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On Bessel series expressions for some lattice sums: II

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Abstract

In part I (Kanemitsu S *et al* 2003 *J. Northwest University*) we have made explicit use of the Mellin–Barnes integrals to prove the Chowla–Selberg-type Bessel series expressions for zeta-functions associated with lattice structures. In this paper we shall make implicit use of Mellin–Barnes integrals, as embedded in our theory of modular relations and functional equations, to reveal relationships between the structure of Madelung constants of the NaCl and CsCl lattices. Namely, we shall elucidate the relation between the structures of the NaCl lattice and those of the CsCl lattice, so to speak using the symmetry of the zeta-function, i.e. using their functional equations. Thus we shall emphasize the symmetry properties of the zeta-functions, restoring the Schlömilch series and Hardy's theory of K-Bessel functions, to prove the functional equations, and then to prove the recurrence relations for the lattice zeta-functions.

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Dedicated to Professor Kiyoshi Kikukawa on his sixtieth birthday

1. Introduction

The Madelung constant $\alpha_3(\mathrm{NaCl})$ for the (three-dimensional) NaCl crystal lattice is given by (-1) times the special value of the associated lattice zeta-function at $s = \frac{1}{2}$

$$\varphi_3(s) = \sum_{\underline{m}\in\mathbb{Z}^3}{}' \frac{(-1)^{s(\underline{m})}}{|\underline{m}|^{2s}} \qquad \sigma = \mathrm{Re}\, s > \frac{3}{2}$$

where $\underline{m} = (m_1, m_2, m_3)$ runs through all integer triples, the prime on the summation sign indicates that not all the entries of $\underline{m}$ are zero, $s(\underline{m})$ signifies the sum $m_1 + m_2 + m_3$, and $|\underline{m}| = \sqrt{m_1^2 + m_2^2 + m_3^2}$ gives the length of $\underline{m}$ (cf, e.g., [2, 3, 9, 21]).

In part I [15], we have given Bessel series expressions for the lattice sum zeta-functions generalizing those for CsCl structures as well as NaCl structures above, in a similar form as given by earlier authors [11]. The method used is a successful application of the Mellin–Barnes integrals, the analytic equivalent of the binomial theorem. This method was revived by recent applications of many Japanese number theorists in the mean square problems (cf [18]), but prior to this, Hardy [10] had already used it in his study of series and integrals involving binary quadratic forms, to which we shall make a contribution here. Then Koshlyakov [17] used it in the study of quadratic fields, and Berndt [1] made a very successful use of it to complete the theory of the Epstein zeta-function [19, 20].

In this paper we shall prove a recurrence formula for the κ-dimensional NaCl lattice zeta-function

$$\varphi_\kappa(s) = \sum_{\underline{m}\in\mathbb{Z}^\kappa}{}' \frac{(-1)^{s(\underline{m})}}{E(\underline{m})^s} \qquad \sigma > \frac{\kappa}{2} \tag{1.1}$$

where as above

$$E(\underline{m}) = m_1^2 + \cdots + m_\kappa^2 \qquad s(\underline{m}) = m_1 + \cdots + m_\kappa \tag{1.2}$$

with a generalized Dirichlet series admitting a Bessel series expression. From this we may inductively deduce a Bessel series expression for $\varphi_\kappa(s)$ itself. Since the main interest is in the case of $\varphi_3(s)$, the recurrence formula, containing $\varphi_2(s)$ and $\varphi_1(s)$, gives an immediate means for rapid calculation of the Madelung constant.

The method of proof is slightly different from that in part I, in that although we still use Mellin–Barnes integrals, we use them in an implicit form embodied in our theory of modular relations (and functional equations) [13, 14].

Let $Q = (a_{jk})_{j,k}$ be a positive definite matrix of degree κ and $Q(\underline{x}) = Q(x_1, \ldots, x_\kappa) = \sum_{j=1}^{\kappa}\sum_{k=1}^{\kappa} a_{jk}x_jx_k$ denote the corresponding positive definite quadratic form. For $\underline{\gamma} = (\gamma_1, \ldots, \gamma_\kappa)$, $\underline{\delta} = (\delta_1, \ldots, \delta_\kappa)$ let $Z\left|\frac{\underline{\gamma}}{\underline{\delta}}\right|(s)_Q = Z\left|\begin{smallmatrix}\gamma_1, \ldots, \gamma_\kappa\\ \delta_1, \ldots, \delta_\kappa\end{smallmatrix}\right|(s)_Q$ denote the associated Epstein zeta-function defined by

$$Z\left|\frac{\underline{\gamma}}{\underline{\delta}}\right|(s)_Q = Z\left|\begin{matrix}\gamma_1, \ldots, \gamma_\kappa\\ \delta_1, \ldots, \delta_\kappa\end{matrix}\right|(s)_Q = \sum_{\substack{\underline{m}\in\mathbb{Z}^\kappa\\ Q(\underline{m}+\underline{\gamma})\neq 0}} \frac{\mathrm{e}^{2\pi \mathrm{i}\underline{m}\cdot\underline{\delta}}}{Q(\underline{m}+\underline{\gamma})^{s/2}} \tag{1.3}$$

where $\underline{m} = (m_1, \ldots, m_\kappa) \in \mathbb{Z}^\kappa$ and $\underline{m}\cdot\underline{\delta}$ signifies the inner product $m_1\delta_1 + \cdots + m_\kappa\delta_\kappa$.

The Epstein zeta-function $Z\left|\frac{\underline{\gamma}}{\underline{\delta}}\right|(s)_Q$ satisfies the functional equation

$$\pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right) Z\left|\frac{\underline{\gamma}}{\underline{\delta}}\right|(s)_Q = \frac{\mathrm{e}^{-2\pi \mathrm{i}\underline{\gamma}\cdot\underline{\delta}}}{\sqrt{\det Q}}\pi^{-\frac{\kappa-s}{2}}\Gamma\left(\frac{\kappa-s}{2}\right) Z\left|\frac{\underline{\delta}}{-\underline{\gamma}}\right|(\kappa-s)_{Q^{-1}} \tag{1.4}$$

where Q^{-1} is the reciprocal form of Q (cf [7]).

Our $\varphi_\kappa(s)$ is a special case of $Z\left|\frac{\underline{\gamma}}{\underline{\delta}}\right|(s)_Q$ with $\underline{\gamma} = \underline{0}$, $\underline{\delta} = \underline{1/2} = \left(\frac{1}{2}, \ldots, \frac{1}{2}\right)$, $Q(\underline{x}) = |\underline{x}|^2 = x_1^2 + \cdots + x_\kappa^2$ and s replaced by $2s$

$$\varphi_\kappa(s) = Z\left|\frac{0}{\underline{1/2}}\right|(2s)_E \tag{1.5}$$

whose functional equation assumes the form

$$\pi^{-s}\Gamma(s)\varphi_\kappa(s) = \pi^{-(\frac{\kappa}{2}-s)}\Gamma\left(\frac{\kappa}{2}-s\right)\psi_\kappa\left(\frac{\kappa}{2}-s\right) \tag{1.6}$$

where

$$\psi_\kappa(s) = Z\left|\begin{matrix}\underline{1/2}\\ \underline{0}\end{matrix}\right|(2s)_E = \sum_{\underline{m}\in\mathbb{Z}^\kappa} \frac{1}{|\underline{m}+\underline{1/2}|^{2s}}. \tag{1.7}$$

For the CsCl crystal lattice with Cs^+ at the origin, the Madelung constant is given as the special value of the associated lattice zeta-function at $s = 1/2$

$$-\left(\frac{3}{4}\right)^s \xi_3(s) = \left(\frac{3}{4}\right)^s Z\left|\begin{matrix}\frac{1}{2} & \frac{1}{2} & \frac{1}{2}\\ 0 & 0 & 0\end{matrix}\right|(2s)_E - \left(\frac{3}{4}\right)^s Z\left|\begin{matrix}0 & 0 & 0\\ 0 & 0 & 0\end{matrix}\right|(2s)_E \tag{1.8}$$

where we note that $Z\left|\begin{smallmatrix}\frac{1}{2} & \frac{1}{2} & \frac{1}{2}\\ 0 & 0 & 0\end{smallmatrix}\right|(2s)_E$ occurring in the first term on the right-hand side of (1.8) is exactly the Dirichlet series $\psi_3(s)$ in (1.7) which appears in the functional equation (1.6) (cf section 3), and where

$$-\left(\frac{3}{4}\right)^s \xi_3(s) = -3^s Z\left|\begin{matrix}\underline{0}\\ \underline{1/2}\end{matrix}\right|(2s)_Q \qquad \text{with} \quad Q = \begin{pmatrix} 3 & -1 & -1\\ -1 & 3 & -1\\ -1 & -1 & 3\end{pmatrix}.$$

A consequence of relation (1.8) and its counterpart

$$Z\left|\begin{matrix}\underline{0}\\ \underline{1/2}\end{matrix}\right|(1)_Q = \frac{1}{2\pi}\left\{Z\left|\begin{matrix}\underline{0}\\ \underline{0}\end{matrix}\right|(2)_E - Z\left|\begin{matrix}\underline{0}\\ \underline{1/2}\end{matrix}\right|(2)_E\right\}$$

$$Z\left|\begin{matrix}\underline{0}\\ \underline{1/2}\end{matrix}\right|(1)_E = \frac{2}{\pi}\left\{Z\left|\begin{matrix}\underline{0}\\ \underline{0}\end{matrix}\right|(2)_Q - Z\left|\begin{matrix}\underline{0}\\ \underline{1/2}\end{matrix}\right|(2)_Q\right\}$$

shows the duality between NaCl and CsCl lattices (one is a dual of a sublattice of the other). A more thorough study of this and more will be conducted elsewhere.

In this paper we shall dwell on the effective use of the functional equation and its equivalents satisfied by the lattice zeta-function in question, first because these are lacking in most research by scholars of physical-chemical disciplines, except for Zucker [24] who derives the functional equations for $\sum \frac{1}{(m^2+n^2)^s}$, and secondly because it gives a clear picture of the duality of the lattice structure of NaCl and CsCl, and for other possible dual crystals.

Thus, in section 2.1 we shall first use Hautot's idea of using Schlömilch series to yield the Bessel series expression for $Z(s) = \sum'_{m,n} \frac{1}{(m^2+dn^2)^s}$ whence we deduce the functional equation for it. This Bessel series expansion is due to Chowla and Selberg [6, 19] and might be named after them, though the Chowla–Selberg formula usually refers to another formula.

Then we go to section 2.2 where we shall study Hardy's long-forgotten paper [10] and deduce the functional equation for the Epstein zeta-function $\zeta_Q(s) = \sum'_{m,n} \frac{1}{Q(m,n)^s}$, where $Q = Q(m,n) = am^2 + bmn + cn^2$ denotes a positive definite (binary) quadratic form, by completing his proof (Hardy confessed that he could not deduce the functional equation).

In section 3 we shall prove a recurrence formula for the κ-dimensional NaCl crystal zeta-function $\varphi_\kappa(s)$ and for the CsCl zeta-function $\psi_\kappa(s)$ referred to above, with a generalized Dirichlet series admitting the Bessel series expression.

We use the following standard notation. In the following $s = \sigma + \mathrm{i}t$ denotes a complex variable.

$\Gamma(s)$ denotes the gamma function defined by

$$\Gamma(s) = \int_0^\infty \mathrm{e}^{-u} u^{s-1}\,\mathrm{d}u \qquad \sigma > 0.$$

We introduce two basic Dirichlet series $\zeta(s)$, $\beta(s)$,

$$\zeta(s) = \sum_{n=1}^\infty \frac{1}{n^s} \qquad \sigma > 1$$

which is called the Riemann zeta-function, while

$$\beta(s) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{(2n-1)^s}$$

is identical with one of Dirichlet's L-functions

$$\beta(s) = L(s, \chi_4) = \sum_{n=1}^{\infty} \frac{\chi_4(n)}{n^s}$$

where $\chi_4(n)$ is defined to be 1, -1 or 0 according as $n \equiv 1 \pmod 4$, $n \equiv -1 \pmod 4$ or $n \equiv 0 \pmod 2$, respectively.

We use the standard Bessel functions

$$J_\nu(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\Gamma(\nu+n+1)} \left(\frac{z}{2}\right)^{\nu+2n} \tag{1.9}$$

denoting the ordinary Bessel function of the first kind, which is used in connection with Schlömilch series in section 2.1. $K_\nu(z)$ denotes the modified Bessel function defined either by

$$K_\nu(z) = \frac{1}{2}\int_0^\infty \exp\left(-\frac{1}{2}z(u+u^{-1})\right) u^{-\nu-1}\,\mathrm{d}u \tag{1.10}$$

or by

$$K_\nu(z) = \frac{\pi}{2}\frac{I_{-\nu}(z) - I_\nu(z)}{\sin \pi\nu} \tag{1.11}$$

(the limit is to be taken for $\nu \in \mathbb{Z}$) with $I_\nu(z)$ denoting the Bessel function

$$I_\nu(z) = \sum_{n=0}^{\infty} \frac{1}{n!\Gamma(\nu+n+1)} \left(\frac{z}{2}\right)^{\nu+2n}.$$

K_ν is used in the context of the inverse Heaviside integral (in (2.9))

$$\frac{1}{2\pi\mathrm{i}}\int_{(c)} \Gamma\left(s+\frac{\mu+\nu}{2}\right)\Gamma\left(s+\frac{\mu-\nu}{2}\right) x^{-s}\,\mathrm{d}s = 2x^{\mu/2}K_\nu(2\sqrt{x}) \tag{1.12}$$

valid for $c + \mathrm{Re}\,\frac{\mu+\nu}{2} \geqslant \mathrm{Re}\,\nu > 0$, where $\int_{(c)}$ denotes the vertical integral $\sigma = c$, $-\infty < t < \infty$.

In section 3 we use the following Mellin–Barnes integral:

$$\Gamma(s)(1+\lambda)^{-s} = \frac{1}{2\pi\mathrm{i}}\int_{(c)} \Gamma(s+z)\Gamma(-z)\lambda^z\,\mathrm{d}z \tag{1.13}$$

which holds under the condition $|\arg\lambda| < \pi$, $-\mathrm{Re}\,s < c < 0$.

We also need the following well-known formulae:

$$K_{n+\frac{1}{2}}(x) = \sqrt{\frac{\pi}{2x}}\mathrm{e}^{-x}\sum_{r=0}^{n}\frac{(n+r)!}{r!(n-r)!(2x)^r} \qquad (n \in \mathbb{N}\cup\{0\}) \tag{1.14}$$

$$K_\nu(x) \sim \sqrt{\frac{\pi}{2x}}\,\mathrm{e}^{-x}\sum_{r=0}^{\infty}\frac{\Gamma\left(\nu+r+\frac{1}{2}\right)}{\Gamma\left(\nu-r+\frac{1}{2}\right)r!(2x)^r} \qquad \left(|\arg x| < \frac{3\pi}{2}\right)$$

$$= O(x^{-\frac{1}{2}}\,\mathrm{e}^{-x}) \qquad \text{as } x \to \infty. \tag{1.15}$$

In the following $\sum_{n\in\mathbb{N}}$ means the summation over $n = 1, 2, \ldots$, $\sum_{m\in\mathbb{Z}}$ or $\sum_{m,n}$ etc means the summation over all integers, and the prime on the summation means that some terms are omitted which give rise to singularities of summands.

2. Bessel series for Epstein zeta-functions

2.1. Bessel series for $\sum'_{m,n} \frac{1}{(m^2+dn^2)^s}$ *via Schlömilch series*

We shall prove the following Chowla–Selberg-type identity, the formula itself was known to Kober [16, p 620, (5*a*)].

Theorem 1. *The zeta-function*

$$Z(s) = Z(s,d) = \sum_{m,n}{}' \frac{1}{(m^2+dn^2)^s} \qquad (d>0)$$

admits the Bessel series expression

$$Z(s) = 2\zeta(2s) + \frac{2\sqrt{\pi}}{d^{s-\frac{1}{2}}}\frac{\Gamma\left(s-\frac{1}{2}\right)}{\Gamma(s)}\zeta(2s-1) + \frac{8\pi^s}{d^{\frac{s}{2}-\frac{1}{4}}\Gamma(s)}\sum_{n=1}^{\infty} n^{s-\frac{1}{2}}\sigma_{1-2s}(n)K_{s-\frac{1}{2}}(2\pi\sqrt{d}n) \tag{2.1}$$

where $\sigma_a(n) = \sum_{d|n} d^a$ *denotes the sum of a*th *powers of divisors of n.*

For the proof we use the following results on Schlömilch series.

Lemma 1.
(i) [22, p 386] *For* $\mathrm{Re}\, s > 0$, $\mathrm{Re}\,(a \pm \mathrm{i}b) > 0$, *we have*

$$(a^2+b^2)^{-s} = \frac{2^{1-2s}\sqrt{\pi}}{\Gamma(s)}\int_0^{\infty} x^{2s-1}\,\mathrm{e}^{-ax}\frac{J_{s-\frac{1}{2}}(bx)}{(bx/2)^{s-1/2}}\,\mathrm{d}x.$$

(ii) (Schlömilch series, cf [11]). The Schlömilch series

$$g_s(x) = \frac{1}{2\Gamma(s+1)} + \sum_{m=1}^{\infty}\frac{J_s(mx)}{(mx/2)^s} = \frac{1}{2}\sum_{m=-\infty}^{\infty}\frac{J_s(mx)}{(mx/2)^s}$$

can be computed to be

$$g_s(x) = \begin{cases} \dfrac{\sqrt{\pi}}{x\Gamma\left(s+\frac{1}{2}\right)} & \text{for} \quad 0<x<2\pi \\[2ex] \dfrac{\sqrt{\pi}}{x\Gamma\left(s+\frac{1}{2}\right)} + \dfrac{2\sqrt{\pi}}{x\Gamma\left(s+\frac{1}{2}\right)}\displaystyle\sum_{n=1}^{q}\left(1-\left(\frac{2\pi n}{x}\right)^2\right)^{s-\frac{1}{2}} & \text{for} \quad 2q\pi<x<2(q+1)\pi. \end{cases}$$

(iii) The integral transform

$$Q_s(b) = \int_0^{\infty} \mathrm{e}^{-bx}x^{2s}g_s(x)\,\mathrm{d}x \qquad \mathrm{Re}\, s>0 \quad \mathrm{Re}\, b>0$$

has the expansion

$$Q_s(b) = 2^{2s-1}b^{-2s}\Gamma(s) + 2\left(\frac{2\pi}{b}\right)^s\sum_{l=1}^{\infty}(2l)^s K_s(2\pi bl).$$

Proof of theorem 1. We separate the part with $n=0$ from the sum to get

$$Z(s) = 2\zeta(2s) + \sum_{n=-\infty}^{\infty}{}'\sum_{m=-\infty}^{\infty}(dn^2+m^2)^{-s}.$$

We use lemma 1 (i) with $a=\sqrt{d}|n|$, $b=m$ and sum them for $m,n\in\mathbb{Z}$ for $\sigma>1$. Then

$$Z(s) = 2\zeta(2s) + \frac{2^{1-2s}\sqrt{\pi}}{\Gamma(s)}\sum_{n=-\infty}^{\infty}{}'\int_0^{\infty}x^{2s-1}\,\mathrm{e}^{-\sqrt{d}|n|x}\sum_{m=-\infty}^{\infty}\frac{J_{s-\frac{1}{2}}(mx)}{(mx/2)^{s-\frac{1}{2}}}\,\mathrm{d}x \tag{2.2}$$

where the inversion of order of the infinite sum and integration is justified by absolute convergence.

Since the innermost sum on the right-hand side is a Schlömilch series $2g_s(x)$, the integral in (2.2) can be evaluated in view of lemma 1(ii) in terms of Bessel series.

We record the process of transformations for the sake of completeness,

$$\begin{aligned} Z(s) &= 2\zeta(2s) + \frac{2^{2-2s}\sqrt{\pi}}{\Gamma(s)} \sum_{n=-\infty}^{\infty}{}' \int_0^{\infty} \exp(-\sqrt{d}|n|x) x^{2(s-\frac{1}{2})} g_{s-\frac{1}{2}}(x)\,\mathrm{d}x \\ &= 2\zeta(2s) + \frac{2^{2-2s}\sqrt{\pi}}{\Gamma(s)} \sum_{n=-\infty}^{\infty}{}' Q_{s-\frac{1}{2}}(\sqrt{d}|n|) \\ &= 2\zeta(2s) + \frac{\sqrt{\pi}}{\Gamma(s)} \sum_{n=-\infty}^{\infty}{}' (\sqrt{d}|n|)^{-2(s-\frac{1}{2})} \Gamma\left(s - \frac{1}{2}\right) \\ &\quad + \frac{4\pi^s}{d^{\frac{1}{2}(s-\frac{1}{2})}\Gamma(s)} \sum_{n=-\infty}^{\infty}{}' \sum_{l=1}^{\infty} \left(\frac{l}{|n|}\right)^{s-\frac{1}{2}} K_{s-\frac{1}{2}}(2\pi\sqrt{d}|n|l) \end{aligned}$$

whence (2.1) follows on writing $ln = m$ and introducing the σ-function. This completes the proof. □

Remark. As was pointed out by Chowla and Selberg ([19, section 5]), the Bessel series expression for $Z(s)$ implies its functional equation

$$\left(\frac{\pi}{\sqrt{d}}\right)^{-s} \Gamma(s)Z(s) = \left(\frac{\pi}{\sqrt{d}}\right)^{-(1-s)} \Gamma(1-s)Z(1-s). \tag{2.3}$$

This Hecke-type functional equation is the one which is satisfied by the Epstein zeta-function $\zeta_Q(s)$ associated with a positive definite (binary) quadratic form $Q = Q(m,n) = am^2 + 2bmn + cn^2$:

$$\pi^{-s}\Gamma(s)\zeta_Q(s) = |d|^{-\frac{1}{2}}\pi^{-(1-s)}\Gamma(1-s)\zeta_{Q^{-1}}(1-s) \tag{2.4}$$

where $d = b^2 - ac < 0$ denotes the discriminant and Q^{-1} denotes the reciprocal of Q given by

$$Q^{-1}(m,n) = \frac{1}{|d|}(cm^2 - 2bmn + an^2). \tag{2.5}$$

The functional equation for the zeta-function (1.4) of a positive definite quadratic form in κ variables was first proved by Epstein [7] by using the ϑ-transformation formula (or in other words, the Poisson summation formula in k dimensions.) Zucker [24] used similar methods to deduce functional equations for $Z(s)$ and also for the three-dimensional sum $\sum\sum\sum' \frac{1}{(l^2+m^2+n^2)^s}$.

2.2. *Hardy's argument*

Here we take up Hardy's idea of using the K-Bessel function, which is under our general spectrum in this paper, and prove the functional equation (2.4) by completing his argument.

Proof of functional equation (2.4) in terms of Hardy. We slightly change Hardy's notation, and write $Q = Q(m,n) = am^2 + 2bmn + cn^2$ instead of his $\alpha m^2 + 2\beta mn + \gamma n^2$. Define

$$\zeta_Q(s) = \sum_{m,n}{}' \frac{1}{Q(m,n)^s} \qquad \sigma > 1. \tag{2.6}$$

We use Hardy's normalized K-Bessel function $\psi_z(x)$ defined for $x > 0$, $z \in \mathbb{C}$ by ([10])

$$\psi_z(x) = x^{\frac{z+1}{2}} K_{z+\frac{1}{2}}(2x) = \int_0^\infty \exp(-t^2 - (x^2/t^2))t^z \,\mathrm{d}t \tag{2.7}$$

(cf (1.10)), 'normalized' in the sense that

$$\lim_{x\to 0+} \psi_z(x) = \frac{1}{2}\Gamma\left(\frac{z+1}{2}\right). \tag{2.8}$$

We use the Heaviside integral ([10, (30)], cf (1.12))

$$\int_0^\infty \psi_z(x)x^{s-1}\,\mathrm{d}x = \frac{1}{4}\Gamma\left(\frac{s}{2}\right)\Gamma\left(\frac{z+s+1}{2}\right) \tag{2.9}$$

valid for $\sigma > 0$ ($\mathrm{Re}\, z \geqslant -1$). We also use the function ([10, (25)])

$$\begin{aligned}\chi_z(u) &= \sum_{m,n} \psi_z(\pi\sqrt{Q}u)\\ &= \sum_{m,n} \psi_z\big(\pi\sqrt{am^2+2bmn+cn^2}u\big)\end{aligned} \tag{2.10}$$

and the theta-series

$$\vartheta(z)_Q = \sum_{m,n} \mathrm{e}^{-Q\pi z} \tag{2.11}$$

and recall its transformation formula ([7], [10, (69)])

$$\vartheta(z)_Q = \frac{1}{z\sqrt{|d|}}\vartheta\left(\frac{1}{z}\right)_{Q^{-1}} \tag{2.12}$$

with the inverse Q^{-1} defined by (2.5).

We note the consequence of (2.10) and (2.11)

$$\chi_z\left(\frac{\kappa}{\pi}\right) = \sum_{m,n}\psi_z(\kappa\sqrt{Q}) = \int_0^\infty \mathrm{e}^{-t^2}t^z\vartheta\left(\frac{\kappa^2}{\pi t^2}\right)_Q \mathrm{d}t. \tag{2.13}$$

Now, noting that the term corresponding to (0, 0) is missing in the defining sum of $\zeta_Q(s)$, we have, instead of [10, (76)],

$$\frac{1}{4}\Gamma(s)\Gamma\left(s+\frac{z+1}{2}\right)\pi^{-2s}\zeta_Q(s) = \int_0^\infty \left\{\chi_z(u) - \frac{1}{2}\Gamma\left(\frac{z+1}{2}\right)\right\}u^{2s-1}\,\mathrm{d}u \qquad \sigma > 1. \tag{2.14}$$

Then we follow Riemann's second proof of the functional equation for the Riemann zeta-function and split the range of integration into two—(0, 1) and (1, ∞)—and note that the integral extended over $1 < u$ represents an analytic function of s, all over $\mathbb{C}$.

To transform $\int_0^1 = \int_0^1 \left[\chi_z(u) - \frac{1}{2}\Gamma\left(\frac{z+1}{2}\right)\right]u^{2s-1}\,\mathrm{d}u$ we substitute (2.13) with $\kappa = \pi u$. Then we get

$$\begin{aligned}\int_0^1 &= \int_0^1 \chi_z(u)u^{2s-1}\,\mathrm{d}u - \frac{1}{2}\Gamma\left(\frac{z+1}{2}\right)\int_0^1 u^{2s-1}\,\mathrm{d}u\\ &= \int_0^1 u^{2s-1}\,\mathrm{d}u\int_0^\infty \mathrm{e}^{-t^2}t^z\vartheta\left(\frac{\pi u^2}{t^2}\right)_Q \mathrm{d}t - \frac{1}{2}\Gamma\left(\frac{z+1}{2}\right)\frac{1}{2s}\\ &= \int_0^\infty \mathrm{e}^{-t^2}t^z\int_0^1\vartheta\left(\frac{\pi u^2}{t^2}\right)_Q u^{2s-1}\,\mathrm{d}u\,\mathrm{d}t - \frac{1}{4s}\Gamma\left(\frac{z+1}{2}\right)\end{aligned} \tag{2.15}$$

with the interchange of the order of integration being justified by absolute convergence.

Applying the transformation formula (2.12), we rewrite the inner integral on the right-hand side of (2.15) as

$$\int_0^1 \frac{t^2}{\pi u^2\sqrt{|d|}}\vartheta\left(\frac{t^2}{\pi u^2}\right)_{Q^{-1}} u^{2s-1}\,\mathrm{d}u = \frac{t^2}{\pi\sqrt{|d|}}\left\{\int_0^1\left(\vartheta\left(\frac{t^2}{\pi u^2}\right)_{Q^{-1}}-1\right)u^{2s-3}\,\mathrm{d}u+\frac{1}{2s-2}\right\}. \tag{2.16}$$

Substituting (2.16) into (2.15), we see that

$$\int_0^1\left\{\chi_z(u)-\frac{1}{2}\Gamma\left(\frac{z+1}{2}\right)\right\}u^{2s-1}\,\mathrm{d}u = \frac{1}{\pi\sqrt{|d|}}\int_0^\infty \mathrm{e}^{-t^2}t^{z+2}\,\mathrm{d}t\int_0^1\left(\vartheta\left(\frac{t^2}{\pi u^2}\right)_{Q^{-1}}-1\right)u^{2s-3}\,\mathrm{d}u + \frac{1}{4\pi\sqrt{|d|}}\frac{1}{s-1}\Gamma\left(\frac{z+3}{2}\right)-\frac{1}{4s}\Gamma\left(\frac{z+1}{2}\right). \tag{2.17}$$

Finally, the change of variables u into u^{-1} in the inner integral on the right-hand side of (2.17) gives

$$\int_0^1\left(\vartheta\left(\frac{t^2}{\pi u^2}\right)_{Q^{-1}}-1\right)u^{2s-3}\,\mathrm{d}u=\int_1^\infty\left(\vartheta\left(\frac{t^2u^2}{\pi}\right)_{Q^{-1}}-1\right)u^{-2s+1}\,\mathrm{d}u$$

which is absolutely convergent over all the s-plane, and therefore, by changing the order of integration, we conclude that

$$\int_0^1\left\{\chi_z(u)-\frac{1}{2}\Gamma\left(\frac{z+1}{2}\right)\right\}u^{2s-1}\,\mathrm{d}u = \frac{1}{\pi\sqrt{|d|}}\int_1^\infty\int_0^\infty \mathrm{e}^{-t^2}t^{z+2}\left(\vartheta\left(\frac{t^2u^2}{\pi}\right)_{Q^{-1}}-1\right)u^{-2s+1}\,\mathrm{d}t\,\mathrm{d}u + \frac{\Gamma\left(\frac{z+3}{2}\right)}{4\pi\sqrt{|d|}}\frac{1}{s-1}-\frac{\Gamma\left(\frac{z+1}{2}\right)}{4}\frac{1}{s} \tag{2.18}$$

valid for all $s\in\mathbb{C}$.

Now we suppose $\operatorname{Re}s<0$, and apply a similar argument to the integral over $(1,\infty)$. First, replace u by $1/u$.

Corresponding to (2.15), we have

$$\int_1^\infty\left\{\chi_z(u)-\frac{1}{2}\Gamma\left(\frac{s+1}{2}\right)\right\}u^{2s-1}\,\mathrm{d}u = \int_0^\infty \mathrm{e}^{-t^2}t^z\,\mathrm{d}t\int_1^\infty\vartheta\left(\frac{\pi u^2}{t^2}\right)_Q u^{2s-1}\,\mathrm{d}u+\frac{\Gamma\left(\frac{z+1}{2}\right)}{4s}. \tag{2.19}$$

In place of (2.16) we have

$$\int_1^\infty\vartheta\left(\frac{\pi u^2}{t^2}\right)_Q u^{2s-1}\,\mathrm{d}u=\frac{t^2}{\pi\sqrt{|d|}}\left\{\int_1^\infty\left(\vartheta\left(\frac{t^2}{\pi u^2}\right)_{Q^{-1}}-1\right)u^{2s-3}\,\mathrm{d}u-\frac{1}{2s-2}\right\} \tag{2.20}$$

whence as a substitute of (2.17) we have

$$\int_1^\infty \left[\chi_z(u) - \frac{1}{2}\Gamma\left(\frac{s+1}{2}\right)\right] u^{2s-1}\,\mathrm{d}u$$
$$= \frac{1}{\pi\sqrt{|d|}}\int_0^\infty \mathrm{e}^{-t^2} t^{z+2}\int_0^1 \left(\vartheta\left(\frac{t^2u^2}{\pi}\right)_{Q^{-1}} - 1\right) u^{1-2s}\,\mathrm{d}t\,\mathrm{d}u$$
$$- \frac{\Gamma\left(\frac{s+3}{2}\right)}{4\pi\sqrt{|d|}}\frac{1}{s-1} + \frac{\Gamma\left(\frac{z+1}{2}\right)}{4}\frac{1}{s}. \tag{2.21}$$

And finally we obtain the counterpart of (2.18)

$$\int_1^\infty \left\{\chi_z(u) - \frac{1}{2}\Gamma\left(\frac{s+1}{2}\right)\right\} u^{2s-1}\,\mathrm{d}u$$
$$= \frac{1}{\pi\sqrt{|d|}}\int_0^1 u^{-2s+1}\int_0^\infty \mathrm{e}^{-t^2} t^{z+2}\left(\vartheta\left(\frac{t^2u^2}{\pi}\right)_{Q^{-1}} - 1\right)\mathrm{d}t\,\mathrm{d}u$$
$$- \frac{\Gamma\left(\frac{s+3}{2}\right)}{4\pi\sqrt{|d|}}\frac{1}{s-1} + \frac{\Gamma\left(\frac{z+1}{2}\right)}{4}\frac{1}{s}. \tag{2.22}$$

Substituting (2.18) and (2.22) into (2.14) gives

$$\frac{1}{4}\Gamma(s)\Gamma\left(s+\frac{z+1}{2}\right)\pi^{-2s}\zeta_Q(s)$$
$$= \frac{1}{\pi\sqrt{|d|}}\int_0^\infty u^{-2s+1}\int_0^\infty \mathrm{e}^{-t^2} t^{z+2}\left(\vartheta\left(\frac{t^2u^2}{\pi}\right)_{Q^{-1}} - 1\right)\mathrm{d}t\,\mathrm{d}u \tag{2.23}$$

whereby we note that the range of integral with respect to u is $0 < u < \infty$.

Again, a change of variable u to u^{-1} leads to

$$\frac{1}{4}\Gamma(s)\Gamma\left(s+\frac{z+1}{2}\right)\pi^{-2s}\zeta_Q(s)$$
$$= \frac{1}{\pi\sqrt{|d|}}\int_0^\infty u^{2s-3}\int_0^\infty \mathrm{e}^{-t^2} t^{z+2}\left(\vartheta\left(\frac{t^2}{\pi u^2}\right)_{Q^{-1}} - 1\right)\mathrm{d}t\,\mathrm{d}u. \tag{2.24}$$

Now the inner integral on the right-hand side can be evaluated as in Hardy ([10, p 372], the last two lines)

$$\int_0^\infty \mathrm{e}^{-t^2} t^{z+2}\left(\vartheta\left(\frac{t^2}{\pi u^2}\right)_{Q^{-1}} - 1\right)\mathrm{d}t = \frac{1}{2}\Gamma\left(\frac{z+3}{2}\right)\sum_{m,n}{}'\left(1+\frac{Q^{-1}}{\sqrt{|d|}u^2}\right)^{-\frac{1}{2}(z+3)}$$

which we substitute into (2.24) to obtain

$$\frac{1}{4}\Gamma(s)\Gamma\left(s+\frac{z+1}{2}\right)\pi^{-2s}\zeta_Q(s)$$
$$= \frac{\Gamma\left(\frac{z+3}{2}\right)}{2\pi\sqrt{|d|}}\sum_{m,n}{}'\int_0^\infty\left(1+\frac{cm^2-2bmn+an^2}{\sqrt{|d|}u^2}\right)^{-\frac{1}{2}(z+3)} u^{2s-3}\,\mathrm{d}u. \tag{2.25}$$

Recalling the formula ([10, (77)])

$$\sum_{m\cdot n}{}' \int_0^\infty \left(1+\frac{cm^2-2bmn+an^2}{\sqrt{|d|}u^2}\right)^{-\frac{1}{2}(z+3)} u^{2s-3}\,\mathrm{d}u$$

$$= \frac{1}{2}\frac{\Gamma(1-s)\Gamma\left(s+\frac{z+1}{2}\right)}{\Gamma\left(\frac{z+3}{2}\right)} \sum_{m,n}{}' \left(\frac{\sqrt{|d|}}{cm^2-2bmn+an^2}\right)^{1-s} \tag{2.26}$$

we finally arrive at the formula

$$\frac{1}{4}\Gamma(s)\Gamma\left(s+\frac{z+1}{2}\right)\pi^{-2s}\zeta_Q(s) = \frac{1}{4\pi}\Gamma(1-s)\Gamma\left(s+\frac{z+1}{2}\right)|d|^{\frac{1}{2}-s}\zeta_{Q^{-1}}(1-s). \tag{2.27}$$

The functional equation (2.4) is nothing but formula (2.27) expressed in more symmetric form. This completes the proof of (2.4).

We remark that formula (2.26) depends on the inverse Mellin–Barnes integral (cf section 1 and (1.13)). □

3. Bessel series expressions for Madelung constants of the NaCl and CsCl lattices

Our purpose is to prove the following two theorems which exhibit the duality between NaCl and CsCl structures.

Theorem 2. *For the NaCl lattice zeta-function $\varphi_\kappa(s)$ defined by (1.1), we have*

$$\pi^{-s}\Gamma(s)\left(\varphi_{\kappa+1}(s)-\varphi_\kappa(s)\right) = 2^{\kappa+2}\sum_{\underline{k}\in\mathbb{N}^\kappa}|\underline{k-1/2}|^{s-\frac{\kappa}{2}}\sum_{m\in\mathbb{N}}(-1)^m m^{\frac{\kappa}{2}-s}K_{s-\frac{\kappa}{2}}(2\pi m|\underline{k-1/2}|) \tag{3.1}$$

for $\kappa \geqslant 1$.

Corollary 1. *Let $\alpha_\kappa(NaCl)$ be a κ-dimensional Madelung constant for NaCl defined by $\alpha_\kappa(NaCl) = -\varphi_\kappa(1/2)$. Then we have*

(i) $\alpha_1(NaCl) = 2\log 2.$

(ii)
$$\begin{aligned}\alpha_2(NaCl) &= 4(1-\sqrt{2})\zeta(1/2)\,L(1/2,\chi_4)\\ &= 8\sum_{k,m\in\mathbb{N}}(-1)^{m-1}K_0(\pi m(2k-1)) + 2\log 2\\ &= 8\sum_{m\in\mathbb{N}}K_0(\pi m)\sigma_0(m) - 24\sum_{m\in\mathbb{N}}K_0(2\pi m)\sigma_0(m)\\ &\quad + 16\sum_{m\in\mathbb{N}}K_0(4\pi m)\sigma_0(m) + 2\log 2\end{aligned}$$

where in the first equality, $L(s,\chi_4)$ is the Dirichlet L-function for χ_4 defined in section 1 and in the second and third equalities, K_0 stands for the modified Bessel functions defined by (1.10) and (1.11), and $\sigma_0(n)$ is the number of divisors of n, i.e., $\sigma_0(n) = \sum_{d|n} 1$.

(iii)
$$\alpha_3(NaCl) = \alpha_2(NaCl) + 16\sum_{k_1,k_2\in\mathbb{N}}\frac{1}{\sqrt{(2k_1-1)^2+(2k_2-1)^2}} \times \frac{1}{\exp\left(\pi\sqrt{(2k_1-1)^2+(2k_2-1)^2}\right)+1}.$$

For the normalized CsCl crystal lattice with Cs^+ at the origin, the Cs^+ ions are at $\underline{m} = (l, m, n) \in \mathbb{Z}^3$ while the Cl^- ions are at $\underline{m + 1/2}$ with $\underline{m} \in \mathbb{Z}^3$. Hence the CsCl lattice zeta-function $M_3(s)$, up to a magnification factor, is given by

$$\sum_{\underline{m}\in\mathbb{Z}^3}{}' \frac{-1}{\left(\left(\frac{2}{\sqrt{3}}l\right)^2 + \left(\frac{2}{\sqrt{3}}m\right)^2 + \left(\frac{2}{\sqrt{3}}n\right)^2\right)^s} + \sum_{\underline{m}\in\mathbb{Z}^3} \frac{1}{\left(\left(\frac{2}{\sqrt{3}}\left(l+\frac{1}{2}\right)\right)^2 + \left(\frac{2}{\sqrt{3}}\left(m+\frac{1}{2}\right)\right)^2 + \left(\frac{2}{\sqrt{3}}\left(n+\frac{1}{2}\right)\right)^2\right)^s}$$

which is precisely (1.8)

$$\left(\frac{3}{4}\right)^s \psi_3(s) - \left(\frac{3}{4}\right)^s Z_3(s) \tag{3.2}$$

where

$$\psi_3(s) = \sum_{\underline{m}\in\mathbb{Z}^3} \frac{1}{|\underline{m+1/2}|^{2s}} \qquad \text{and} \qquad Z_3(s) = \sum_{\underline{m}\in\mathbb{Z}^3}{}' \frac{1}{|\underline{m}|^{2s}}.$$

In view of (3.2), we introduce the κ-dimensional CsCl lattice zeta-function $\xi_\kappa(s)$ and Madelung constant through

$$\xi_\kappa(s) = Z_\kappa(s) - \psi_\kappa(s) \tag{3.3}$$

and

$$\alpha_\kappa(\mathrm{CsCl}) = -\frac{\sqrt{\kappa}}{2}\xi_\kappa\left(\frac{1}{2}\right) \tag{3.4}$$

where $\psi_\kappa(s)$ is defined by (1.7) and

$$Z_\kappa(s) = Z\begin{vmatrix} 0\cdots 0 \\ 0\cdots 0 \end{vmatrix}(2s)_E = \sum_{\underline{m}\in\mathbb{Z}^\kappa}{}' \frac{1}{|\underline{m}|^{2s}} \tag{3.5}$$

is the Epstein zeta-function for the identity matrix E studied extensively in part I.

Theorem 3. *The CsCl lattice zeta-function $\xi_\kappa(s)$ defined by (3.3) satisfies*

$$\begin{aligned}\pi^{-s}\Gamma(s)\xi_{\kappa+1}(s) &= 4\sum_{m\in\mathbb{N}}\sum_{\underline{k}\in\mathbb{Z}^\kappa}{}' m^{\frac{\kappa}{2}-s}|\underline{k}|^{s-\frac{\kappa}{2}}K_{s-\frac{\kappa}{2}}(2\pi m|\underline{k}|) \\ &\quad - 4\sum_{m\in\mathbb{N}}\sum_{\underline{k}\in\mathbb{Z}^\kappa}{}' \left(m-\frac{1}{2}\right)^{\frac{\kappa}{2}-s}(-1)^{s(\underline{k})}|\underline{k}|^{s-\frac{\kappa}{2}}K_{s-\frac{\kappa}{2}}\left(2\pi\left(m-\frac{1}{2}\right)|\underline{k}|\right) \\ &\quad + \pi^{-s}\Gamma(s)Z_\kappa(s) + \pi^{-s+\frac{\kappa}{2}}\Gamma\left(s-\frac{\kappa}{2}\right)\xi_1\left(s-\frac{\kappa}{2}\right),\end{aligned}$$

where $|\underline{k}| = \sqrt{k_1^2 + \cdots + k_\kappa^2}$ and $s(\underline{k}) = k_1 + \cdots + k_\kappa$ for $\underline{k} = (k_1, \ldots, k_\kappa)$.

Corollary 2. *The Madelung constants $\alpha_1(CsCl)$ and $\alpha_2(CsCl)$ are the same as those of NaCl respectively, while for the three-dimensional CsCl lattice, it is given by*

$$\begin{aligned}\alpha_3(CsCl) &= -\frac{\sqrt{3}}{2}\xi_3\left(\frac{1}{2}\right) \\ &= -\sqrt{3}\sum_{(k_1,k_2)\neq(0,0)} \frac{1}{\sqrt{k_1^2+k_2^2}}\frac{1}{\exp\left(2\pi\sqrt{k_1^2+k_2^2}\right)-1} \\ &\quad + 2\sqrt{3}\sum_{(k_1,k_2)\neq(0,0)} \frac{(-1)^{k_1+k_2}}{\sqrt{k_1^2+k_2^2}}\frac{1}{\sinh\left(\pi\sqrt{k_1^2+k_2^2}\right)} + \frac{\sqrt{3}(\sqrt{2}+1)}{2}\alpha_2(CsCl) - \frac{\sqrt{3}\pi}{8}.\end{aligned}$$

We note that the equalities $\alpha_j(\text{CsCl}) = \alpha_j(\text{NaCl})$ ($j = 1, 2$) are also observed by the structure of crystals of CsCl and NaCl.

To prove these theorems we recall Hecke's theory of functional equations developed by Berndt [1] and by us [13, 14].

Definition. *The two Dirichlet series $\varphi(s)$ and $\psi(s)$ formed from*

$$0 < \lambda_1 < \lambda_2 < \cdots \qquad 0 < \mu_1 < \mu_2 < \cdots$$

and $\{a_n\}$, $\{b_n\}$,

$$\varphi(s) = \sum_{n=1}^{\infty} \frac{a_n}{\lambda_n^s} \qquad \psi(s) = \sum_{n=1}^{\infty} \frac{b_n}{\mu_n^s},$$

absolutely convergent in some half-plane, are said to satisfy Hecke's functional equation ($A > 0, c \in \mathbb{C}$ constants)

$$A^{-s}\Gamma(s)\varphi(s) = cA^{-(\delta-s)}\Gamma(\delta - s)\psi(\delta - s) \tag{3.6}$$

if there exists a function $\chi(s) = \chi_A(s)$ holomorphic outside a compact set $\mathcal{S}$, convex in any finite strip, coinciding with $A^{-s}\Gamma(s)\varphi(s)$ and $cA^{-(\delta-s)}\Gamma(\delta - s)\psi(\delta - s)$ in the respective region of absolute convergence.

Define the residual function $P(x)$ by

$$P(x) = P_A(x) = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} \chi_A(s) x^{-s} \,\mathrm{d}s \tag{3.7}$$

where $\mathcal{C}$ is a closed curve or curves enclosing $\mathcal{S}$.

Then we have the following lemma.

Lemma 2 ([1, 14])**.** *The Hurwitz-type Dirichlet series $\varphi(s, \alpha)$ associated with $\varphi(s)$*

$$\varphi(s, \alpha) = \sum_{n=1}^{\infty} \frac{a_n}{(\lambda_n + \alpha)^s} \tag{3.8}$$

admits the representation

$$A^{-s}\Gamma(s)\varphi(s, \alpha) = 2c\alpha^{\frac{\delta-s}{2}} \sum_{n=1}^{\infty} b_n \mu_n^{\frac{s-\delta}{2}} K_{s-\delta}(2A\sqrt{\alpha\mu_n}) + \int_0^{\infty} \mathrm{e}^{-\alpha A u} u^{s-1} P(u) \,\mathrm{d}u, \tag{3.9}$$

for $\sigma > \max\left\{\delta - \frac{1}{2}, -1\right\}$, $s \neq 0$.

Conversely, if $\varphi(s, \alpha)$ satisfies (3.9), then (3.6) holds.

We apply this with the following designations: $\{\lambda_n\}$ is the sequence of all possible values of $|\underline{m}|^2 = m_1^2 + \cdots + m_\kappa^2$ arranged in increasing order and $a_n = \sum_{|\underline{m}|^2=\lambda_n} (-1)^{s(\underline{m})}$ and similarly, $\{\mu_n\}$ is the sequence of all possible values of $|\underline{m + 1/2}|^2$ arranged in increasing order and $b_n = \sum_{|\underline{m+1/2}|^2=\mu_n} 1$.

Then the lattice zeta-functions

$$\varphi_\kappa(s) = \sum_{n=1}^{\infty} \frac{a_n}{\lambda_n^s} = \sum_{\underline{m}\in\mathbb{Z}^\kappa}{}' \frac{(-1)^{s(\underline{m})}}{|\underline{m}|^{2s}}$$

and

$$\psi_\kappa(s) = \sum_{n=1}^{\infty} \frac{b_n}{\mu_n^s} = \sum_{\underline{m}\in\mathbb{Z}^\kappa} \frac{1}{|\underline{m + 1/2}|^{2s}}$$

satisfy the Hecke functional equation (1.6); thus $A = \pi, c = 1, \delta = \kappa/2$ (recall (1.5) and (1.7)), as a special case of Epstein's result [7]. From the modular relation (for which we refer to [13, 14]), we may prove that the residual function is

$$P(x) = P_A(x) = -1. \tag{3.10}$$

Therefore its Borel transform $\int_0^\infty e^{-\alpha\pi u} u^{s-1} P(u)\, du$ is $-\Gamma(s)(\alpha\pi)^{-s}$.

Hence lemma 2 reads

$$\pi^{-s}\Gamma(s)\varphi_\kappa(s,\alpha) = 2\alpha^{\frac{\kappa/2-s}{2}} \sum_{\underline{k}\in\mathbb{Z}^\kappa} |\underline{k+1/2}|^{s-\frac{\kappa}{2}} K_{s-\frac{\kappa}{2}}(2\pi\sqrt{\alpha}|\underline{k+1/2}|) - \frac{\Gamma(s)}{(\alpha\pi)^s}. \tag{3.11}$$

We are now in a position to establish the following lemma.

Lemma 3. *For the NaCl lattice zeta-function* $\varphi_\kappa(s)$ *we have*

(i) $\varphi_1(s) = (2^{1-2s}-1)Z_1(s) = 2(2^{1-2s}-1)\zeta(2s)$,

(ii) $\varphi_2(s) = (2^{1-s}-1)Z_2(s) = 4(2^{1-s}-1)\zeta(s)L(s,\chi_4)$,

(iii) $\varphi_{\kappa+1}(s) - \varphi_\kappa(s) = 2\sum_{m\in\mathbb{N}}(-1)^m\varphi_\kappa(s,m^2) + \varphi_1(s)$.

Proof. (i) and (ii) can be proved directly from the definition and the standard decomposition of the Dedekind zeta-function of the Gaussian field $\mathbb{Q}(i)$ into the product of the Riemann zeta-function and Dirichlet L-function going back to Gauss (cf part I, (3.4)).

To prove (iii) we separate the sum over $(\underline{m}, m_{\kappa+1}) = (m_1, \ldots, m_\kappa, m_{\kappa+1})$ into three parts: $m_{\kappa+1} \neq 0$ and $\underline{m} \neq 0$; $m_{\kappa+1} \neq 0$ and $\underline{m} = \underline{0}$; and $\underline{m} \neq \underline{0}$ and $m_{\kappa+1} = 0$. Then

$$\varphi_{\kappa+1}(s) = \sum_{0\neq m_{\kappa+1}\in\mathbb{Z}} (-1)^{m_{\kappa+1}} \sum_{\underline{0}\neq\underline{m}\in\mathbb{Z}^\kappa} \frac{(-1)^{s(\underline{m})}}{\left(|\underline{m}|^2 + m_{\kappa+1}^2\right)^s} + \sum_{0\neq m_{\kappa+1}\in\mathbb{Z}} \frac{(-1)^{m_{\kappa+1}}}{m_{\kappa+1}^{2s}} + \varphi_\kappa(s)$$

which amounts to (iii) on account of (3.8), and the proof is complete. □

Proof of theorem 2. Multiplying both sides of lemma 3 (iii) by $\pi^{-s}\Gamma(s)$ and applying (3.11) to each $\varphi_\kappa(s, m^2)$, we have the assertion of theorem 2. □

Proof of corollary 1. (i) follows by taking the limit as $s \to \frac{1}{2}$ of lemma 3 (i).

The first equality in (ii) is a consequence of lemma 3 (ii).

The second equality is a consequence of theorem 2 with $\kappa = 1$, $s = \frac{1}{2}$ and (i).

To prove the third equality, we introduce the divisor function

$$\sigma_0^*(n) = \sum_{d|n}(-1)^d. \tag{3.12}$$

We may easily prove that

$$\sigma_0^*(n) = -\sigma_0(n) + \begin{cases} 0 & n \text{ odd} \\ 2\sigma_0(\frac{n}{2}) & n \text{ even.} \end{cases} \tag{3.13}$$

Noting that the sum in the second equality can be expressed as

$$\sum_{k,m}(-1)^{m-1}K_0(\pi mk) - \sum_{k,m}(-1)^{m-1}K_0(2\pi mk)$$

or

$$-\sum_{m\in\mathbb{N}} K_0(\pi m)\sigma_0^*(m) + \sum_{m\in\mathbb{N}} K_0(2\pi m)\sigma_0^*(m)$$

we may apply (3.13) to conclude the third equality.

Finally, we turn to the proof of (iii). Recalling that $K_{\frac{1}{2}}(z) = \sqrt{\frac{\pi}{2z}}\, e^{-z}$ (from (1.14)), we deduce from (3.1) with $s = \frac{1}{2}$, $\kappa = 2$

$$\varphi_3\left(\frac{1}{2}\right) - \varphi_2\left(\frac{1}{2}\right) = 2^3 \sum_{k_1,k_2\in\mathbb{N}} \frac{1}{\sqrt{\left(k_1-\frac{1}{2}\right)^2+\left(k_2-\frac{1}{2}\right)^2}}$$
$$\times \sum_{m=1}^{\infty}(-1)^m \exp\left(-2\pi\sqrt{\left(k_1-\tfrac{1}{2}\right)^2+\left(k_2-\tfrac{1}{2}\right)^2}\right)^m$$

whose inner sum is the geometric series with the sum

$$-\frac{1}{\exp\left(2\pi\sqrt{\left(k_1-\frac{1}{2}\right)^2+\left(k_2-\frac{1}{2}\right)^2}\right)+1}$$

and (iii) follows. (Compare [11].) □

Lemma 4. *For the CsCl lattice zeta-function $\xi_\kappa(s)$ and $Z_\kappa(s)$, we have*

(i) $\xi_1(s) = 2^{2s}\varphi_1(s)$,

(ii) $\xi_2(s) = \dfrac{1}{2^{1-s}-1}\varphi_2(s) - \dfrac{\pi^{2s-1}\Gamma(1-s)}{\Gamma(s)}\varphi_2(1-s)$

(iii) $Z_{\kappa+1}(s) - Z_\kappa(s) = \sum_{0\neq m\in\mathbb{Z}} Z_\kappa(s,m^2) + Z_1(s)$.

Proof. (i) is obtained from $\psi_1(s) = (2^{2s}-1)Z_1(s)$ and lemma 3(i). (ii) is a consequence of the functional equation (1.6) and lemma 3(ii). For (iii), we separate the defining sum for $Z_{\kappa+1}(s)$ as in the proof of lemma 3(iii) and obtain the equality immediately. □

Proof of theorem 3. The proof goes along the same lines as that of theorem 2.

First, we recall from (1.7) that

$$\psi_{\kappa+1}(s) = \sum_{m_{\kappa+1}\in\mathbb{Z}}\sum_{\underline{m}\in\mathbb{Z}^\kappa} \frac{1}{(|\underline{m+1/2}|^2+(m_{\kappa+1}+1/2)^2)^s}$$
$$= \sum_{m\in\mathbb{Z}} \psi_\kappa\left(s, \left(m+\frac{1}{2}\right)^2\right) \tag{3.14}$$

where we wrote $\psi_{\kappa+1}(s) = Z\left|\begin{smallmatrix}1/2\\ \underline{0}\end{smallmatrix}\right|(2s)_E$, and $\psi_\kappa(s,\alpha)$ is the Hurwitz-type Dirichlet series associated with $\psi_\kappa(s)$ (cf (3.8)). □

Now we view (1.6) in the reverse way, i.e. $\varphi_\kappa\left(\frac{\kappa}{2}-s\right)$ as the mirror image. Using the modular relation, we may prove that the residual function is given by $x^{-\kappa/2}$, and therefore its Borel transform is

$$\frac{\Gamma\left(s-\frac{\kappa}{2}\right)}{(\alpha\pi)^{s-\frac{\kappa}{2}}}.$$

Thus, as a counterpart of (3.11), we deduce from lemma 2 that

$$\pi^{-s}\Gamma(s)\psi_\kappa(s,\alpha) = 2\alpha^{\frac{\kappa/2-s}{2}} \sum_{\underline{k}\in\mathbb{Z}^\kappa}{}' (-1)^{s(\underline{k})}|\underline{k}|^{s-\frac{\kappa}{2}} K_{s-\frac{\kappa}{2}}(2\pi\sqrt{\alpha}|\underline{k}|) + \Gamma\left(s-\frac{\kappa}{2}\right)(\alpha\pi)^{-s+\frac{\kappa}{2}}. \tag{3.15}$$

Substituting (3.15) with $\alpha = (m + 1/2)^2$ into (3.14), we conclude that

$$\begin{aligned}
\pi^{-s}\Gamma(s)\psi_{\kappa+1}(s)& \\
&= 2\sum_{m\in\mathbb{Z}}\left|m+\frac{1}{2}\right|^{\frac{\kappa}{2}-s}\sum_{\underline{k}\in\mathbb{Z}^\kappa}{}' (-1)^{s(\underline{k})}|\underline{k}|^{s-\frac{\kappa}{2}}K_{s-\frac{\kappa}{2}}\left(2\pi\left|m+\frac{1}{2}\right||\underline{k}|\right) \\
&\quad + \pi^{-s+\frac{\kappa}{2}}\Gamma\left(s-\frac{\kappa}{2}\right)\psi_1\left(s-\frac{\kappa}{2}\right) \\
&= 4\sum_{m\in\mathbb{N}}\left(m-\frac{1}{2}\right)^{\frac{\kappa}{2}-s}\sum_{\underline{k}\in\mathbb{Z}^\kappa}{}' (-1)^{s(\underline{k})}|\underline{k}|^{s-\frac{\kappa}{2}}K_{s-\frac{\kappa}{2}}\left(2\pi\left(m-\frac{1}{2}\right)|\underline{k}|\right) \\
&\quad + \pi^{-s+\frac{\kappa}{2}}\Gamma\left(s-\frac{\kappa}{2}\right)\psi_1\left(s-\frac{\kappa}{2}\right) \qquad (3.16)
\end{aligned}$$

which is valid for $\sigma > \frac{\kappa}{2}$ in the first place.

It is $Z_\kappa(s) = Z\Big|{}^{0\cdots 0}_{0\cdots 0}\Big|(2s)_E$ that satisfies the recurrence relation, which however is a special case of theorem 2 in part I. Thus we shall first indicate the proof based on lemma 2.

The functional equation (1.6) remains the same, with $Z_\kappa(s)$ itself as the mirror image, and the residual function can be computed to be $x^{-\frac{\kappa}{2}} - 1$.

Corresponding to (3.11) and (3.15), we have

$$\pi^{-s}\Gamma(s)Z_\kappa(s,\alpha) = 2\alpha^{\frac{\kappa/2-s}{2}}\sum_{\underline{k}\in\mathbb{Z}^\kappa}{}' |\underline{k}|^{s-\frac{\kappa}{2}}K_{s-\frac{\kappa}{2}}(2\pi\sqrt{\alpha}|\underline{k}|) + \frac{\Gamma(s-\frac{\kappa}{2})}{(\alpha\pi)^{s-\frac{\kappa}{2}}} - \frac{\Gamma(s)}{(\alpha\pi)^s}.$$

Hence from (iii) of lemma 4,

$$\begin{aligned}
\pi^{-s}\Gamma(s)\{Z_{\kappa+1}(s) - Z_\kappa(s)\} &= 4\sum_{m\in\mathbb{N}}\sum_{\underline{k}\in\mathbb{Z}^\kappa}{}' m^{\frac{\kappa}{2}-s}|\underline{k}|^{s-\frac{\kappa}{2}}K_{s-\frac{\kappa}{2}}(2\pi m|\underline{k}|) \\
&\quad + \pi^{-s+\frac{\kappa}{2}}\Gamma\left(s-\frac{\kappa}{2}\right)Z_1\left(s-\frac{\kappa}{2}\right) \qquad (3.17)
\end{aligned}$$

which coincides with the special case of (2.17*a*) of part I (with $Q = E$) after slight modifications.

Substituting (3.16) and (3.17) into (3.3), we obtain the formula corresponding to (3.1) for the CsCl lattice zeta-function

$$\begin{aligned}
\pi^{-s}\Gamma(s)\xi_{\kappa+1}(s) &= 4\sum_{m\in\mathbb{N}}\sum_{\underline{k}\in\mathbb{Z}^\kappa}{}' m^{\frac{\kappa}{2}-s}|\underline{k}|^{s-\frac{\kappa}{2}}K_{s-\frac{\kappa}{2}}(2\pi m|\underline{k}|) \\
&\quad - 4\sum_{m\in\mathbb{N}}\sum_{\underline{k}\in\mathbb{Z}^\kappa}{}' \left(m-\frac{1}{2}\right)^{\frac{\kappa}{2}-s}(-1)^{s(\underline{k})}|\underline{k}|^{s-\frac{\kappa}{2}}K_{s-\frac{\kappa}{2}}\left(2\pi\left(m-\frac{1}{2}\right)|\underline{k}|\right) \\
&\quad + \pi^{-s}\Gamma(s)Z_\kappa(s) + \pi^{-s+\frac{\kappa}{2}}\Gamma\left(s-\frac{\kappa}{2}\right)\xi_1\left(s-\frac{\kappa}{2}\right) \qquad (3.18)
\end{aligned}$$

which is the assertion of theorem 3.

Proof of corollary 2. The assertions for α_1(CsCl) and α_2(CsCl) are obtained from lemma 4. For α_3(CsCl), it is enough to prove

$$\xi_1\left(-\tfrac{1}{2}\right) = -\tfrac{1}{8}$$

which is easily seen from the equality $\psi_1(s) = (2^{2s} - 1)Z_1(s)$. □

Corollary 3. *The Euler constant γ is expressed by*

$$\gamma = -4 \sum_{k,m\in\mathbb{N}} K_0(2\pi mk) + 4(1+\sqrt{2}) \sum_{k,m\in\mathbb{N}} (-1)^k K_0(\pi(2m-1)k) + \log 2\pi - \sqrt{2}\log 2.$$

Proof. From theorem 3, we have

$$\begin{aligned}\xi_2\left(\frac{1}{2}\right) &= 8 \sum_{k,m\in\mathbb{N}} K_0(2\pi mk) - 8 \sum_{k,m\in\mathbb{N}} (-1)^k K_0(2\pi(2m-1)k) \\ &\quad + \lim_{s\to\frac{1}{2}} \left\{\pi^{-s}\Gamma(s)Z_1(s) + \pi^{-s+\frac{1}{2}}\Gamma\left(s-\frac{1}{2}\right)\xi_1\left(s-\frac{1}{2}\right)\right\} \\ &= 8 \sum_{k,m\in\mathbb{N}} K_0(2\pi mk) - 8 \sum_{k,m\in\mathbb{N}} (-1)^k K_0(2\pi(2m-1)k) + 2\gamma - 2\log 2\pi.\end{aligned}$$

This gives an expression for α_2(CsCl) by the *K*-Bessel series. Combining this expression and the second equality of corollary 2 (ii), we get the assertion of corollary 3. □

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