or $\beta < \alpha$ and $b \geq 1$, the (1.8) doesn't have any minimizer. In other cases it does have a minimizer.*

Proof. It is easy to see that when $y \to +\infty$, we have

$$\mathcal{Y}(\alpha; x+iy) = \sum_{(m,n)\in\mathbb{Z}^2\setminus\{0\}} \frac{e^{-\pi\alpha\left(m^2y+\frac{(mx+n)^2}{y}\right)}}{m^2y+\frac{(mx+n)^2}{y}} \to 2y\sum_{n=1}^{+\infty}\frac{1}{n^2}e^{-\pi\alpha\frac{(mx+n)^2}{y}} \sim \frac{\pi^2}{3}y. \tag{6.12}$$

Then if $b > 1$,

$$\mathcal{Y}(\alpha; iy) - b\mathcal{Y}(\beta; iy) \to -\infty, \tag{6.13}$$

which means the (1.8) does not have any minimizer. If $b < 1$,

$$\mathcal{Y}(\alpha; iy) - b\mathcal{Y}(\beta; iy) \to +\infty, \tag{6.14}$$

which means the (1.8) does have a minimizer. If $b = 1$,

$$\mathcal{Y}(\alpha; z) - \mathcal{Y}(\beta; z) = \pi\int_\alpha^\beta \theta(t; s)\,dt.$$

The conclusion is obvious. □

Lemma 6.7. *For any $\beta > \alpha > 0$, $b \in (-\infty, 1]$, the minimizer of (1.8) is $e^{i\frac{\pi}{3}}$.*

Proof. By the relation between $\theta(\alpha; z)$ and $\mathcal{Y}(\alpha; z)$, we get the following facts directly.

$$\frac{\partial}{\partial\alpha}\mathcal{Y}(\alpha; z) = -\pi\theta(\alpha; z). \tag{6.15}$$

Using this, we obtain

$$\frac{\partial^2}{\partial\alpha\partial x}\mathcal{Y}(\alpha; z) = -\pi\frac{\partial}{\partial x}\theta(\alpha; z) > 0, \tag{6.16}$$

and

$$\frac{\partial^2}{\partial\alpha\partial y}\mathcal{Y}(\alpha; z) = -\pi\frac{\partial}{\partial y}\theta(\alpha; z) < 0. \tag{6.17}$$

Therefore, for any $\beta > \alpha > 0$, and $0 < b \leq 1$, we have

$$\frac{\partial}{\partial y}\mathcal{Y}(\alpha; z) - b\frac{\partial}{\partial y}\mathcal{Y}(\beta; z) > \frac{\partial}{\partial y}\mathcal{Y}(\alpha; z) - b\frac{\partial}{\partial y}\mathcal{Y}(\alpha; z) \geq 0. \tag{6.18}$$

$$\frac{\partial}{\partial x}\mathcal{Y}(\alpha; z) - b\frac{\partial}{\partial x}\mathcal{Y}(\beta; z) < \frac{\partial}{\partial x}\mathcal{Y}(\alpha; z) - b\frac{\partial}{\partial x}\mathcal{Y}(\alpha; z) \leq 0. \tag{6.19}$$

This implies that the minimizer is $e^{i\frac{\pi}{3}}$. □

Lemma 6.8. *For $\alpha \geq 1$ with $\alpha \geq \beta$, the minimizer of (1.8) only occurs on the curve $\Gamma_a \cup \Gamma_b$.*

Proof.

$$\begin{aligned}\mathcal{Y}(\alpha; z) - b\mathcal{Y}(\beta; z) &= \pi \int_{\alpha}^{+\infty} \theta(s; z) - 1\, ds - b\pi \int_{\beta}^{+\infty} \theta(s; z) - 1\, ds \\ &= (1-b)\pi \int_{\alpha}^{+\infty} \theta(s; z) - 1\, ds - b\pi \int_{\beta}^{\alpha} \theta(s; z) - 1\, ds.\end{aligned} \tag{6.20}$$

When $\alpha > \beta \geq 1$, (4.5) yields

$$\begin{aligned}&\frac{\frac{\partial}{\partial y}\int_{\alpha}^{+\infty} \theta(s; z) - 1\, ds}{\frac{\partial}{\partial x}\int_{\alpha}^{+\infty} \theta(s; z) - 1\, ds} = \frac{\int_{\alpha}^{+\infty} \frac{\partial}{\partial y}\theta(s; z)\, ds}{\int_{\alpha}^{+\infty} \frac{\partial}{\partial x}\theta(s; z)\, ds} < \frac{\frac{\partial}{\partial y}\theta(\alpha; z)}{\frac{\partial}{\partial x}\theta(\alpha; z)} \\ &< \frac{\int_{\beta}^{\alpha} \frac{\partial}{\partial y}\theta(s; z)\, ds}{\int_{\beta}^{\alpha} \frac{\partial}{\partial x}\theta(s; z)\, ds} = \frac{\frac{\partial}{\partial y}\int_{\beta}^{\alpha} \theta(s; z) - 1\, ds}{\frac{\partial}{\partial x}\int_{\beta}^{\alpha} \theta(s; z) - 1\, ds}.\end{aligned} \tag{6.21}$$

By Proposition 3.8, we obtain that the minimizer of (1.8) only occurs on the curve $\Gamma_a \cup \Gamma_b$.

When $\alpha \geq \frac{1}{\beta} > 1 > \beta$,

$$\begin{aligned}\int_{\beta}^{\alpha} \theta(s; z) - 1\, ds &= \int_{1}^{\alpha} \theta(s; z) - 1\, ds + \int_{\beta}^{1} \theta(s; z) - 1\, ds \\ &= \int_{1}^{\alpha} \theta(s; z) - 1\, ds + \int_{1}^{\frac{1}{\beta}} \frac{1}{s}\Big(\theta(s; z) - 1\Big)\, ds + \beta - \log\beta - 1.\end{aligned} \tag{6.22}$$

Using (4.5) again, we get

$$\frac{\frac{\partial}{\partial y}\int_{\alpha}^{+\infty} \theta(s; z)\, ds}{\frac{\partial}{\partial x}\int_{\alpha}^{+\infty} \theta(s; z)\, ds} < \frac{\frac{\partial}{\partial y}\theta(\alpha; z)}{\frac{\partial}{\partial x}\theta(\alpha; z)} < \frac{\frac{\partial}{\partial y}\int_{\beta}^{\alpha} \theta(s; z)\, ds}{\frac{\partial}{\partial x}\int_{\beta}^{\alpha} \theta(s; z)\, ds}. \tag{6.23}$$

By Proposition 3.8 again, we get the same conclusion.

When $\frac{1}{\beta} > \alpha > 1 > \beta$,

$$\begin{aligned}\int_{\beta}^{\alpha} \theta(s; z) - 1\, ds &= \int_{1}^{\alpha} \theta(s; z) - 1\, ds + \int_{1}^{\frac{1}{\beta}} \Big(\theta(s; z) - 1\Big)\frac{1}{s}\, ds + \beta - \log\beta - 1 \\ &= \int_{1}^{\alpha} \theta(s; z) - 1\, ds + \int_{1}^{\alpha} \Big(\theta(s; z) - 1\Big)\frac{1}{s}\, ds + \int_{\alpha}^{\frac{1}{\beta}} \Big(\theta(s; z) - 1\Big)\frac{1}{s}\, ds + \beta - \log\beta - 1.\end{aligned} \tag{6.24}$$

$$\int_{\alpha}^{+\infty} \theta(s; z)\, ds = \int_{\alpha}^{\frac{1}{\beta}} \theta(s; z)\, ds + \int_{\frac{1}{\beta}}^{+\infty} \theta(s; z)\, ds. \tag{6.25}$$

By Lemma 6.1, we have

$$\frac{\frac{\partial}{\partial y}\int_{\alpha}^{\frac{1}{\beta}} \theta(s;z)\,ds}{\frac{\partial}{\partial x}\int_{\alpha}^{\frac{1}{\beta}} \theta(s;z)\,ds} < \frac{\frac{\partial}{\partial y}\int_{\alpha}^{\frac{1}{\beta}} \theta(s;z)\frac{1}{s}\,ds}{\frac{\partial}{\partial x}\int_{\alpha}^{\frac{1}{\beta}} \theta(s;z)\frac{1}{s}\,ds}. \tag{6.26}$$

By (4.5), we get

$$\frac{\frac{\partial}{\partial y}\int_{\frac{1}{\beta}}^{+\infty} \theta(s;z)\,ds}{\frac{\partial}{\partial x}\int_{\frac{1}{\beta}}^{+\infty} \theta(s;z)\,ds} < \frac{\frac{\partial}{\partial y}\int_{\alpha}^{\frac{1}{\beta}} \theta(s;z)\,ds}{\frac{\partial}{\partial x}\int_{\alpha}^{\frac{1}{\beta}} \theta(s;z)\,ds}. \tag{6.27}$$

Using the same analysis on $[1,\alpha]$, we get

$$\frac{\frac{\partial}{\partial y}\int_{\alpha}^{\frac{1}{\beta}} \theta(s;z)\frac{1}{s}\,ds}{\frac{\partial}{\partial x}\int_{\alpha}^{\frac{1}{\beta}} \theta(s;z)\frac{1}{s}\,ds} < \frac{\frac{\partial}{\partial y}\int_{1}^{\alpha} \theta(s;z)\,ds}{\frac{\partial}{\partial x}\int_{1}^{\alpha} \theta(s;z)\,ds} < \frac{\frac{\partial}{\partial y}\int_{1}^{\alpha} \theta(s;z)\frac{1}{s}\,ds}{\frac{\partial}{\partial x}\int_{1}^{\alpha} \theta(s;z)\frac{1}{s}\,ds}. \tag{6.28}$$

Combining (6.26), (6.27) and (6.28), we have

$$\frac{\frac{\partial}{\partial y}\int_{\alpha}^{+\infty} \theta(s;z)-1\,ds}{\frac{\partial}{\partial x}\int_{\alpha}^{+\infty} \theta(s;z)-1\,ds} < \frac{\frac{\partial}{\partial y}\int_{\beta}^{\alpha} \theta(s;z)-1\,ds}{\frac{\partial}{\partial x}\int_{\beta}^{\alpha} \theta(s;z)-1\,ds}. \tag{6.29}$$

Other cases are obvious. □

6.3 Other potentials

Proof of Theorem 1.11. By Laplace transform, we have

$$\mathcal{F}_i(z) = \int_1^{+\infty} \theta(t;z)(\hat{\mu}_{f_i}(t) + \frac{1}{t}\hat{\mu}_{f_i}(\frac{1}{t}))\,dt, \tag{6.30}$$

which can be rewritten as

$$\mathcal{F}_i(z) = \int_1^{+\infty} (\theta(t;z)-1)(\hat{\mu}_{f_i}(t) + \frac{1}{t}\hat{\mu}_{f_i}(\frac{1}{t}))\,dt + \int_1^{+\infty} (\frac{1}{t}-\frac{1}{t^2})\hat{\mu}_{f_i}(\frac{1}{t})\,dt. \tag{6.31}$$

Moreover, we have

$$\frac{\frac{\partial}{\partial y}\mathcal{F}_i(z)}{\frac{\partial}{\partial x}\mathcal{F}_i(z)} = \frac{\frac{\partial}{\partial y}\int_1^{+\infty} \theta(t;z)(\hat{\mu}_{f_i}(t) + \frac{1}{t}\hat{\mu}_{f_i}(\frac{1}{t}))\,dt}{\frac{\partial}{\partial x}\int_1^{+\infty} \theta(t;z)(\hat{\mu}_{f_i}(t) + \frac{1}{t}\hat{\mu}_{f_i}(\frac{1}{t}))\,dt}. \tag{6.32}$$

Without loss of generality, we can assume $\frac{\hat{\mu}_{f_1}(t)+\frac{1}{t}\hat{\mu}_{f_1}(\frac{1}{t})}{\hat{\mu}_{f_2}(t)+\frac{1}{t}\hat{\mu}_{f_2}(\frac{1}{t})}$ is increasing for $t \in (1, +\infty)$. Then by Lemma 6.1, we have

$$
\begin{aligned}
&\int_1^{+\infty} \frac{\frac{\partial}{\partial y}\theta(t;z)}{-\frac{\partial}{\partial x}\theta(t;z)} \frac{\hat{\mu}_{f_1}(t)+\frac{1}{t}\hat{\mu}_{f_1}(\frac{1}{t})}{\hat{\mu}_{f_2}(t)+\frac{1}{t}\hat{\mu}_{f_2}(\frac{1}{t})} \left(-\frac{\partial}{\partial x}\theta(t;z)(\hat{\mu}_{f_2}(t)+\frac{1}{t}\hat{\mu}_{f_2}(\frac{1}{t}))\right) dt \\
&\cdot \int_1^{+\infty} \left(-\frac{\partial}{\partial x}\theta(t;z)(\hat{\mu}_{f_2}(t)+\frac{1}{t}\hat{\mu}_{f_2}(\frac{1}{t}))\right) dt \\
> &\int_1^{+\infty} \frac{\hat{\mu}_{f_1}(t)+\frac{1}{t}\hat{\mu}_{f_1}(\frac{1}{t})}{\hat{\mu}_{f_2}(t)+\frac{1}{t}\hat{\mu}_{f_2}(\frac{1}{t})} \left(-\frac{\partial}{\partial x}\theta(t;z)(\hat{\mu}_{f_2}(t)+\frac{1}{t}\hat{\mu}_{f_2}(\frac{1}{t}))\right) dt \\
&\cdot \int_1^{+\infty} \frac{\frac{\partial}{\partial y}\theta(t;z)}{-\frac{\partial}{\partial x}\theta(t;z)} \left(-\frac{\partial}{\partial x}\theta(t;z)(\hat{\mu}_{f_2}(t)+\frac{1}{t}\hat{\mu}_{f_2}(\frac{1}{t}))\right) dt.
\end{aligned}
\tag{6.33}
$$

Shifting terms gives

$$
\frac{\frac{\partial}{\partial y}\int_1^{+\infty}\theta(t;z)(\hat{\mu}_{f_1}(t)+\frac{1}{t}\hat{\mu}_{f_1}(\frac{1}{t}))\,dt}{\frac{\partial}{\partial x}\int_1^{+\infty}\theta(t;z)(\hat{\mu}_{f_1}(t)+\frac{1}{t}\hat{\mu}_{f_1}(\frac{1}{t}))\,dt} < \frac{\frac{\partial}{\partial y}\int_1^{+\infty}\theta(t;z)(\hat{\mu}_{f_2}(t)+\frac{1}{t}\hat{\mu}_{f_2}(\frac{1}{t}))\,dt}{\frac{\partial}{\partial x}\int_1^{+\infty}\theta(t;z)(\hat{\mu}_{f_2}(t)+\frac{1}{t}\hat{\mu}_{f_2}(\frac{1}{t}))\,dt}, \tag{6.34}
$$

which finishes the proof. □

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