

# ON THE REGULAR PART OF BLOCH GREEN FUNCTION: ANALYTICAL FORMULA AND CRITICAL POINTS

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ABSTRACT. This paper is concerned with the regular part of the Bloch Green's function in a Wigner-Seitz lattice cell. We first give a new fast converging series expression. Then we derive an explicit expression using some Dedekind eta functions when the Bloch vector  $\mathbf{k}$  are some rational numbers. Finally we study its critical points.

## 1. THE BLOCH GREEN'S FUNCTION ON THE LATTICE AND MAIN RESULTS

In studying of the stability of localized lattice patterns for reaction-diffusion systems (Gierer-Meinhardt, Schnakenberg) in  $\mathbb{R}^2$ , a Bloch Green's function is introduced in [7, 8]. For a general complex nonzero Bloch vector  $\mathbf{k}$ , the Bloch Green's function takes complex form. However its regular part, as seen below, is shown to be real (Lemma 2.1, [7]). The stability of lattice patterns is determined by max-min properties of the regular part of the Bloch Green's function. In this paper our primary goal is to establish new analytical formula of the regular part and study its critical points. For more background on the regular part of the Bloch Green's function and its application in biological pattern formation, we refer to recent survey article by Ward [17]. For the lattice sum and related physical models we refer to Linton [11, 12].

We first introduce Bravais lattice cell. Let  $\mathbf{l}_1$  and  $\mathbf{l}_2$  be two linearly independent vectors in  $\mathbb{R}^2$ , with angle  $\theta$  between them. The Bravais lattice  $\Lambda$  is then defined by

$$\Lambda = \{m\mathbf{l}_1 + n\mathbf{l}_2 \mid m, n \in \mathbb{Z}\}.$$

The parallelogram generated by the vectors  $\mathbf{l}_1$  and  $\mathbf{l}_2$  is called primitive cell, whose area is denoted as  $|\Lambda|$ . The *Wigner-Seitz or Voronoi* cell centered at a given lattice point of  $\Lambda$  consists of all points in the plane that are closer to this point than to any other lattice point. The *Wigner-Seitz* cell is a convex polygon with the same area as the parallelogram  $\mathbf{l}_1 \times \mathbf{l}_2$ . We denote the *Wigner-Seitz* or *Voronoi* cell at the origin as  $\Omega$ . For a *Wigner-Seitz* cell  $\Omega$  and vector  $\mathbf{k} \neq 0$ , the Bloch Green's function  $G(\mathbf{x}; \mathbf{k})$  is defined to satisfy

$$\begin{cases} -\Delta G(\mathbf{x}; \mathbf{k}) = \delta(\mathbf{x}), & \mathbf{x} = (x_1, x_2) \in \Omega \\ G(\mathbf{x} + \mathbf{l}; \mathbf{k}) = e^{-2\pi i \mathbf{k} \cdot \mathbf{l}} G(\mathbf{x}; \mathbf{k}), & \mathbf{l} \in \Lambda \end{cases} \quad (1.1)$$

where  $\mathbf{x} = (x_1, x_2)$  belongs to Voronoi cell  $\Omega$  and the Bloch vector  $\mathbf{k}$  belongs to the dual lattice (sometimes known as the reciprocal lattice):

$$\Lambda^* = \{\mathbf{d} \mid \mathbf{d} \cdot \mathbf{l} \in \mathbb{Z}, \forall \mathbf{l} \in \Lambda\}.$$

It follows that the dual lattice satisfies

$$(\Lambda^*)^* = \Lambda; \quad |\Lambda^*| = \frac{1}{|\Lambda|}.$$

In the following, we parameterize  $\Lambda^*$  as  $\{n\mathbf{d}_1 + m\mathbf{d}_2, (m, n) \in \mathbb{Z}^2\}$ , where  $\mathbf{d}_1 = (1, 0)$ ,  $\mathbf{d}_2 = (x, y)$ ,  $y > 0$ . Hence  $\Lambda = (\Lambda^*)^* = \{m\mathbf{l}_1 + n\mathbf{l}_2, (m, n) \in \mathbb{Z}^2\}$ , where  $\mathbf{l}_1 = (1, -\frac{x}{y})$ ,  $\mathbf{l}_2 = (0, \frac{1}{y})$ . Thus  $|\Lambda| = |\mathbf{l}_1 \wedge \mathbf{l}_2| = \frac{1}{y}$ .

Formally the Bloch Green's function can be constructed as the sum of free-space Green's functions:

$$G(\mathbf{x}; \mathbf{k}) = \sum_{\mathbf{l} \in \Lambda} G_0(\mathbf{x} + \mathbf{l}) e^{2\pi i \mathbf{k} \cdot \mathbf{l}}, \quad (1.2)$$

where the free-space Green's function  $G_0(\mathbf{x})$  satisfies

$$-\Delta G_0(\mathbf{x}) = \delta(\mathbf{x}). \quad (1.3)$$

To calculate the summation in (1.2), we use the Poisson summation formula for Fourier transform on the lattice, which says that

$$\sum_{\mathbf{l} \in \Lambda} f(\mathbf{x} + \mathbf{l}) e^{2\pi i \mathbf{k} \cdot \mathbf{l}} = \frac{1}{|\Lambda|} \sum_{\mathbf{d} \in \Lambda^*} \widehat{f}(\mathbf{d} - \mathbf{k}) e^{2\pi i \mathbf{x} \cdot (\mathbf{d} - \mathbf{k})}, \quad (1.4)$$

where  $\Lambda^*$  is the dual lattice of  $\Lambda$ . Here we adopt the following definition of Fourier transform

$$\widehat{f}(\xi) = \int_{\mathbb{R}^2} e^{-2\pi i \mathbf{x} \cdot \xi} f(\mathbf{x}) d\mathbf{x}.$$

By this definition, for the Gaussian distribution and Dirac measure centered at  $\mathbf{b}$ , there holds

$$\widehat{e^{-\pi|\mathbf{x}|^2}} = e^{-\pi|\xi|^2}, \quad \widehat{\delta(\mathbf{x} - \mathbf{b})} = e^{-2\pi i \mathbf{b} \cdot \xi}. \quad (1.5)$$

To introduce the formula for the Bloch Green's function, we introduce some notations first. Let  $\mathbf{k} = k_1 + ik_2$  be the Bloch wave vector and  $\mathbf{l}_1$  and  $\mathbf{l}_2$  be the generator of the lattice, i.e.,

$$\Lambda = \Lambda(\mathbf{l}_1, \mathbf{l}_2) := \mathbf{l}_1 \mathbb{Z} + \mathbf{l}_2 \mathbb{Z} := \{m\mathbf{l}_1 + n\mathbf{l}_2 \mid (m, n) \in \mathbb{Z}^2\}.$$

If we treat  $\mathbf{d}_1, \mathbf{d}_2, \mathbf{l}_1, \mathbf{l}_2$  as complex variables, we denote  $\tau = x + iy$  as quotient of the basis:

$$\tau = -\frac{\mathbf{l}_1}{\mathbf{l}_2} = \frac{\mathbf{d}_2}{\mathbf{d}_1}.$$

By rotation we may assume that  $Im(\tau) > 0$ . Let  $\mathbf{x} = (x_1, x_2)$  be the vector variable of the Bloch Green's function. For simplicity in computations, we also denote that

$$u = x \cdot x_1 + y \cdot x_2, \quad v = x_1. \quad (1.6)$$

By taking Fourier transform in (1.3), we have

$$\widehat{G}_0(\mathbf{p}) = \frac{1}{4\pi^2 |\mathbf{p}|^2}. \quad (1.7)$$

Combining (1.2), (1.4) and (1.7), we obtain the following formula for the Bloch Green's function

$$G(\mathbf{x}; \mathbf{k}) = \frac{y}{4\pi^2} \sum_{\mathbf{d} \in \Lambda^*} \frac{e^{2\pi i \mathbf{x} \cdot (\mathbf{d} - \mathbf{k})}}{|\mathbf{d} - \mathbf{k}|^2} = \frac{1}{4\pi^2} e^{-2\pi i (\mathbf{k} \cdot \mathbf{x})} \sum_{(m, n) \in \mathbb{Z}^2} e^{2\pi i (mu + nv)} \frac{y}{|m\tau + n - \mathbf{k}|^2}. \quad (1.8)$$

Let

$$E_{u, v, \mathbf{k}}(\tau) = \sum_{(m, n) \in \mathbb{Z}^2} e^{2\pi i (mu + nv)} \frac{y}{|m\tau + n - \mathbf{k}|^2}. \quad (1.9)$$

Then the Bloch Green's function can be written as

$$G(\mathbf{x}; \mathbf{k}) = \frac{1}{4\pi^2} e^{-2\pi i (\mathbf{k} \cdot \mathbf{x})} E_{u, v, \mathbf{k}}(\tau).$$

The regular part of the Bloch Green's function is then defined by

$$R(\tau, \mathbf{k}) = \lim_{\mathbf{x} \rightarrow 0} \left( G(\mathbf{x}, \mathbf{k}) + \frac{1}{2\pi} \log \left| \frac{\mathbf{x}}{\sqrt{|\Lambda|}} \right| \right). \quad (1.10)$$

(The factor  $\sqrt{|\Lambda|}$  appears in above definition due to the scaling of the lattice cell area.)

In terms of  $E_{u, v, \mathbf{k}}(\tau)$ , the regular part of the Bloch Green's function can be expressed as

$$R(\tau, \mathbf{k}) = \lim_{\mathbf{x} \rightarrow 0} \left( \frac{1}{4\pi^2} E_{u, v, \mathbf{k}}(\tau) + \frac{1}{2\pi} \log \left| \frac{\mathbf{x}}{\sqrt{|\Lambda|}} \right| \right). \quad (1.11)$$

In [7], the authors derived the following formula of  $R(\tau, \mathbf{k})$  involving a parameter  $\eta$  (in the spirit of Beylkin et al. [3])

$$R(\tau, \mathbf{k}) = \sum_{\mathbf{d} \in \Lambda^*} \exp\left(-\frac{|2\pi\mathbf{d} - \mathbf{k}|^2}{4\eta^2}\right) \frac{1}{|2\pi\mathbf{d} - \mathbf{k}|^2} + \sum_{\mathbf{l} \in \Lambda, \mathbf{l} \neq \mathbf{0}} e^{i\mathbf{k} \cdot \mathbf{l}} F_{sing}(\mathbf{l}) - \frac{\gamma}{4\pi} - \frac{\log \eta}{2\pi}, \quad (1.12)$$

where  $F_{sing}(\mathbf{l}) = E_1(|\mathbf{l}|^2\eta^2)/(4\pi)$ ,  $E_1(z) = \int_z^\infty t^{-1}e^{-t}dt$  is the exponential integral and  $\gamma$  is the Euler constant. Here finding the optimal  $\eta$  is critical in numerical computing. Furthermore, they also derived the following leading-order asymptotic behavior of  $R(\tau, \mathbf{k})$ ,

$$R(\tau, \mathbf{k}) \sim \frac{1}{\mathbf{k}^T \mathbf{Q} \mathbf{k}}, \text{ as } \mathbf{k} \rightarrow 0, \quad (1.13)$$

where the positive-definite matrix  $\mathbf{Q}$  is defined in terms of the parameters of the Wigner-Seitz cell.

As one can see from (1.12), the right hand side involves an artificial parameter  $\eta$ . The role of  $\eta$  is to facilitate numerical computations. Our first result in this paper is the following general form of  $R(\tau, \mathbf{k})$  which is expressed by double series with exponential factors.

**Theorem 1.1.** *Let  $\tau = x + iy, y > 0, \mathbf{k} = k_1 + ik_2$ . The regular part of the Bloch Green's function has the form:*

$$\begin{aligned} R(\tau, \mathbf{k}) &= \frac{(e^{2k_2\pi} - e^{-2k_2\pi})y}{4\pi k_2(e^{2k_2\pi} + e^{-2k_2\pi} - 2\cos(2k_1\pi))} \\ &\quad - \frac{1}{2\pi} \log |2\pi\sqrt{y}| \\ &\quad + \frac{k_2^2}{2\pi y^2} \sum_{n=1}^{\infty} \frac{1}{n(n - \frac{k_2}{y})(n + \frac{k_2}{y})} \\ &\quad + \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{1}{n - \frac{k_2}{y}} \sum_{m=1}^{\infty} e^{-2\pi m(ny - k_2)} \cos(2\pi m(nx - k_1)) \\ &\quad + \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{1}{n + \frac{k_2}{y}} \sum_{m=1}^{\infty} e^{-2\pi m(ny + k_2)} \cos(2\pi m(nx + k_1)). \end{aligned} \quad (1.14)$$

**Remark 1.1.** *When  $y$  is large, the first and second terms in (1.14) determine the leading order behavior of  $R(\tau, \mathbf{k})$ . That is,*

$$R(\tau, \mathbf{k}) \sim \left( \frac{(e^{2k_2\pi} - e^{-2k_2\pi})}{4\pi k_2(e^{2k_2\pi} + e^{-2k_2\pi} - 2\cos(2k_1\pi))} y - \frac{1}{2\pi} \log |2\pi\sqrt{y}| \right), \quad y \gg 1. \quad (1.15)$$

**Remark 1.2.** *We can rewrite the third term in (1.14) by the Digamma function which is defined as*

$$\psi(z) := \frac{\partial}{\partial z} \{\ln \Gamma(z)\} = \frac{\Gamma'(z)}{\Gamma(z)}.$$

*Then the third part in (1.14) can be rewritten as*

$$\frac{t^2}{2\pi} \sum_{n=1}^{\infty} \frac{1}{n(n-t)(n+t)} = \frac{1}{4\pi} (2\psi(1) - \psi(1-t) - \psi(1+t)),$$

*where  $t = \frac{k_2}{y}$  and we use the following summation formula ([1])*

$$\psi(x) - \psi(y) = (x - y) \sum_{k=0}^{\infty} \frac{1}{(n+x)(n+y)}.$$

**Remark 1.3.** *The fourth and fifth parts in (1.15) are harmonic although they are double series.*

**Remark 1.4.** *Observe that the series in (1.15) are fast converging due to the exponential factors.*

**Remark 1.5.** Finally we give another equivalent formula. First, we give precise domain of Bloch wave vector  $\mathbf{k}$  and its parametrization. From equation (1.1), by uniqueness of the solution of the periodical boundary PDE, the Bloch Green's function  $G(\mathbf{x}; \mathbf{k})$  satisfies

$$G(\mathbf{x}; \mathbf{k} + \Lambda^*) = G(\mathbf{x}; \mathbf{k}).$$

It implies the periodicity of  $R(\mathbf{x}; \mathbf{k})$ . That is,

$$\begin{aligned} R(\tau; \mathbf{k} + \Lambda^*) &= \lim_{\mathbf{x} \rightarrow \mathbf{0}} \left( G(\mathbf{x}; \mathbf{k} + \Lambda^*) + \frac{1}{2\pi} \log \left| \frac{\mathbf{x}}{\sqrt{|\Lambda|}} \right| \right) \\ &= \lim_{\mathbf{x} \rightarrow \mathbf{0}} \left( G(\mathbf{x}; \mathbf{k}) + \frac{1}{2\pi} \log \left| \frac{\mathbf{x}}{\sqrt{|\Lambda|}} \right| \right) \\ &= R(\tau; \mathbf{k}). \end{aligned}$$

Therefore, we can restrict Bloch wave vector  $\mathbf{k}$  in the fundamental cell of  $\Lambda^*$ . Equivalently,

$$\mathbf{k} \in \{s\mathbf{d}_1 + t\mathbf{d}_2 = ty\mathbf{i} + (s + tx)\mathbf{j} \mid s, t \in [0, 1]\},$$

where  $\mathbf{d}_1, \mathbf{d}_2$  are the basis of  $\Lambda^*$ . We can further parameterize  $\mathbf{k}$  as

$$\mathbf{k} = ty\mathbf{i} + (s + tx)\mathbf{j} \mid s, t \in [0, 1], \text{ i.e., } k_2 = ty, k_1 = s + tx; s, t \in [0, 1].$$

With this parametrization, by (1.15), we can obtain an alternative form of the regular part of the Bloch Green's function. That is,

$$\begin{aligned} R(\tau, \xi) &= \frac{(e^{2ty\pi} - e^{-2ty\pi})}{4\pi t(e^{2ty\pi} + e^{-2ty\pi} - 2\cos(2(s + tx)\pi))} \\ &\quad - \frac{1}{2\pi} \log |2\pi\sqrt{y}| \\ &\quad + \frac{t^2}{2\pi} \sum_{n=1}^{\infty} \frac{1}{n(n-t)(n+t)} \\ &\quad + \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{1}{n-t} \sum_{m=1}^{\infty} e^{-2\pi m(n-t)y} \cos(2\pi m((n-t)x - s)) \\ &\quad + \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{1}{n+t} \sum_{m=1}^{\infty} e^{-2\pi m(n+t)y} \cos(2\pi m((n+t)x + s)), \end{aligned} \tag{1.16}$$

where  $\tau = (x, y), \xi = (s, t)$  and  $s, t \in [0, 1]$ .

When  $\mathbf{k} = k$  is a real number we have a more precise formula:

**Theorem 1.2.** The regular part of the Bloch Green's function when  $\mathbf{k} = k$  is a real number can be written as

$$R_k(\tau) := R(\tau, \mathbf{k}) = \frac{y}{4\sin^2(\pi k)} - \frac{1}{2\pi} \log \sqrt{y} - \frac{1}{2\pi} \log 2\pi - \frac{1}{2\pi} \sum_{n=1}^{\infty} \cos(2\pi nk) \log |1 - q^n|^2, \tag{1.17}$$

where  $q = e^{2\pi i\tau}, \tau = x + iy$ .

Next we analyze the asymptotic behavior of  $R(\tau, \mathbf{k})$  when  $\mathbf{k} \rightarrow 0$ . We first define the periodic Green's function

$$\begin{cases} -\Delta G_0(\mathbf{x}; \tau) = \delta(\mathbf{x}) - \frac{1}{|\Omega|}, & \mathbf{x} \in \Omega \\ \int_{\Omega} G_0(\mathbf{x}; \tau) d\mathbf{x} = 0 \\ G_0(\mathbf{x} + \mathbf{l}; \tau) = G_0(\mathbf{x}; \tau), & \mathbf{l} \in \Lambda \end{cases} \tag{1.18}$$

and its regular part

$$R_0(\tau) = \lim_{\mathbf{x} \rightarrow \mathbf{0}} \left( G_0(\mathbf{x}; \tau) + \frac{1}{2\pi} \log \left| \frac{\mathbf{x}}{\sqrt{|\Lambda|}} \right| \right) \tag{1.19}$$

which has the following form (Chen-Oshita [5]; see also Lin-Wang [10] and Sandier-Serfaty [14])

$$\begin{aligned} R_0(\tau) &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}| - \frac{1}{2\pi} \log |q^{1/12} \prod_{n=1}^{\infty} (1 - q^n)^2| \\ &= -\frac{1}{2\pi} \log 2\pi - \frac{1}{4\pi} \log |Im(\tau)\eta(\tau)|, \end{aligned} \quad (1.20)$$

where  $q = e^{2\pi i\tau}$ ,  $\tau = x + iy$  and  $\eta(\tau) = q^{\frac{1}{6}} \prod_{n=1}^{\infty} (1 - q^n)^4$ .

**Remark 1.6.** For the vortex lattice problem, the re-normalized energy is expressed by the regular part of the Green's function on the periodic lattice (i.e.,  $\mathbf{k} = \mathbf{0}$  in our setting, (1.20) and (1.17)), see Sandier-Serfaty [14]. To model di-block copolymers, one uses the Helmholtz free energy. One also reduces the energy to regular part of the Green's function on the periodic lattice, see Chen-Oshita [5]. Therefore, by finding the minimum of regular part of the Green's function, it is proved that the hexagonal or triangular lattice minimizes the energy functional. See more discussions in the last Section.

**Remark 1.7.**  $R_0(\tau)$  and the properties of  $G_0$  also play important role in analyzing bubbling solutions to mean field equations. See Lin-Wang [10].

Then we have the following asymptotic behavior.

**Theorem 1.3.** As  $\mathbf{k} \rightarrow 0$ ,  $R(\tau, \mathbf{k})$  converges to regular part of the periodic Green's function:

$$\lim_{\mathbf{k} \rightarrow \mathbf{0}} \left( R(\tau, \mathbf{k}) - \frac{y}{4\pi^2 |\mathbf{k}|^2} \right) = R_0(\tau). \quad (1.21)$$

**Remark 1.8.** The limit formula (1.21) provides the precise asymptotic behavior as  $\mathbf{k} \rightarrow 0$  in contrast to the leading order asymptotic behavior proved in (1.13) [Lemma 2.2, [7]].

It turns out that when  $\mathbf{k}$  are some given rational numbers, the regular part of the Bloch Green's function are closely related to  $R_0(\tau)$  (see (1.3)).

**Theorem 1.4.** When  $\mathbf{k}$  are real numbers ( $\frac{1}{2}$ ,  $\frac{1}{3}$ ,  $\frac{1}{4}$  and  $\frac{1}{6}$ ), the regular part of the Bloch Green's function can be linearly expanded by  $R_0(\tau)$  with different frequencies. More precisely,

$$\begin{aligned} R_{\frac{1}{2}}(\tau) &= -R_0(\tau) + 2R_0(2\tau) + \frac{1}{2\pi} \log 2 \\ R_{\frac{1}{3}}(\tau) &= -\frac{1}{2}R_0(\tau) + \frac{3}{2}R_0(3\tau) + \frac{3}{8\pi} \log 3 \\ R_{\frac{1}{4}}(\tau) &= R_{\frac{1}{2}}(2\tau) + \frac{1}{2\pi} \log \sqrt{2} \\ &= -R_0(2\tau) + 2R_0(4\tau) + \frac{1}{2\pi} \log \frac{4}{2^{1/2}} \\ R_{\frac{1}{6}}(\tau) &= -\frac{1}{2}R_{\frac{1}{2}}(\tau) + \frac{3}{2}R_{\frac{1}{2}}(3\tau) + \frac{3}{8\pi} \log 3 \\ &= \frac{1}{2}R_0(\tau) - R_0(2\tau) - \frac{3}{2}R_0(3\tau) + 3R_0(6\tau) + \frac{1}{2\pi} \log 2 + \frac{3}{8\pi} \log 3. \end{aligned} \quad (1.22)$$

**Remark 1.9.** As we can see in the last section, all the critical points of  $R_0(\tau)$  can be classified. (See also Lin-wang [10].) By the linear expansions in (1.22), we can obtain critical points of  $R(\tau, \mathbf{k})$  immediately when  $\mathbf{k}$  are  $\frac{1}{2}$ ,  $\frac{1}{3}$ ,  $\frac{1}{4}$  and  $\frac{1}{6}$ .

Finally we discuss critical points of the regular part of the Bloch Green's function. This is related to the following conjecture (Conjecture 6.1, [7]):

**Conjecture** [Iron-Rumsey-Ward-Wei [7]]: Within the class of Bravais lattice of a common area,  $\min_{\mathbf{k}} R(\tau, \mathbf{k})$  is maximized for a regular hexagonal lattice. Namely, consider the following max-min problem

$$\max_{\tau} \min_{\mathbf{k}} R(\tau, \mathbf{k}). \quad (1.23)$$

The optimal lattice is a regular hexagonal lattice, i.e.,  $\tau = \frac{1}{2} + i\frac{\sqrt{3}}{2}$ .

In [7, 8], they showed numerically that the maximizer of the objective function  $\max_{\tau} \min_{\mathbf{k}} R(\tau, \mathbf{k})$  determines the optimal lattice of periodic solutions in reaction diffusion systems.

Our last result provides evidence of the Conjecture. It says the hexagonal pattern is indeed an nondegenerate saddle point of  $R(\tau, \mathbf{k})$ .

**Theorem 1.5.** *There is a  $\tilde{k}_2 \sim 0.3$  such that  $(\tau, \mathbf{k}) = (\frac{1}{2} + i\frac{\sqrt{3}}{2}, \frac{1}{2} + i\tilde{k}_2)$  (which corresponds to hexagonal lattice) is an nondegenerate saddle point (local  $\max_{\tau} \min_{\mathbf{k}}$ ) for  $R(\tau, \mathbf{k})$ .*

The paper is organised as follows. In Section 2, we derive the general form of the Bloch Green's function when  $\mathbf{k}$  is any complex number[Theorem 1.1]. In Section 3, we prove Theorem 1.2 by the method from number theory, which is an analogue in calculating the Kronecker second limit formula. We also derive the asymptotic formula[Theorem 1.3]. In Section 4, we further study the structures of regular part of the Bloch Green's function by eta function/Euler modular form. Section 5 aims to locate some critical points of  $R(\tau, \mathbf{k})$  and derive the local extreme properties. In particular, we give some numerical information about the maxmin point in the Conjecture [Theorem 1.5].

There are many references on lattice sum, for example see sum on rectangular lattice and arbitrary lattice in [4] and [16] respectively. Here the new ingredient in our problem is not only lattice sum on arbitrary lattice, but also we need to find the regular part of the lattice sum and derive its fine analytic properties. For this we use heavily the Kronecker second limit formula (see, for example, S. Lang [9]).

## 2. PROOF OF THEOREM 1.1

In this section, we derive the general formula (1.14) for  $R(\tau, \mathbf{k})$ .

One simple but very useful idea in calculating the conditionally convergent series, initiated in analytic number theory by Siegel [15], is the following elementary algebraic identity

$$\frac{1}{|z|^2} = \frac{1}{z\bar{z}} = \frac{1}{\bar{z}-z} \left( \frac{1}{z} - \frac{1}{\bar{z}} \right). \quad (2.1)$$

Using (1.9) and (2.1), one deduces that

$$\begin{aligned} & y^{-1} E_{u,v,\mathbf{k}}(\tau) \\ &= \sum_{(m,n) \in \mathbb{Z}^2} e^{2\pi i(mv+nu)} \frac{1}{|m\tau + n - \mathbf{k}|^2} = \sum_{(m,n) \in \mathbb{Z}^2} e^{2\pi i(mv+nu)} \frac{1}{(m\tau + n - \mathbf{k})(m\bar{\tau} + n - \bar{\mathbf{k}})} \\ &= \sum_{n \in \mathbb{Z}} e^{2\pi i nu} \frac{1}{n(\bar{\tau} - \tau) + 2k_2 i} \sum_{m \in \mathbb{Z}} e^{2\pi i mv} \left( \frac{1}{n\tau + m - \mathbf{k}} - \frac{1}{n\bar{\tau} + m - \bar{\mathbf{k}}} \right) \\ &= \sum_{n \in \mathbb{Z}} e^{2\pi i nu} \frac{1}{n(\bar{\tau} - \tau) + 2k_2 i} \left( \sum_{m=1}^{\infty} e^{2\pi i mv} \left( \frac{1}{n\tau + m - \mathbf{k}} - \frac{1}{n\bar{\tau} + m - \bar{\mathbf{k}}} \right) \right. \\ &\quad \left. + \sum_{m=1}^{\infty} e^{-2\pi i mv} \left( \frac{1}{n\tau - m - \mathbf{k}} - \frac{1}{n\bar{\tau} - m - \bar{\mathbf{k}}} \right) \right) + \sum_{n \in \mathbb{Z}} e^{2\pi i nu} \frac{1}{n(\bar{\tau} - \tau) + 2k_2 i} \left( \frac{1}{n\tau - \mathbf{k}} - \frac{1}{n\bar{\tau} - \bar{\mathbf{k}}} \right) \\ &= \sum_{n \in \mathbb{Z}} \frac{e^{2\pi i nu}}{n(\bar{\tau} - \tau) + 2k_2 i} \sum_{m=1}^{\infty} \left( \left( \frac{e^{2\pi i mv}}{m + n\tau - \mathbf{k}} - \frac{e^{-2\pi i mv}}{m - (n\tau - \mathbf{k})} \right) - \left( \frac{e^{2\pi i mv}}{m + n\bar{\tau} - \bar{\mathbf{k}}} - \frac{e^{-2\pi i mv}}{m - (n\bar{\tau} - \bar{\mathbf{k}})} \right) \right) \\ &\quad + \sum_{m=1}^{\infty} e^{-2\pi i mv} \left( \frac{1}{n\tau - m - \mathbf{k}} - \frac{1}{n\bar{\tau} - m - \bar{\mathbf{k}}} \right) + \sum_{n \in \mathbb{Z}} e^{2\pi i nu} \frac{1}{n(\bar{\tau} - \tau) + 2k_2 i} \left( \frac{1}{n\tau - \mathbf{k}} - \frac{1}{n\bar{\tau} - \bar{\mathbf{k}}} \right). \end{aligned} \quad (2.2)$$

The above expression is a form of the Bloch Green's function. One may also deduce the Bloch Green's function by using product of many theta functions, see [12].

Observing that in each bracket of the expression of the Bloch Green's function in (2.2), we have two symmetric expressions to be taken summation. By Siegel [15], we have the following summation formula for two symmetric expressions

$$\sum_{m=1}^{\infty} \left( \frac{e^{2\pi i m u}}{z+m} + \frac{e^{-2\pi i m u}}{z-m} \right) = 2\pi i \frac{e^{-2\pi i u z}}{1-e^{-2\pi i z}} - \frac{1}{z}. \quad (2.3)$$

Thus  $E_{u,v,\mathbf{k}}(\tau, s)$  can be further simplified as

$$\begin{aligned} y^{-1} E_{u,v,\mathbf{k}}(\tau, s) &= \sum_{n \in \mathbb{Z}} \frac{\pi e^{2\pi i n u}}{k_2 - n y} \left( \frac{e^{-2\pi i v(n\tau - \mathbf{k})}}{1 - e^{-2\pi i(n\tau - \mathbf{k})}} - \frac{e^{-2\pi i v(n\bar{\tau} - \bar{\mathbf{k}})}}{1 - e^{-2\pi i(n\bar{\tau} - \bar{\mathbf{k}})}} \right) \\ &\quad + \sum_{n \in \mathbb{Z}} (e^{2\pi i n u} - 1) \frac{1}{n(\bar{\tau} - \tau) + 2k_2 i} \left( \frac{1}{n\tau - \mathbf{k}} - \frac{1}{n\bar{\tau} - \bar{\mathbf{k}}} \right) \\ &:= J_1 + J_2, \end{aligned} \quad (2.4)$$

where  $J_1$  and  $J_2$  are defined above. For the second part  $J_2$  in (2.4), applying the elementary algebraic identity (2.1), we have

$$J_2 = \sum_{n \in \mathbb{Z}} (e^{2\pi i n u} - 1) \frac{1}{|n - \mathbf{k}|^2}. \quad (2.5)$$

So  $J_2$  is an absolutely convergent series and  $J_2 = 0$  if  $u = 0$ . For the first part  $J_1$  in (2.4), we use the well known geometric series, that is

$$\frac{1}{1-r} = \sum_{n=0}^{\infty} r^n, \quad r \text{ is a complex number and } |r| < 1.$$

By further dividing  $n$  into three cases  $n > 0$ ,  $n = 0$  and  $n < 0$  respectively, we have

$$\begin{aligned} J_1 &= \frac{\pi}{k_2} \left( \frac{e^{2\pi i v \mathbf{k}}}{1 - e^{2\pi i \mathbf{k}}} - \frac{e^{2\pi i v \bar{\mathbf{k}}}}{1 - e^{2\pi i \bar{\mathbf{k}}}} \right) + \sum_{n \neq 0, n \in \mathbb{Z}} \frac{\pi e^{2\pi i n u}}{k_2 - n y} \left( \frac{e^{-2\pi i v(n\tau - \mathbf{k})}}{1 - e^{-2\pi i(n\tau - \mathbf{k})}} - \frac{e^{-2\pi i v(n\bar{\tau} - \bar{\mathbf{k}})}}{1 - e^{-2\pi i(n\bar{\tau} - \bar{\mathbf{k}})}} \right) \\ &= \frac{\pi}{k_2} \left( \frac{e^{2\pi i v \mathbf{k}}}{1 - e^{2\pi i \mathbf{k}}} - \frac{e^{2\pi i v \bar{\mathbf{k}}}}{1 - e^{2\pi i \bar{\mathbf{k}}}} \right) \\ &\quad + \sum_{n=1}^{\infty} \frac{\pi}{n y - k_2} \left( e^{2\pi i(nu - v(n\bar{\tau} - \bar{\mathbf{k}}))} + \sum_{m=1}^{\infty} e^{2\pi i(m-v)(n\tau - \mathbf{k})} + e^{-2\pi i(m+v)(n\bar{\tau} - \bar{\mathbf{k}})} \right) \\ &\quad + \sum_{n=1}^{\infty} \frac{\pi}{n y + k_2} \left( e^{2\pi i(nu + v(n\tau + \mathbf{k}))} + \sum_{m=1}^{\infty} e^{2\pi i(m+v)(n\tau + \mathbf{k})} + e^{-2\pi i(m-v)(n\bar{\tau} + \bar{\mathbf{k}})} \right). \end{aligned} \quad (2.6)$$

Now we can reform  $J_1$  in a symmetric way and further divide it into four parts to be computed in different ways. That is,

$$\begin{aligned} J_1 &= \frac{\pi}{k_2} \left( \frac{e^{2\pi i v \mathbf{k}}}{1 - e^{2\pi i \mathbf{k}}} - \frac{e^{2\pi i v \bar{\mathbf{k}}}}{1 - e^{2\pi i \bar{\mathbf{k}}}} \right) \\ &\quad + \frac{\pi}{y} \sum_{n=1}^{\infty} \left( \frac{1}{n - \frac{k_2}{y}} e^{2\pi i(n(u - v\bar{\tau}) + v\bar{\mathbf{k}})} + \frac{1}{n + \frac{k_2}{y}} e^{2\pi i(n(u + v\tau) + v\mathbf{k})} \right) \\ &\quad + \frac{\pi}{y} \sum_{n=1}^{\infty} \frac{1}{n - \frac{k_2}{y}} \sum_{m=1}^{\infty} e^{2\pi i(m-v)(n\tau - \mathbf{k})} + e^{-2\pi i(m+v)(n\bar{\tau} - \bar{\mathbf{k}})} \\ &\quad + \frac{\pi}{y} \sum_{n=1}^{\infty} \frac{1}{n + \frac{k_2}{y}} \sum_{m=1}^{\infty} e^{2\pi i(m+v)(n\tau + \mathbf{k})} + e^{-2\pi i(m-v)(n\bar{\tau} + \bar{\mathbf{k}})} \\ &:= J_{10} + J_{11} + J_{12} + J_{13}, \end{aligned} \quad (2.7)$$

where  $J_{1j}, j = 0, 1, 2, 3$  are defined at above.

The four parts in (2.7) will be dealt with separately. First, for  $J_{10}$ , direct calculation shows that

$$J_{10}|_{v=0} = \frac{\pi(e^{2k_2\pi} - e^{-2k_2\pi})}{k_2(e^{2k_2\pi} + e^{-2k_2\pi} - 2\cos(2k_1\pi))}. \quad (2.8)$$

For the part  $J_{11}$ , the series is conditionally convergent, hence one can not take limit  $\mathbf{x} \rightarrow \mathbf{0}$  directly. Instead, we single out the singular part and nonsingular part in reformulating the series. That is,

$$\begin{aligned} J_{11} &= \frac{\pi}{y} \sum_{n=1}^{\infty} \left( \frac{1}{n - \frac{k_2}{y}} e^{2\pi i(n(u-v\bar{\tau})+v\bar{\mathbf{k}})} + \frac{1}{n + \frac{k_2}{y}} e^{2\pi i(n(u+v\tau)+v\mathbf{k})} \right) \\ &= \frac{\pi}{y} \sum_{n=1}^{\infty} \frac{1}{n} \left( e^{2\pi i(n(u-v\bar{\tau})+v\bar{\mathbf{k}})} + e^{2\pi i(n(u+v\tau)+v\mathbf{k})} \right) \\ &\quad + \frac{k_2\pi}{y^2} \sum_{n=1}^{\infty} \left( \frac{1}{n(n - \frac{k_2}{y})} e^{2\pi i(n(u-v\bar{\tau})+v\bar{\mathbf{k}})} - \frac{1}{n(n + \frac{k_2}{y})} e^{2\pi i(n(u+v\tau)+v\mathbf{k})} \right) \\ &= \frac{\pi}{y} \left( e^{2\pi i v \bar{\mathbf{k}}} \log(1 - e^{2\pi i(u-v\bar{\tau})}) + e^{2\pi i v \mathbf{k}} \log(1 - e^{2\pi i(u+v\tau)}) \right) \\ &\quad + \frac{k_2\pi}{y^2} \sum_{n=1}^{\infty} \left( \frac{1}{n(n - \frac{k_2}{y})} e^{2\pi i(n(u-v\bar{\tau})+v\bar{\mathbf{k}})} - \frac{1}{n(n + \frac{k_2}{y})} e^{2\pi i(n(u+v\tau)+v\mathbf{k})} \right) \\ &:= J_{111} + J_{112}, \end{aligned} \quad (2.9)$$

where  $J_{111}, J_{112}$  is the singular part and nonsingular part respectively. Using the same notations in (1.6), the singular part  $J_{111}$  can be handled by

$$\begin{aligned} &\lim_{\mathbf{x} \rightarrow \mathbf{0}} \left( e^{2\pi i v \bar{\mathbf{k}}} \log(1 - e^{2\pi i(u-v\bar{\tau})}) + e^{2\pi i v \mathbf{k}} \log(1 - e^{2\pi i(u+v\tau)}) + 2 \log \left| \frac{\mathbf{x}}{\sqrt{|\Lambda|}} \right| \right) \\ &= \lim_{\mathbf{x} \rightarrow \mathbf{0}} \left( \log(1 - e^{2\pi i(u-v\bar{\tau})}) + \log(1 - e^{2\pi i(u+v\tau)}) + 2 \log |\sqrt{y} \cdot \mathbf{x}| \right) \\ &= \lim_{\mathbf{x} \rightarrow \mathbf{0}} \left( 2 \log |1 - e^{2\pi i(u-v\bar{\tau})}| + 2 \log |\sqrt{y} \cdot \mathbf{x}| \right) \\ &= -2 \log 2\pi - 2 \log \sqrt{y}. \end{aligned} \quad (2.10)$$

For the nonsingular part  $J_{112}$ , letting  $\mathbf{x} \rightarrow \mathbf{0}$  hence  $u, v \rightarrow 0$ , one deduces

$$\begin{aligned} J_{112} &= \frac{k_2\pi}{y^2} \sum_{n=1}^{\infty} \left( \frac{1}{n(n - \frac{k_2}{y})} - \frac{1}{n(n + \frac{k_2}{y})} \right) \\ &= \frac{2\pi k_2^2}{y^3} \sum_{n=1}^{\infty} \frac{1}{n(n - \frac{k_2}{y})(n + \frac{k_2}{y})}. \end{aligned} \quad (2.11)$$

For the remainder terms  $J_{12}, J_{13}$  in (2.7), by taking limit directly, we have

$$\begin{aligned} \lim_{\mathbf{x} \rightarrow \mathbf{0}} (J_{12} + J_{13}) &= \frac{\pi}{y} \sum_{n=1}^{\infty} \frac{1}{n - \frac{k_2}{y}} \sum_{m=1}^{\infty} 2e^{-2\pi m(ny-k_2)} \cos(2\pi m(nx - k_1)) \\ &\quad + \frac{\pi}{y} \sum_{n=1}^{\infty} \frac{1}{n + \frac{k_2}{y}} \sum_{m=1}^{\infty} 2e^{-2\pi m(ny+k_2)} \cos(2\pi m(nx + k_1)). \end{aligned} \quad (2.12)$$

Combining all the computations above, we are ready to derive the regular part of the Bloch Green's function from its definition, i.e.,



$$\begin{aligned}
R(\tau, \mathbf{k}) &= \lim_{\mathbf{x} \rightarrow 0} \left( \frac{1}{4\pi^2} E_{u,v,\mathbf{k}}(\tau) + \frac{1}{2\pi} \log \left| \frac{\mathbf{x}}{\sqrt{|\Lambda|}} \right| \right) \\
&= \lim_{\mathbf{x} \rightarrow 0} \left( \frac{y}{4\pi^2} (J_1 + J_2) + \frac{1}{2\pi} \log |\sqrt{y} \cdot \mathbf{x}| \right) \\
&= \lim_{\mathbf{x} \rightarrow 0} \left( \frac{y}{4\pi^2} (J_{10} + J_{11} + J_{12} + J_{13} + J_2) + \frac{1}{2\pi} \log |\sqrt{y} \cdot \mathbf{x}| \right) \\
&= \lim_{\mathbf{x} \rightarrow 0} \frac{y}{4\pi^2} \left( J_{10} + (J_{111} + \frac{2\pi}{y} \log |\sqrt{y} \cdot \mathbf{x}|) + J_{112} + J_{12} + J_{13} + J_2 \right).
\end{aligned}$$

Combining (2.5), (2.8), (2.10), (2.11), and (2.12), we obtain formula (1.14) for  $R(\tau, \mathbf{k})$ . These complete the proof of Theorem 1.1.

### 3. PROOF OF THEOREM 1.2 AND THEOREM 1.3

In this section, we will use a different method to calculate the regular part of the Bloch Green's function when  $\mathbf{k}$  is a real number. We first recall the following Fourier transformation formula

$$f(\widehat{\mathbf{A}\mathbf{x} + \mathbf{b}}) = e^{2\pi i \mathbf{b} \cdot \mathbf{A}^{-\mathbf{T}} \xi} \frac{1}{|\det \mathbf{A}|} \widehat{f}(\mathbf{A}^{-\mathbf{T}} \xi), \quad (3.1)$$

where  $\mathbf{A}^{-\mathbf{T}}$  can be defined as the transpose of the inverse.

From (3.1) and Poisson summation formula (1.4), we obtain the following summation identity

$$\sum_{n \in \mathbb{Z}} e^{-\pi t(n+mx-k_1)^2} e^{2\pi i n v} = \sum_{n \in \mathbb{Z}} t^{-1/2} e^{2\pi i(k_1-mx)(\nu+n)} e^{-\frac{\pi}{t}(\nu+n)^2},$$

where  $u, v, k_1, k_2$  are real numbers.

We define

$$E_{u,v,\mathbf{k}}(\tau, s) = \sum_{(m,n) \in \mathbb{Z}^2} e^{2\pi i(mu+nv)} \frac{y^s}{|m\tau + n - \mathbf{k}|^{2s}} \quad (3.2)$$

where  $\tau = x + iy$  is in the upper plane and  $\mathbf{k} = k_1 + ik_2$ . The sum being taken for all integers  $m\tau + n - \mathbf{k} \neq 0$ . The series converges for  $Re(s) > 1$ . Then

$$E_{u,v,\mathbf{k}}(\tau) = \lim_{s \rightarrow 1^+} E_{u,v,\mathbf{k}}(\tau, s).$$

The problem is transferred to find the limit formula of  $E_{u,v,\mathbf{k}}$  as  $s \rightarrow 1^+$ . This is an analogue to the Kronecker second limit. To calculate the Kronecker second limit formula of the  $E_{u,v,\mathbf{k}}$ , we follow the calculation as in S. Lang [9], where the classical Kronecker first and second limit formulas are computed explicitly.

We start with the scaling (by parameter  $a$ ) of the Gamma function

$$\frac{\pi^{-s} \Gamma(s)}{a^s} = \int_0^\infty e^{-\pi a t} t^s \frac{dt}{t}. \quad (3.3)$$

Therefore, by splitting off the sum taken for  $m = 0$ , one has

$$\begin{aligned}
y^{-s} E_{u,v,\mathbf{k}}(\tau, s) &= \sum_{(m,n) \in \mathbb{Z}^2} e^{2\pi i(mu+nv)} \frac{1}{((my - k_2)^2 + (n + mx - k_1)^2)^s} \\
&= \sum_{n \in \mathbb{Z}} e^{2\pi i n v} \frac{1}{k_2^2 + (n - k_1)^2} \\
&\quad + \sum_{m \neq 0, m \in \mathbb{Z}} e^{2\pi i m u} \sum_{n \in \mathbb{Z}} e^{2\pi i n v} \frac{1}{((my - k_2)^2 + (n + mx - k_1)^2)^s} \\
&= I_1 + I_2.
\end{aligned}$$

$I_1$  and  $I_2$  will be calculated differently. For  $I_1(v = 0)$ , by (2.3), we can get the explicit summation formula as follows

$$\begin{aligned} I_1 &= \sum_{n \in \mathbb{Z}} \frac{1}{k_2^2 + (n - k_1)^2} = \sum_{n \in \mathbb{Z}} \frac{1}{(n - (ik_2 + k_1))(n - (-ik_2 + k_1))} \\ &= \frac{\pi(e^{2k_2\pi} - e^{-2k_2\pi})}{2k_2(\frac{e^{2k_2\pi} + e^{-2k_2\pi}}{2} - \cos(2k_1\pi))}, \quad \forall k_1, k_2 \in \mathbb{R}, k_1^2 + k_2^2 \neq 0. \end{aligned} \quad (3.4)$$

In particular if  $k_2 = 0$ , we have

$$\sum_{m \in \mathbb{Z}} \frac{e^{2\pi i m u}}{(m - z)^2} = \frac{\pi^2 e^{2\pi i z u} (1 - u + u e^{-2\pi i z})}{\sin^2(\pi z)}.$$

For the second part  $I_2$ , we use the scaling of the Gamma function (3.3). Then one rewrites  $I_2$  by exponential functions

$$\begin{aligned} I_2 &= \sum_{m \neq 0, m \in \mathbb{Z}} e^{2\pi i m} \sum_{n \in \mathbb{Z}} e^{2\pi i n v} \frac{1}{((m y - k_2)^2 + (n + m x - k_1)^2)^s} \\ &= \frac{\pi^s}{\Gamma(s)} \sum_{m \neq 0, m \in \mathbb{Z}} e^{2\pi i m u} e^{-\pi t (m y - k_2)^2} \int_0^\infty \sum_{n \in \mathbb{Z}} e^{2\pi i n v} e^{-\pi t (n + m x - k_1)^2} t^s \frac{dt}{t} \\ &= \frac{\pi^s}{\Gamma(s)} \sum_{m \neq 0, m \in \mathbb{Z}} e^{2\pi i m u} e^{-\pi t (m y - k_2)^2} \int_0^\infty \sum_{n \in \mathbb{Z}} e^{2\pi i (k_1 - m x)(v + n)} e^{-\frac{\pi}{t}(v + n)^2} t^{s - \frac{1}{2}} \frac{dt}{t}. \end{aligned}$$

When  $s = 1$ , we summarize the terms by

$$\begin{aligned} I_2 &= \pi \sum_{m \neq 0, m \in \mathbb{Z}} e^{2\pi i m(u - vx)} \sum_{n \in \mathbb{Z}} e^{2\pi i n(k_1 - mx)} \int_0^\infty e^{-\pi(t(m y - k_2)^2 + (n + v)^2/t)} t^{1/2} \frac{dt}{t} \\ &= \pi \sum_{m \neq 0, m \in \mathbb{Z}} e^{2\pi i m(u - vx)} \sum_{n \in \mathbb{Z}} e^{2\pi i n(k_1 - mx)} \frac{1}{|m y - k_2|} e^{-2\pi |m y - k_2| \cdot |n + v|}, \end{aligned}$$

where we use the following integral

$$K_{\frac{1}{2}}(a, b) = \int_0^\infty e^{-(a^2 t + \frac{b^2}{t})} t^{\frac{1}{2}} \frac{dt}{t} = \frac{\sqrt{\pi}}{a} e^{-2ab}.$$

When  $k_2 = 0$ , we can proceed with the help of the following summation formula:

$$\sum_{n=1}^{\infty} \frac{r^n}{n} = -\log(1 - r), \quad |r| < 1.$$

For  $I_2$ , we only need to calculate its value at  $s = 0, k_2 = 0$ . By taking first  $n = 0$  and using the double sum  $\sum_{m \neq 0} = \sum_{m=1}^{\infty} + \sum_{m=-1}^{-\infty}$ , we get the following summation formula:

$$\begin{aligned} &\sum_{m=1}^{\infty} \frac{1}{m} e^{2\pi i m((u - vx) + iyv)} + \sum_{m=1}^{\infty} \frac{1}{m} e^{2\pi i m(-(u - vx) + iyv)} \\ &= -\log(1 - e^{2\pi i(u - v\bar{\tau})})(1 - e^{-2\pi i(u - v\tau)}). \end{aligned}$$

Notice that  $m(u - vx) + n(k_1 - mx) + i|m| \cdot y \cdot |n + v|$  can be rewritten as  $m(u - v\bar{\tau} - n\bar{\tau}) + nk_1$  if  $mn > 0$  and  $m(u - v\tau - n\tau) + nk_1$  if  $mn < 0$ . Then for  $I_2$ , we have

$$\begin{aligned}
I_2 &= \frac{\pi}{y} \sum_{m \neq 0, m \in \mathbb{Z}} e^{2\pi i m(u-vx)} \sum_{n \in \mathbb{Z}} e^{2\pi i n(k_1 - mx)} \frac{1}{|m|} e^{-2\pi |my| \cdot |n+v|} \\
&= \frac{\pi}{y} \left( \sum_{m \neq 0, n=0} + \sum_{m>0, n>0} + \sum_{m<0, n<0} + \sum_{m>0, n<0} + \sum_{m<0, n>0} \right) \\
&= \frac{\pi}{y} \left( -\log(1 - e^{2\pi i(u-v\bar{\tau})})(1 - e^{-2\pi i(u-v\tau)}) - \sum_{n=1}^{\infty} e^{2\pi i n k_1} \log(1 - e^{2\pi i(u-v\bar{\tau}-n\bar{\tau})}) \right. \\
&\quad - \sum_{n=1}^{\infty} e^{-2\pi i n k_1} \log(1 - e^{2\pi i(v\bar{\tau}-n\bar{\tau}-u)}) - \sum_{n=1}^{\infty} e^{-2\pi i n k_1} \log(1 - e^{2\pi i(u-v\tau+n\tau)}) \\
&\quad \left. - \sum_{n=1}^{\infty} e^{2\pi i n k_1} \log(1 - e^{2\pi i(-u+v\tau+n\tau)}) \right) \\
&= \frac{\pi}{y} \left( -\log(1 - q_{\bar{z}})(1 - q_{-z}) - \sum_{n=1}^{\infty} e^{2\pi i n k_1} \log(|1 - q_{\bar{\tau}}^n q_z|^2) - \sum_{n=1}^{\infty} e^{-2\pi i n k_1} \log(|1 - q_{\bar{\tau}}^n / q_z|^2) \right) \\
&= \frac{\pi}{y} \left( -\log(|1 - q_z|^2) + 4\pi v y - \sum_{n=1}^{\infty} e^{2\pi i n k_1} \log(|1 - q_{\bar{\tau}}^n q_z|^2) - \sum_{n=1}^{\infty} e^{-2\pi i n k_1} \log(|1 - q_{\bar{\tau}}^n / q_z|^2) \right).
\end{aligned}$$

Here we have used the notations  $z = u - v\tau$ ,  $q_z = e^{2\pi i z}$ .

Therefore, combining all the calculation above, we have the Kronecker second limit of our  $E_{u,v,\mathbf{k}}(\tau, s)$  defined in (3.2) as follows

$$\begin{aligned}
E_{u,v,\mathbf{k}}(\tau) &= \lim_{s \rightarrow 1^+} E_{u,v,\mathbf{k}}(\tau, s) = \frac{\pi^2 e^{2\pi i z u} (1 - u + u e^{-2\pi i z})}{\sin^2(\pi k_1)} y + \pi \left( -\log(|1 - q_z|^2) + 4\pi^2 v y \right. \\
&\quad \left. - 2\pi \sum_{n=1}^{\infty} e^{2\pi i n k_1} \log(|1 - q_{\bar{\tau}}^n q_z|^2) - 2\pi \sum_{n=1}^{\infty} e^{-2\pi i n k_1} \log(|1 - q_{\bar{\tau}}^n / q_z|^2) \right) \\
&= 2\pi \left( q_{\bar{\tau}}^{\frac{1}{4} \frac{e^{2\pi i z u} (1 - u + u e^{-2\pi i z})}{\sin^2(\pi k_1)}} - \log |1 - q_z| + 2\pi v y \right. \\
&\quad \left. - \sum_{n=1}^{\infty} e^{2\pi i n k_1} \log |1 - q_{\bar{\tau}}^n q_z| - \sum_{n=1}^{\infty} e^{-2\pi i n k_1} \log |1 - q_{\bar{\tau}}^n / q_z| \right). \tag{3.5}
\end{aligned}$$

In (3.5), to obtain the regular part, we still need to calculate  $\lim_{u+iv \rightarrow 0} \log |1 - q_z|$ . In view of the notations in (1.6), we have

$$\begin{aligned}
&\lim_{\mathbf{x}=(x_1, x_2) \rightarrow \mathbf{0}} \left( -\frac{1}{2\pi} \log |1 - q_z| + \frac{1}{2\pi} \log \left| \frac{\mathbf{x}}{\sqrt{|\Lambda|}} \right| \right) \\
&= \lim_{\mathbf{x}=(x_1, x_2) \rightarrow \mathbf{0}} \left( -\frac{1}{2\pi} \log |1 - e^{2\pi y(x_1 + ix_2)}| + \frac{1}{2\pi} \log |\sqrt{y} \cdot \mathbf{x}| \right) \\
&= -\frac{1}{2\pi} \log \sqrt{y} - \frac{1}{2\pi} \log 2\pi. \tag{3.6}
\end{aligned}$$

For the remainder terms in  $E_{u,v,\mathbf{k}}(\tau)$  (3.5), it is straightforward to take limit since there are no singularities in the functions. Therefore, combining (1.11), we obtain Theorem 1.2.

To prove Theorem 1.3, we will use summation formula (3.4) in proving Theorem 1.2 and the main result in Theorem 1.1. By (3.4), one recognizes that the first part in (1.14) can be expanded

by singular and nonsingular part respectively in the following formula

$$\begin{aligned} \frac{(e^{2k_2\pi} - e^{-2k_2\pi})y}{4k_2\pi(e^{2k_2\pi} + e^{-2k_2\pi} - 2\cos(2k_1\pi))} - \frac{y}{4\pi|\mathbf{k}|^2} &= \frac{y}{4\pi^2} \left( \sum_{n \in \mathbb{Z}} \frac{1}{k_2^2 + (n - k_1)^2} - \frac{1}{k_2^2 + k_1^2} \right) \\ &= \frac{y}{4\pi^2} \sum_{n \in \mathbb{Z}, n \neq 0} \frac{1}{k_2^2 + (n - k_1)^2}. \end{aligned}$$

Now it is clear that

$$\lim_{\mathbf{k} \rightarrow \mathbf{0}} \left( \frac{(e^{2k_2\pi} - e^{-2k_2\pi})y}{4k_2\pi(e^{2k_2\pi} + e^{-2k_2\pi} - 2\cos(2k_1\pi))} - \frac{y}{4\pi|\mathbf{k}|^2} \right) = \frac{y}{4\pi^2} \sum_{n \in \mathbb{Z}, n \neq 0} \frac{1}{n^2} = \frac{y}{12}.$$

Once this is done, it is straightforward to find the limit formula in Theorem 1.3 by Theorem 1.1 after some elementary computation which we omit the details here.

#### 4. PROOF OF THEOREM 1.4

In this section, we give relatively concise expressions for regular part of the Bloch Green's function when  $\mathbf{k}$  are some given rational real numbers by using the fourth order Dedekind eta function. Note that the eta function is invariant under the modular group as we will see below.

Recall the Dedekind eta function as defined by

$$\eta_D(z) = e^{\frac{\pi iz}{12}} \prod_{n=1}^{\infty} (1 - e^{2\pi inz}).$$

It satisfies following two important properties of  $\eta_D(z)$  (see Apostol [2]):

$$\begin{aligned} \eta_D(\tau + 1) &= e^{\frac{\pi i}{12}} \eta_D(\tau), \\ \eta_D\left(-\frac{1}{\tau}\right) &= \sqrt{-i\tau} \eta_D(\tau). \end{aligned}$$

The eta function will be used in the current paper is

$$\eta(z) = \eta_D^4(z).$$

Then one has

$$\begin{aligned} \eta(\tau + 1) &= e^{\frac{\pi i}{3}} \eta(\tau), \\ \eta\left(-\frac{1}{\tau}\right) &= -\tau^2 \eta(\tau). \end{aligned}$$

Hence

$$\begin{aligned} |Im(\tau + 1)\eta(\tau + 1)| &= |Im(\tau)\eta(\tau)|, \\ |Im\left(-\frac{1}{\tau}\right)\eta\left(-\frac{1}{\tau}\right)| &= |Im(\tau)\eta(\tau)|. \end{aligned}$$

Note that the Modular group is generated by  $S : \tau \rightarrow \tau + 1$  and  $T : \tau \rightarrow -\frac{1}{\tau}$ . It follows that the function  $|Im(\tau)\eta(\tau)|$  is invariant under the Modular group. That is,

$$|Im(\Gamma(1)\tau)\eta(\Gamma(1)\tau)| = |Im(\tau)\eta(\tau)|.$$

Here the Modular group is

$$\Gamma(1)\tau = \left\{ \frac{a\tau + b}{c\tau + d} \mid ad - bc = 1; a, b, c, d \in \mathbb{Z} \right\}. \quad (4.1)$$

Our results in this section show that the regular part of the Bloch Green's function is related the function  $\log |Im(\tau)\eta(\tau)|$  and can be expressed by a linear combination of functions like  $|Im(\tau)\eta(\tau)|$  with different "frequencies".

We consider the case  $k_2 = 0$ . As in (1.17)[Theorem 1.2], we have

$$\begin{aligned} R_k(\tau) &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}q^{C(k)}| - \frac{1}{2\pi} \sum_{n=1}^{\infty} \cos(2\pi nk) \log |(1 - q^n)^2| \\ &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}| - \frac{1}{2\pi} \log |q^{C(k)} \prod_{n=1}^{\infty} (1 - q^n)^{2 \cos(2\pi nk)}|, \end{aligned} \quad (4.2)$$

where  $q = e^{2\pi i\tau}$ ,  $\tau = x + iy$  and

$$C(k) = \frac{1}{4\pi^2} \sum_{n \in \mathbb{Z}, k \in (0,1)} \frac{1}{|n - k|^2} = \frac{1}{4 \sin^2(\pi k)}.$$

Since

$$\lim_{k \rightarrow 0} \left( C(k) - \frac{1}{4\pi^2 k^2} \right) = \frac{1}{12},$$

we have

$$\lim_{k \rightarrow 0} \left( R_k(\tau) - \frac{y}{4\pi^2 k^2} \right) = R_0(\tau). \quad (4.3)$$

where  $R_0(\tau)$  is defined in (1.20) (Chen-Oshita [5]). This is the weak version of Theorem 1.3.

In the following, we will derive simplified forms of  $R_k(\tau)$  with  $k = \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{6}$  based on the eta functions.

We first consider  $R_{\frac{1}{2}}(\tau)$  by writing it in Euler modular form:

$$\begin{aligned} R_{\frac{1}{2}}(\tau) &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}q^{1/4}| + \frac{1}{2\pi} \log \left| \frac{\prod_{n=1}^{\infty} (1 - q^n)^2}{\prod_{n=1}^{\infty} (1 - q^{2n})^4} \right| \\ &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}| + \frac{1}{2\pi} \log \left| \frac{\eta^{1/2}(\tau)}{\eta(2\tau)} \right|, \quad \tau = x + iy \\ &= -\frac{1}{2\pi} \log 2\pi + \frac{1}{4\pi} \log |Im(\tau)\eta(\tau)| - \frac{1}{2\pi} \log |Im(2\tau)\eta(2\tau)| + \frac{1}{2\pi} \log 2. \end{aligned} \quad (4.4)$$

A theta function expression related to  $R_{\frac{1}{2}}(\tau)$  is

$$\theta_2(0, q) = \theta_{10}(0; \tau) = \frac{2\eta^2(2\tau)}{\eta(\tau)}.$$

Then we have  $R_{\frac{1}{2}}(\tau)$  expressed by theta function. That is,

$$R_{\frac{1}{2}}(\tau) = -\frac{1}{4\pi} \log |y\theta_{10}(\tau)| - \frac{1}{4\pi} \log |2\pi^2|.$$

For  $k = \frac{1}{3}$ , again by reforming it in Euler modular form, one deduces

$$\begin{aligned} R_{\frac{1}{3}}(\tau) &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}q^{1/3}| - \frac{1}{2\pi} \sum_{n=1}^{\infty} \cos\left(\frac{2\pi}{3}(3n-1)\right) \log |(1 - q^{3n-1})^2| \\ &\quad - \frac{1}{2\pi} \sum_{n=1}^{\infty} \cos\left(\frac{2\pi}{3}(3n-2)\right) \log |(1 - q^{3n-2})^2| - \frac{1}{2\pi} \sum_{n=1}^{\infty} \cos\left(\frac{2\pi}{3}(3n)\right) \log |(1 - q^{3n})^2| \\ &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}| + \frac{1}{2\pi} \log \left| \frac{q^{1/24} \prod_{n=1}^{\infty} (1 - q^n)}{(q^3)^{3/24} \prod_{n=1}^{\infty} (1 - (q^3)^n)^3} \right| \\ &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}| + \frac{1}{2\pi} \log \left| \frac{\eta^{1/4}(\tau)}{\eta^{3/4}(3\tau)} \right|, \quad \tau = x + iy \\ &= -\frac{1}{2\pi} \log 2\pi + \frac{1}{8\pi} \log |Im(\tau)\eta(\tau)| - \frac{3}{8\pi} \log |Im(3\tau)\eta(3\tau)| + \frac{3}{8\pi} \log 3. \end{aligned} \quad (4.5)$$

Next, for  $k = \frac{1}{4}, \frac{1}{6}$ , in a similar way by reforming the series in quotients of infinite products, one deduces that

$$\begin{aligned} R_{\frac{1}{4}}(\tau) &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}q^{1/2}| + \frac{1}{2\pi} \sum_{n=1}^{\infty} \log \left| \frac{(1-(q^2)^{2n-1})^2}{(1-(q^2)^{2n})^2} \right| \\ &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}| + \frac{1}{2\pi} \log \left| \frac{\eta^{1/2}(2\tau)}{\eta(4\tau)} \right|, \tau = x + iy \\ &= -\frac{1}{2\pi} \log 2\pi + \frac{1}{4\pi} \log |Im(2\tau)\eta(2\tau)| - \frac{1}{2\pi} \log |Im(4\tau)\eta(4\tau)| + \frac{1}{2\pi} \log \frac{4}{2^{1/2}}, \end{aligned} \quad (4.6)$$

and

$$\begin{aligned} R_{\frac{1}{6}}(\tau) &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}q| + \frac{1}{2\pi} \log \left| \prod_{n=1}^{\infty} \frac{(1-(q^2)^n)^2(1-(q^3)^n)^3}{(1-q^n)(1-(q^6)^n)^6} \right| \\ &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}| + \frac{1}{2\pi} \log \left| \frac{(q^2)^{1/12} \prod_{n=1}^{\infty} (1-(q^2)^n)^2 \cdot (q^3)^{1/8} \prod_{n=1}^{\infty} (1-(q^3)^n)^3}{q^{1/24} \prod_{n=1}^{\infty} (1-q^n) \cdot (q^6)^{1/4} \prod_{n=1}^{\infty} (1-(q^6)^n)^6} \right| \\ &= -\frac{1}{2\pi} \log |2\pi\sqrt{y}| + \frac{1}{2\pi} \log \left| \frac{\eta^{1/2}(2\tau)\eta^{3/4}(3\tau)}{\eta^{1/4}(\tau)\eta^{6/4}(6\tau)} \right| \\ &= -\frac{1}{2\pi} \log 2\pi + \frac{1}{4\pi} \log |Im(2\tau)\eta(2\tau)| + \frac{3}{8\pi} \log |Im(3\tau)\eta(3\tau)| \\ &\quad - \frac{1}{8\pi} \log |Im(\tau)\eta(\tau)| - \frac{3}{4\pi} \log |Im(6\tau)\eta(6\tau)| + \frac{1}{2\pi} \log \frac{6^{3/2}}{2^{1/2}3^{3/4}}. \end{aligned} \quad (4.7)$$

Now Theorem 1.4 follows from the simplified expressions in (4.4), (4.5), (4.6), and (4.7).

At the end of this section, we give some asymptotic behavior of  $R_{\frac{1}{2}}(\tau) - aR_0(\tau)$ , where  $a$  is a parameter. We start with the asymptotic behavior of  $\log |y\eta(iy)|$  by direct computation,

$$\log |y\eta(iy)| = -\frac{\pi}{3}y + \log y + o(\log y), \quad y \rightarrow +\infty. \quad (4.8)$$

By the invariance property, that is,  $|y\eta(iy)| = |\frac{1}{y}\eta(i\frac{1}{y})|$ , the limit behavior of  $\log |y\eta(iy)|$  at  $\infty$  (4.8) implies the limit behavior around zero. That is,

$$\log |y\eta(iy)| = -\frac{\pi}{3y} + \log \frac{1}{y} + o(\log \frac{1}{y}), \quad y \rightarrow 0^+. \quad (4.9)$$

For the asymptotic behavior of  $R_{\frac{1}{2}}(\tau) - aR_0(\tau)$  on the vertical line  $x = 0$ , combining (4.8) and (4.9), we have

$$\begin{aligned} R_{\frac{1}{2}}(\tau) - aR_0(\tau) &= \frac{1}{12}(3-a)y + \frac{a-1}{4\pi} \log y + o(\log y), \quad y \rightarrow +\infty, \\ &= -\frac{a-1}{12y} + \frac{a}{4\pi} \log \frac{1}{y} + o(\log \frac{1}{y}), \quad y \rightarrow 0^+. \end{aligned} \quad (4.10)$$

To ensure that  $R_{\frac{1}{2}}(\tau) - aR_0(\tau)$  has a maximum at some inside point of the upper plane, we need  $a \geq 3$ .

## 5. CRITICAL POINTS, EXTREME PROPERTIES AND PROOF OF THEOREM 1.5

In this section, we aim to study the critical points of  $R(\tau, \mathbf{k})$ , in view of the Conjecture stated at the end of Section 1. Although we have the explicit expression of  $R(\tau, \mathbf{k})$ , we are unable to find all the critical points of  $R(\tau, \mathbf{k})$  due to its complicated structure; in particular, locating all the max min points of  $R(\tau, \mathbf{k})$  seems difficult, which is exactly connect to Conjecture in the introduction.

As  $\mathbf{k} \rightarrow 0$ ,  $R(\tau, \mathbf{k})$  converges to  $R_0(\tau)$  with respect to the Bloch wave number  $\mathbf{k}$ , see (1.21) (Theorem 1.3). On the other hand, when  $k = \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{6}$ ,  $R(\tau, \mathbf{k})$  can be written linearly by  $R_0(\tau)$  [Theorem 1.4]. These facts motivate us to use the critical points of  $R_0(\tau)$  to find the critical points of  $R(\tau, \mathbf{k})$ .

To classify all the critical points of  $R_0(\tau)$ , we first study the monotonicity properties of  $R_0(\tau)$ . The horizontal monotonicity of  $R_0(\tau)$  was proved in Chen-Oshita [5], but this is not enough to classify all the critical points of  $R_0(\tau)$ . We then turn to construct the vertical monotonicity of  $R_0(\tau)$  [(5) in 5.1]. This also provides an alternative approach to find the minimum of  $R_0(\tau)$ . This is contained in the following proposition whose proof will be given at the end of the section.

**Proposition 5.1.** *For  $R_0(\tau)$ , the following properties hold*

- (1)  $\frac{\partial}{\partial y}R_0(0, y) \geq 0$  for  $y \geq 1$ , with “=” when  $y = 1$ ;
- (2)  $R_0(\frac{1}{2}, y)$  has and only has three critical points. They are  $\{\frac{\sqrt{3}}{6}, \frac{1}{2}, \frac{\sqrt{3}}{2}\}$ ;
- (3) Special values on the critical points are equal:  $R_0(0, 1) = R_0(\frac{1}{2}, \frac{1}{2})$ ,  $R_0(\frac{1}{2}, \frac{\sqrt{3}}{2}) = R_0(\frac{1}{2}, \frac{\sqrt{3}}{6})$ ;
- (4)  $\frac{\partial}{\partial y}|_{x^2+y^2=1}R_0(x, y) \geq 0$  for  $x \in [0, \frac{1}{2}]$ , with “=” when  $x = 0, \frac{1}{2}$ ;
- (5) On vertical monotonicity on the half fundamental domain.  $\frac{\partial}{\partial y}R_0(x, y) > 0$  on  $\{z = x+iy \in \mathbb{H} : |z| > 1 \text{ and } 0 < \text{Re}(z) < \frac{1}{2}\}$ ;
- (6) There is only one critical point on the line  $x = 0$ , which is  $(0, 1)$ ; there are only three critical points on the line  $x = \frac{1}{2}$ , which are  $(\frac{1}{2}, \frac{1}{2})$ ,  $(\frac{1}{2}, \frac{\sqrt{3}}{2})$ ,  $(\frac{1}{2}, \frac{\sqrt{3}}{6})$ .

We already know that  $R_0(\tau)$  is invariant under the modular group  $\Gamma(1)$  (See (4.1)). Direct calculation shows that  $R_0(\tau)$  is also invariant under the reflective transformation  $z \rightarrow -\bar{z}$ . The fundamental region under  $\Gamma(1)$  and reflective transformation is

$$\{z = x + iy \in \mathbb{H} := (x, y), y > 0 : |z| > 1 \text{ and } 0 < \text{Re}(z) < \frac{1}{2}\}$$

by number theory, see e.g. [6].

In the following Proposition, we show that  $(\frac{1}{2}, \frac{\sqrt{3}}{2})$  is a global minimum point (hence critical point) of  $R_0(\tau)$  [Chen-Oshita [5], Sandier-Serfaty [14]]. Actually, we can classify all the critical points of  $R_0(\tau)$ . In this direction, we also remark to the readers that there are some unknown but maybe interesting connection between our classification results about critical points of  $R_0(\tau)$  and the critical points of  $G_0(\mathbf{x}; \tau)$  as shown in Lin-Wang [10]. Actually,  $R_0(\tau)$  is the regular part of the Green's function  $G_0(\mathbf{x}; \tau)$  ((1.19)). Depending on the lattice structure(i.e.,  $\tau$ ), Lin-Wang [10] showed that the Green's function  $G_0(\mathbf{x}; \tau)$  has either 3 or 5 critical points.

**Proposition 5.2.**  *$R_0(\tau)$  only has two types of critical points, they are nondegenerate.*

- (1) Type 1:

$$(0, 1)/\{\frac{az+b}{cz+d}, a, b, c, d \in \mathbb{Z}, ad - bc = 1 \text{ or } -\bar{z}\},$$

i.e., the represent element is  $(0, 1)$  under the modular group and reflective transformation.

Type 2:

$$(\frac{1}{2}, \frac{\sqrt{3}}{2})/\{\frac{az+b}{cz+d}, a, b, c, d \in \mathbb{Z}, ad - bc = 1 \text{ or } -\bar{z}\};$$

- (2)  $(\frac{1}{2}, \frac{1}{2})$  and  $(\frac{1}{2}, \frac{\sqrt{3}}{6})$  is type 1 and type 2 critical point respectively;
- (3)  $(0, 1)$  is a nondegenerate saddle point and  $(\frac{1}{2}, \frac{\sqrt{3}}{2})$  is a global minimum point; All the critical points of  $R_0(\tau)$  are nondegenerate.

*Proof.* By (5) in Proposition 5.1, it follows that the points  $(0, 1)$  and  $(\frac{1}{2}, \frac{\sqrt{3}}{2})$  are the only critical points of  $R_0(x, y)$  on the region  $\{z = x + iy \in \mathbb{H} : |z| \geq 1 \text{ and } 0 \leq \text{Re}(z) \leq \frac{1}{2}\}$ . All the other critical points on the upper half plane are generated by these two points under the modular group and reflective transformation. This proves (1). (2) follows from (3) in Proposition 5.1. In  $y$  direction,  $(0, 1)$  is a global minimum, see (1) in Proposition 5.1 and (5.5). To complete the proof, we will show that in the  $x$  direction,  $(0, 1)$  is a local maximum point.

Direct calculation shows that

$$\frac{\partial}{\partial x}R_0(\tau) \Big|_{y=1} = \sum_{n=1}^{\infty} \frac{-2ne^{-2\pi n} \sin(2\pi nx)}{1 - 2e^{-2\pi n} \cos(2\pi nx) + e^{-4\pi n}}.$$

Using the elementary trigonometric inequality  $|\sin(na)| \leq n|\sin(a)|$  ( $a$  is any real number) and dividing the summation into  $n = 1$  and  $n \geq 2$ , we have

$$\begin{aligned}
-\frac{\partial}{\partial x} R_0(\tau) \Big|_{y=1} &= \left( \sum_{n=1}^1 + \sum_{n=2}^{\infty} \right) \frac{2ne^{-2\pi n} \sin(2\pi nx)}{1 - 2e^{-2\pi n} \cos(2\pi nx) + e^{-4\pi n}} \\
&\geq \frac{2e^{-2\pi} \sin(2\pi x)}{1 - 2e^{-2\pi} \cos(2\pi x) + e^{-4\pi}} - \sum_{n=2}^{\infty} \frac{2n^2 e^{-2\pi n} \sin(2\pi x)}{1 - 2e^{-2\pi n} \cos(2\pi nx) + e^{-4\pi n}} \\
&\geq 2e^{-2\pi} \sin(2\pi x) \left( \frac{1}{(1 + e^{-2\pi})^2} - \sum_{n=2}^{\infty} \frac{n^2 e^{-2\pi(n-1)}}{(1 - e^{-6\pi})^3} \right) \\
&= e^{-2\pi} \sin(2\pi x) \left( \frac{1}{(1 + e^{-2\pi})^2} - \frac{e^{-2\pi}(4 - 3e^{-2\pi} + e^{-4\pi})}{(1 - e^{-6\pi})^3(1 - e^{-2\pi})^3} \right) \\
&= e^{-2\pi} \sin(2\pi x) (0.9962755500 - 0.0075012615) \\
&\geq 0, \text{ for } x \in [0, \frac{1}{2}],
\end{aligned} \tag{5.1}$$

where we have used the summation formula

$$\sum_{n=2}^{\infty} n^2 r^n = r \left[ r \left[ \frac{r^2}{1-r} \right]' \right]' = \frac{r^2(4 - 3r + r^2)}{(1-r)^3}.$$

Notice that  $\frac{\partial}{\partial x} R_0(\tau) \Big|_{y=1}$  is an odd function, inequality (5.1) implies that  $R_0(\tau) \Big|_{y=1}$  has a local maximum at point  $x = 0$ .

By similar asymptotic analysis in (4.8) and (4.9), we deduce that  $\lim_{y \rightarrow 0^+} R_0(\tau) = +\infty$  and  $\lim_{y \rightarrow +\infty} R_0(\tau) = +\infty$ . This implies that  $R_0(\tau)$  admits a minimum for finite positive  $y$ . We already know that type 1 critical point  $(0, 1)$  is a saddle point. Then the global minimum point must be  $(\frac{1}{2}, \frac{\sqrt{3}}{2})$ . This provides an alternative proof of minimality of  $R_0(\tau)$  on the hexagonal point  $(\frac{1}{2}, \frac{\sqrt{3}}{2})$ .  $\square$

In view of (3) in the following Proposition 5.3, we obtain Theorem 1.5.

**Proposition 5.3.** *On critical points for regular part of the Bloch Green's function, we have*

- (1) *The regular parts  $R_{\frac{1}{2}}(\tau)$ ,  $R_{\frac{1}{3}}(\tau)$ ,  $R_{\frac{1}{4}}(\tau)$  has critical points  $(\frac{1}{2}, \frac{1}{2})$ ,  $(\frac{1}{2}, \frac{\sqrt{3}}{6})$ ,  $(\frac{1}{4}, \frac{1}{4})$  respectively. They all are nondegenerate saddle points;*
- (2) *If  $k = k_1$ , then the regular part  $= R_k(\tau) := R(\tau, k)$  has at least one critical point  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . In  $k$  direction, it is a local minimum; in  $\tau$  direction it is a saddle point.*
- (3) *(General case) The regular part  $R(\tau; \mathbf{k})$  has one critical point  $(\frac{1}{2}, \frac{\sqrt{3}}{2}, \frac{1}{2}, \approx 0.3)$ , which is a local  $\max_{\tau} \min_{\mathbf{k}}$  point. This is a numerical result.*

*Proof.* (1) : It follows from combinatorial identities (1.22) and Proposition 5.2.

(2) : Direct calculation gives  $\frac{\partial}{\partial k} R(\tau; \frac{1}{2}) = 0$  and  $R(\tau; \frac{1}{2}) = R_{\frac{1}{2}}(\tau)$ . Then (2) follows (1).

(3) : To find the critical points of  $R(\tau, \mathbf{k})$ , we need to calculate the partial derivatives. From (1.14), we have

$$\begin{aligned}
\frac{\partial}{\partial x} R(\tau, \mathbf{k}) &= - \sum_{n=1}^{\infty} \frac{n}{n - \frac{k_2}{y}} \sum_{m=1}^{\infty} m e^{-2\pi m(ny - k_2)} \sin(2\pi m(nx - k_1)) \\
&\quad - \sum_{n=1}^{\infty} \frac{n}{n + \frac{k_2}{y}} \sum_{m=1}^{\infty} m e^{-2\pi m(ny + k_2)} \sin(2\pi m(nx + k_1))
\end{aligned} \tag{5.2}$$

and



$$\begin{aligned}
\frac{\partial}{\partial k_1} R(\tau, \mathbf{k}) &= -\frac{y(e^{2k_2\pi} - e^{-2k_2\pi}) \sin(2k_1\pi)}{k_2(e^{2k_2\pi} + e^{-2k_2\pi} - 2\cos(2k_1\pi))^2} \\
&+ \sum_{n=1}^{\infty} \frac{1}{n - \frac{k_2}{y}} \sum_{m=1}^{\infty} m e^{-2\pi m(ny - k_2)} \sin(2\pi m(nx - k_1)) \\
&+ \sum_{n=1}^{\infty} \frac{1}{n + \frac{k_2}{y}} \sum_{m=1}^{\infty} m e^{-2\pi m(ny + k_2)} \sin(2\pi m(nx + k_1)).
\end{aligned} \tag{5.3}$$

It is obvious that  $\frac{\partial}{\partial x} R(x, y; k_1, k_2) = \frac{\partial}{\partial k_2} R(x, y; k_1, k_2) = 0$  if  $x = 0$  or  $\frac{1}{2}$  and  $k_1 = 0$  or  $k_1 = \frac{1}{2}$ .

From (5.2) and (5.3), we fix  $x = \frac{1}{2}, k_1 = \frac{1}{2}$ . Then by numerical finding the zero points of  $\frac{\partial}{\partial y} R(\tau; \mathbf{k}) = 0$  and  $\frac{\partial}{\partial k_1} R(\tau; \mathbf{k}) = 0$ , we obtain the result.  $\square$

**Proposition 5.4.** *On some properties of the regular part of the Bloch Green's function:*

- $R(\tau + 1; \mathbf{k}) = R(\tau; \mathbf{k});$
- $R(\tau; -\mathbf{k}) = R(\tau; \mathbf{k});$
- $R(\tau; \mathbf{k} + 1) = R(\tau; \mathbf{k});$
- $R(1 - \bar{\tau}; \mathbf{k}) = R(\tau; -\bar{\mathbf{k}});$

*Proof.* It follows directly from the formula (1.15).  $\square$

**Proof of Proposition 5.1.**

*Proof.* By straightforward calculation, we have

$$\frac{\partial^2}{\partial y^2} R_0(0, y) = \frac{1}{y^2} + \sum_{n=1}^{\infty} \frac{16\pi^2 n^2 e^{-2n\pi y}}{(1 - e^{-2\pi n y})^2} > 0 \text{ for } y > 0. \tag{5.4}$$

On the other hand,  $R_0(z) = R_0(-\frac{1}{z})$  gives  $R_0(0, y) = R_0(0, \frac{1}{y})$ . Consequently,

$$\frac{\partial}{\partial y} R_0(0, y) = -y^{-2} \frac{\partial}{\partial y} R_0(0, \frac{1}{y}). \tag{5.5}$$

It follows that  $\frac{\partial}{\partial y} R_0(0, 1) = 0$ . Combining (5.4), this proves (1). Since  $R_0(-\bar{z}) = R_0(z)$ , (1) implies that  $(0, 1)$  is a critical point of  $R_0(x, y)$ .

Let  $\tau\xi := -\frac{1}{\bar{\xi}}, \sigma\xi := -\bar{\xi}$ , hence  $\sigma\tau(\frac{1}{2} + iy) = \frac{2}{4y^2+1} + i\frac{4y}{4y^2+1}$ . The invariance of  $R_0(z)$  under the transforms  $\tau, \sigma$  gives

$$|y\eta(\frac{1}{2} + iy)| = |\frac{4y}{4y^2+1}\eta(\frac{2}{4y^2+1} + i\frac{4y}{4y^2+1})| \Rightarrow |\eta(\frac{1}{2} + iy)| = |\frac{4}{4y^2+1}\eta(\frac{2}{4y^2+1} + i\frac{4y}{4y^2+1})|.$$

Differentiating with respect to  $y$ , we have

$$\begin{aligned}
\frac{\partial}{\partial y} \log |\eta(\frac{1}{2} + iy)| &= -\frac{8y}{4y^2+1} + \frac{\partial}{\partial z} \Big|_{z=\frac{2}{4y^2+1}, w=\frac{4y}{4y^2+1}} \log |\eta(z + iw)| \\
&- \frac{4(4y^2-1)}{(4y^2+1)^2} \cdot \frac{\partial}{\partial w} \Big|_{z=\frac{2}{4y^2+1}, w=\frac{4y}{4y^2+1}} \log |\eta(z + iw)|.
\end{aligned} \tag{5.6}$$

On the other hand, direct computation of  $\log |\eta(z, w)|$  gives

$$\frac{\partial}{\partial z} \log |\eta(z + iw)| = \sum_{n=1}^{\infty} \frac{4n\pi e^{-2n\pi w} \sin(2n\pi z)}{1 + e^{-4n\pi w} - 2e^{-2n\pi w} \cos(2n\pi z)}. \tag{5.7}$$

Consequently,

$$\frac{\partial}{\partial z} \Big|_{z=\frac{1}{2}, w=\frac{\sqrt{3}}{2}} \log |\eta(z + iw)| = 0. \tag{5.8}$$

Inserting  $y = \frac{\sqrt{3}}{2}$  in (5.6) and combining (5.8), we have

$$\frac{\partial}{\partial y} \Big|_{y=\frac{\sqrt{3}}{2}} \log |\eta(\frac{1}{2} + iy)| = -\frac{2\sqrt{3}}{3}.$$

Hence  $\frac{\partial}{\partial y} \Big|_{y=\frac{\sqrt{3}}{2}} \log |y\eta(\frac{1}{2} + iy)| = 0$ . Next we derive a functional equation of  $\frac{\partial}{\partial y} R_0(\frac{1}{2}, y)$ . Since  $\xi \mapsto S(\xi) := \frac{\xi-1}{2\xi-1} \in \Gamma(1)$  and  $S(\frac{1}{2} + iy) = \frac{1}{2} + i\frac{1}{4y}$ , one deduces

$$R_0(\frac{1}{2}, y) = R_0(\frac{1}{2}, \frac{1}{4y}). \quad (5.9)$$

It follows that

$$\frac{\partial}{\partial y} R_0(\frac{1}{2}, y) = -\frac{1}{4y^2} \frac{\partial}{\partial y} R_0(\frac{1}{2}, \frac{1}{4y}). \quad (5.10)$$

Combining (5.10), one deduces that  $\frac{\partial}{\partial y} R_0(\frac{1}{2}, y)|_{y=\frac{1}{2}} = 0$ ,  $\frac{\partial}{\partial y} R_0(\frac{1}{2}, y)|_{y=\frac{\sqrt{3}}{6}} = 0$ . Along with the conclusion that the function  $\frac{\partial}{\partial y} R_0(\tau)|_{x=\frac{1}{2}}$  is positive on  $(\frac{\sqrt{3}}{6}, \frac{1}{2})$  and  $(\frac{\sqrt{3}}{2}, 1)$ , negative on  $(0, \frac{\sqrt{3}}{6})$  and  $(\frac{1}{2}, \frac{\sqrt{3}}{2})$  [13], we prove (2), (3).

(4): Consider the composition of the two maps  $z \rightarrow w' = \frac{z}{z+1}$ ,  $w \rightarrow 2w' - 1 = \frac{z-1}{z+1}$ , we have  $R_0(x, y) = R_0(u(x, y), v(x, y))$ , where  $u(x, y) = \frac{x^2+y^2-1}{(x+1)^2+y^2}$ ,  $v(x, y) = \frac{2y}{(x+1)^2+y^2}$ . Now differentiating with respect to  $y$ , we have

$$\frac{\partial}{\partial y} \Big|_{x^2+y^2=1} R_0(x, y) = \frac{x}{1+x} \frac{\partial}{\partial y} R_0(\frac{1}{2}, \frac{\sqrt{1-x^2}}{1+x}). \quad (5.11)$$

Here we have used that  $\frac{\partial v}{\partial y} \Big|_{x^2+y^2=1} = \frac{x}{1+x}$  and  $\frac{\partial}{\partial x} R_0(\frac{1}{2}, y) = 0$  (see (5.7)). Therefore (4) follows from (5.11) and (2).

Consider the transform  $z \rightarrow \frac{z}{z+1} \in \Gamma(1)$  which maps  $i$  to  $\frac{1}{2} + i\frac{1}{2}$ , by invariance property of  $R_0(\tau)$ , we have  $R_0(0, 1) = R_0(\frac{1}{2}, \frac{1}{2})$ .

(5): Note that

$$-\Delta \frac{\partial}{\partial y} R_0(x, y) = 2y^{-3} > 0.$$

Strong maximum principle and (1), (2), (4) imply (5).

(6): In view of (5.7), critical points of  $R_0(0, y)$ ,  $R_0(\frac{1}{2}, y)$  are critical points of  $R_0(x, y)$  automatically.

The proof of Proposition 5.1 is thus completed. □

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