On lattice sums and Wigner limits

David Borwein[a], Jonathan M. Borwein[b], Armin Straub[c]

[a] *Department of Mathematics, Western University, Middlesex College, London, Ontario N6A 3K7, Canada*
[b] *School of Mathematical and Physical Sciences, University of Newcastle, University Drive, Callaghan, NSW 2308, Australia*
[c] *Max-Planck-Institut für Mathematik, Vivatsgasse 7, 53111 Bonn, Germany*

Abstract

Wigner limits are given formally as the difference between a lattice sum, associated to a positive definite quadratic form, and a corresponding multiple integral. To define these limits, which arose in work of Wigner on the energy of static electron lattices, in a mathematically rigorous way one commonly truncates the lattice sum and the corresponding integral and takes the limit along expanding hypercubes or other regular geometric shapes. We generalize the known mathematically rigorous two and three dimensional results regarding Wigner limits, as laid down in [BBS89], to integer lattices of arbitrary dimension. In doing so, we also resolve a problem posed in [BGM+13, Chapter 7].

For the sake of clarity, we begin by considering the simpler case of cubic lattice sums first, before treating the case of arbitrary quadratic forms. We also consider limits taken along expanding hyperballs with respect to general norms, and connect with classical topics such as Gauss's circle problem. An appendix is included to recall certain properties of Epstein zeta functions that are either used in the paper or serve to provide perspective.

Keywords: lattice sums, analytic continuation, Wigner electron sums

1. Introduction

Throughout this paper, $Q(x) = Q(x_1, \dots, x_d)$ is a positive definite quadratic form in d variables with real coefficients and determinant $\Delta > 0$. As proposed in [BGM+13, Chapter 7], we shall examine the behaviour of

$$\sigma_N(s) := \alpha_N(s) - \beta_N(s)$$

as $N \to \infty$, where α_N and β_N are given by

$$\alpha_N(s) := \sum_{n_1=-N}^{N} \cdots \sum_{n_d=-N}^{N} \frac{1}{Q(n_1, \dots, n_d)^s}, \tag{1}$$

$$\beta_N(s) := \int_{-N-1/2}^{N+1/2} \cdots \int_{-N-1/2}^{N+1/2} \frac{\mathrm{d}x_1 \cdots \mathrm{d}x_d}{Q(x_1, \dots, x_d)^s}. \tag{2}$$

As usual, the summation in (1) is understood to avoid the term corresponding to $(n_1, \dots, n_d) = (0, \dots, 0)$. If $\operatorname{Re} s > d/2$, then $\alpha_N(s)$ converges to the Epstein zeta function $\alpha(s) = Z_Q(s)$ as $N \to \infty$. A few basic properties of Z_Q are recollected in Section 2. On the other hand, each integral $\beta_N(s)$ is only defined for $\operatorname{Re} s < d/2$.

A priori it is therefore unclear, for any s, whether the *Wigner limit* $\sigma(s) := \lim_{N\to\infty} \sigma_N(s)$ should exist. In the sequel, we will write $\sigma_Q(s)$ when we wish to emphasize the dependence on the quadratic form Q. For more on the physical background, which motivates the interest in the limit $\sigma(s)$, we refer to Section 1.1 below.

In the case $d = 2$, it was shown in [BBS89, Theorem 1] that the limit $\sigma(s)$ exists in the strip $0 < \operatorname{Re} s < 1$ and that it coincides therein with the analytic continuation of $\alpha(s)$. Further, in the case $d = 3$ with $Q(x) = x_1^2 + x_2^2 + x_3^2$, it was shown in [BBS89, Theorem 3] that the limit $\sigma(s)$ exists for $1/2 < \operatorname{Re} s < 3/2$ as well as for $s = 1/2$. However, it was determined that $\sigma(1/2) - \pi/6 = \lim_{\varepsilon\to 0^+} \sigma(1/2+\varepsilon)$. In other words, the limit $\sigma(s)$ exhibits a jump discontinuity at $s = 1/2$.

It is therefore natural to ask in what senses the phenomenon, observed for the cubic lattice when $d = 3$, extends both to higher dimensions and to more general quadratic forms. We largely resolve the following problem which is a refinement of one posed in the recent book [BGM+13, Chapter 7].

Problem 1.1 (Convergence)**.** For dimension $d > 1$, consider σ_N as above.

> Show that the limit $\sigma(s) := \lim_{N\to\infty} \sigma_N(s)$ exists in the strip $d/2 - 1 < \operatorname{Re} s < d/2$. Does the limit exist for $s = d/2 - 1$? If so, is the limit discontinuous at $s = d/2 - 1$, and can the height of the jump discontinuity be evaluated?

In Proposition 3.1, we show that the limit indeed exists in the strip suggested in Problem 1.1. In the case of $Q(x) := x_1^2 + \cdots + x_d^2$, we then show in Theorem 4.2 that $\sigma(s)$ also converges for $s = d/2 - 1$. As in the case $d = 3$, we find that $\sigma(s)$ has a jump discontinuity, which we evaluate in closed form. In Theorem 4.4 we extend this result less explicitly to arbitrary positive definite quadratic forms Q.

1.1. Motivation and physical background

As described in [BGM+13, Chapter 7]:

> In 1934 Wigner introduced the concept of an electron gas bathed in a compensating background of positive charge as a model for a metal. He suggested that under certain circumstances the electrons would arrange themselves in a lattice, and that the body-centred lattice would be the most stable of the three common cubic structures. Fuchs (1935) appears to have confirmed this in a calculation on copper relying on physical properties of copper. The evaluation of the energy of the three cubic electron lattices under precise conditions was carried out by Coldwell-Horsefall and

Maradudin (1960) and became the standard form for calculating the energy of static electron lattices. In this model electrons are assumed to be negative point charges located on their lattice sites and surrounded by an equal amount of positive charge uniformly distributed over a cube centered at the lattice point.

In three dimensions, this leads precisely to the problem enunciated in the previous section. That is, Wigner, when $d = 3$, $s = 1/2$ and $Q(x) = x_1^2+x_2^2+x_3^2$, proposed considering, after appropriate renormalization, the entity

$$\sigma(s) := \sum_{n_1=-\infty}^{\infty} \cdots \sum_{n_d=-\infty}^{\infty} \frac{1}{Q(n_1,\ldots,n_d)^s} - \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \frac{\mathrm{d}x_1 \cdots \mathrm{d}x_d}{Q(x_1,\ldots,x_d)^s}. \quad (3)$$

As a physicist Wigner found it largely untroubling that in (3) the object of study $\sigma(s)$ never makes unambiguous sense. Nor even does it point the way to formalize its mathematical content. The concept is thus both natural physically and puzzling mathematically for the reasons given above of the non-convergence of the integral whenever the sum converges.

The best-behaved case is that of two dimensions, which is also physically meaningful if used to consider planar lamina. In [BBSZ88, §3] a 'meta-principle' was presented justifying the evaluation of σ as the analytic continuation of $\alpha = Z_Q$. This was followed by a discussion and analysis of various important hexagonal and diamond, cubic and triangular lattices in two and three space [BBSZ88, §4]. In particular, the values of α obtained agreed with values in the physical literature whenever they were known. It was this work which led to the analysis in [BBS89].

The entirety of [BGM+13, Chapter 7] is dedicated to the analysis of such 'electron sums' in two and three dimensions. While we make no direct claim for the physical relevance of the analysis with $d > 3$, the delicacy of the mathematical resolution of Problem 1.1 is certainly informative even just for general forms in three dimensions.

1.2. Structure of the paper

The remainder of the paper is organized as follows. In Section 2, we establish some basic properties of α_N and β_N. Then, in Section 3, we establish convergence in the strip for a general quadratic form (Proposition 3.1). Next, in Section 4, we consider convergence on the boundary of the strip. In particular, we explicitly evaluate the jump discontinuity in the cubic case (Theorem 4.2). In the non-cubic case the same phenomenon is established, though the corresponding evaluation of the jump is less explicit (Theorem 4.4). In Section 5, we consider other limiting procedures which replace limits over expanding cubes by more general convex bodies. The paper concludes with a brief accounting of the underlying theory of cubic lattice sums in Appendix A. For more details the reader is referred to [BGM+13] and the other cited works.

2. Basic analytic properties

Any quadratic form $Q(x) = Q(x_1, \dots, x_d)$ can be expressed as

$$Q(x) = Q_A(x) := x^T A x = \sum_{1 \leqslant i,j \leqslant d} a_{ij} x_i x_j, \tag{4}$$

for a matrix $A = (a_{ij})_{1 \leqslant i,j \leqslant d}$ which is symmetric (that is, $a_{ij} = a_{ji}$ for all $1 \leqslant i, j \leqslant d$). If Q is positive definite, then A is a positive definite matrix of determinant $\Delta = \det(A) > 0$. A basic property of a positive definite matrix A, given in most linear algebra texts, is that it can be decomposed as $A = L^T L$, where L is a non-singular matrix. This property is used implicitly when making coordinate transformations as in (10) and in the proof of Lemma 2.5 below.

As indicated in the introduction, the limit of $\alpha_N(s)$ is the Epstein zeta function

$$\alpha(s) := Z_Q(s) := \sum_{n_1, \dots, n_d}{}' \frac{1}{Q(n_1, n_2, \dots, n_d)^s}. \tag{5}$$

Standard arguments show that $Z_Q(s)$ is an analytic function in the domain $\operatorname{Re} s > d/2$. In fact, see [Eps06] or [BK08, Chapter 2 or 8], the Epstein zeta function $Z_Q(s)$ has a meromorphic continuation to the entire complex plane and satisfies the functional equation

$$\frac{Z_Q(s)\Gamma(s)}{\pi^s} = \frac{1}{\sqrt{\Delta}} \frac{Z_{Q^{-1}}(d/2 - s)\Gamma(d/2 - s)}{\pi^{d/2 - s}}, \tag{6}$$

where $Q(x) = x^T A x$ and $Q^{-1}(x) = x^T A^{-1} x$. Moreover, the only pole of $Z_Q(s)$ occurs at $s = d/2$, is simple, and has residue

$$\operatorname{res}_{d/2} Z_Q(s) = \frac{1}{\sqrt{\Delta}} \frac{\pi^{d/2}}{\Gamma(d/2)}. \tag{7}$$

A particularly important special case of Epstein zeta functions is that of cubic lattice sums, which correspond to the choice $Q(x) = x_1^2 + \cdots + x_d^2$. In Appendix A, we recall some of their basic properties, which provide further context for the questions discussed herein.

These remarks made, it is natural to begin our investigation of Problem 1.1 by discussing some related properties of the limit of $\beta_N(s)$. In the sequel, we use the notation $\|x\|_\infty := \max(|x_1|, \dots, |x_d|)$ for vectors $x = (x_1, \dots, x_d) \in \mathbb{R}^d$.

Proposition 2.1. *Let Q be a d-dimensional positive definite quadratic form of determinant $\Delta > 0$. The integral $\beta_N(s)$ extends meromorphically to the entire complex plane with a single pole at $s = d/2$, which is simple and has residue*

$$\operatorname{res}_{d/2} \beta_N(s) = -\frac{1}{\sqrt{\Delta}} \frac{\pi^{d/2}}{\Gamma(d/2)} = -\operatorname{res}_{d/2} \alpha(s). \tag{8}$$

Proof. The integral $\beta_N(s)$, as defined in (2), is analytic for $\operatorname{Re} s < d/2$. On the other hand, we easily see that the difference

$$\beta_N(s) - \int_{Q(x)\leqslant N} \frac{1}{Q(x)^s}\mathrm{d}x \tag{9}$$

is an entire function in s. The latter integral can be evaluated in closed form. Indeed, for $\operatorname{Re} s < d/2$,

$$\begin{aligned}\int_{Q(x)\leqslant N} \frac{1}{Q(x)^s}\mathrm{d}x &= \frac{1}{\sqrt{\Delta}}\int_{\|x\|_2^2\leqslant N} \frac{1}{\|x\|_2^{2s}}\mathrm{d}x \\ &= \frac{1}{\sqrt{\Delta}}\operatorname{vol}(\mathbb{S}^{d-1})\int_0^{\sqrt{N}} r^{d-1-2s}\mathrm{d}r \\ &= \frac{1}{\sqrt{\Delta}}\frac{N^{d/2-s}}{d/2-s}\frac{\pi^{d/2}}{\Gamma(d/2)}.\end{aligned} \tag{10}$$

In light of (9), this shows that $\beta_N(s)$ has an analytic continuation to the full complex plane with a single pole at $s = d/2$, which is simple and has residue as claimed in (8). The second equality in (8) follows from (7). □

We note that the fact that the residue of $\beta_N(s)$ does not depend on N reflects that, for any $N, M > 0$, the differences $\beta_N(s) - \beta_M(s)$ are, as in (9), entire functions.

We further record that the proof of Proposition 2.1 is related to the following observation. For any reasonable function $F_s : \mathbb{R}^d \to \mathbb{R}$ such that $F_s(\lambda x) = |\lambda|^{-2s}F_s(x)$,

$$\begin{aligned}\int_{\|x\|_\infty\leqslant 1} F_s(x)\mathrm{d}\lambda_d &= \int_0^1\int_{\|x\|_\infty=t} F_s(x)\mathrm{d}\lambda_{d-1}\mathrm{d}t \\ &= \int_0^1 t^{d-1-2s}\int_{\|x\|_\infty=1} F_s(x)\mathrm{d}\lambda_{d-1}\mathrm{d}t \\ &= \frac{1}{d-2s}\int_{\|x\|_\infty=1} F_s(x)\mathrm{d}\lambda_{d-1},\end{aligned} \tag{11}$$

where λ_d denotes the d-dimensional Lebesgue measure and λ_{d-1} the induced $(d-1)$-dimensional surface measure (that is, $\mathrm{d}\lambda_{d-1} = \mathrm{d}x_1\cdots\mathrm{d}x_{j-1}\mathrm{d}x_{j+1}\cdots\mathrm{d}x_d$ on the part of the domain where x_j is constant).

Remark 2.2. Since the notation used in (11) is rather terse, let us, for instance, spell out the crucial first equality. By separating the variable of maximal abso-

lute value and then interchanging summation and integration,

$$\begin{aligned}\int_{\|x\|_\infty\leqslant 1} F_s(x)\mathrm{d}\lambda_d &= 2\sum_{j=1}^{d}\int_0^1\left(\int_{[-x_j,x_j]^{d-1}} F_s(x)\mathrm{d}x_1\cdots\mathrm{d}x_{j-1}\mathrm{d}x_{j+1}\cdots\mathrm{d}x_d\right)\mathrm{d}x_j\\ &= \int_0^1\left(\sum_{j=1}^{d}\int_{\substack{\|x\|=|t|\\ x_j=\pm t}} F_s(x)\mathrm{d}x_1\cdots\mathrm{d}x_{j-1}\mathrm{d}x_{j+1}\cdots\mathrm{d}x_d\right)\mathrm{d}t\\ &= \int_0^1\int_{\|x\|_\infty=t} F_s(x)\mathrm{d}\lambda_{d-1}\mathrm{d}t.\end{aligned}$$

We note that the relation between first and final integral also holds with $\|\cdot\|_\infty$ replaced by $\|\cdot\|_2$ (in which case λ_{d-1} would now refer to the surface measure on the Euclidean sphere $\{x\in\mathbb{R}^d : \|x\|_2 = t\}$). ◊

Based on (11), we obtain the following consequence of Proposition 2.1, which will be important for our purposes later on.

Lemma 2.3. *Let Q be a d-dimensional positive definite quadratic form of determinant $\Delta > 0$. Then we have*

$$\int_{\|x\|_\infty=1}\frac{1}{Q(x)^{d/2}}\mathrm{d}\lambda_{d-1} = \frac{2}{\sqrt{\Delta}}\frac{\pi^{d/2}}{\Gamma(d/2)}. \tag{12}$$

Proof. From the arguments in the proof of Proposition 2.1, we know that

$$\int_{\|x\|_\infty\leqslant 1}\frac{1}{Q(x)^s}\mathrm{d}\lambda_d$$

is a meromorphic function with a simple pole at $s = d/2$. The computation in (11) shows that

$$\int_{\|x\|_\infty=1}\frac{1}{Q(x)^{d/2}}\mathrm{d}\lambda_{d-1} = -2\operatorname{res}_{d/2}\int_{\|x\|_\infty\leqslant 1}\frac{1}{Q(x)^s}\mathrm{d}\lambda_d = \frac{2}{\sqrt{\Delta}}\frac{\pi^{d/2}}{\Gamma(d/2)},$$

with the last equality following in analogy with Proposition 2.1. □

Example 2.4 (Generalized arctan(1))**.** The special case $Q(x) := x_1^2 + \cdots + x_d^2$ results in the integral evaluation

$$\int_{[-1,1]^{d-1}}\frac{1}{(1+x_1^2+\cdots x_{d-1}^2)^{d/2}}\mathrm{d}x = \frac{1}{d}\frac{\pi^{d/2}}{\Gamma(d/2)}, \tag{13}$$

which has been derived in [BB08, Section 5.7.3] as a radially invariant generalization of arctan(1).

Let us indicate an alternative direct derivation of (13). To this end, recall that the gamma function is characterized by

$$\frac{\Gamma(s)}{A^s} = \int_0^\infty t^{s-1}e^{-At}\mathrm{d}t.$$

Applying this integral representation, which is valid for $\operatorname{Re} s > 0$, with $A = 1 + x_1^2 + \cdots x_{d-1}^2$, we find

$$\begin{aligned}
&\int_{[-1,1]^{d-1}} \frac{1}{(1+x_1^2+\cdots x_{d-1}^2)^s} \mathrm{d}x \\
&= \frac{1}{\Gamma(s)} \int_{[-1,1]^{d-1}} \int_0^\infty t^{s-1} e^{-(1+x_1^2+\cdots x_{d-1})t} \mathrm{d}t\mathrm{d}x \\
&= \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t} \int_{[-1,1]^{d-1}} e^{-(x_1^2+\cdots x_{d-1})t} \mathrm{d}x\mathrm{d}t \\
&= \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} e^{-t} \left(\int_{-1}^1 e^{-x^2 t} \mathrm{d}x \right)^{d-1} \mathrm{d}t \\
&= \frac{2}{\Gamma(s)} \int_0^\infty u^{2s-1} e^{-u^2} \left(\int_{-1}^1 e^{-x^2 u^2} \mathrm{d}x \right)^{d-1} \mathrm{d}u.
\end{aligned}$$

In particular, for $s = d/2$,

$$\int_{[-1,1]^{d-1}} \frac{1}{(1+x_1^2+\cdots x_{d-1}^2)^{d/2}} \mathrm{d}x = \frac{2}{\Gamma(d/2)} \int_0^\infty e^{-u^2} \left(u \int_{-1}^1 e^{-x^2 u^2} \mathrm{d}x \right)^{d-1} \mathrm{d}u.$$

Define

$$f(u) = u \int_{-1}^1 e^{-x^2 u^2} \mathrm{d}x,$$

which, in terms of the error function, can be expressed as $f(u) = \sqrt{\pi} \operatorname{erf}(u)$. We note that $f(u) \to \sqrt{\pi}$ as $u \to \infty$. Further, the derivative is simply

$$f'(u) = 2e^{-u^2}.$$

After the substitution $v = f(u)$, we thus find

$$\int_{[-1,1]^{d-1}} \frac{1}{(1+x_1^2+\cdots x_{d-1}^2)^{d/2}} \mathrm{d}x = \frac{1}{\Gamma(d/2)} \int_0^{\sqrt{\pi}} v^{d-1} \mathrm{d}v = \frac{1}{d} \frac{\pi^{d/2}}{\Gamma(d/2)},$$

as claimed. ◊

As in (4), we denote with $Q = Q_A$ the quadratic form $Q(x)$ on $\mathbb{R}^d$ associated with the symmetric matrix $A = (a_{ij})_{1 \leqslant i,j \leqslant d}$. We now record an extension of Lemma 2.3, which will prove useful for our purposes (the case $B = A$ in (14) reduces to (12), and it is the case $B = A^2$ that will appear later). Recall that the *trace* of a square matrix is given by $\operatorname{tr} A = \sum_{j=1}^d a_{jj}$ and defines a Euclidean norm on the symmetric $d \times d$ matrices via $\langle A_1, A_2 \rangle = \operatorname{tr}(A_1 A_2)$.

Lemma 2.5. *For matrices $A, B \in \mathbb{R}^{d \times d}$, with A positive definite,*

$$\int_{\|x\|_\infty = 1} \frac{Q_B(x)}{Q_A(x)^{1+d/2}} \mathrm{d}\lambda_{d-1} = \frac{\operatorname{tr}(BA^{-1})}{\sqrt{\det(A)}} \frac{\pi^{d/2}}{\Gamma(1+d/2)}. \tag{14}$$

Proof. On decomposing A as $A = L^T L$, we find

$$\int_{Q(x)\leqslant 1} \frac{Q_B(x)}{Q_A(x)^{s+1}}\mathrm{d}x = \frac{1}{\det(L)} \int_{\|x\|_2^2\leqslant 1} \frac{Q_C(x)}{\|x\|_2^{2s+2}}\mathrm{d}x,$$

with $C := (L^{-1})^T B L^{-1}$. For the residue of the latter integral only the quadratic terms $C_{11}x_1^2 + \cdots + C_{dd}x_d^2$ in $Q_C(x)$ contribute; indeed, in the present case the contributions of the mixed terms $C_{ij}x_i x_j$, $i \neq j$, integrate to zero. Because of symmetry we thus obtain

$$\begin{aligned}\int_{Q(x)\leqslant 1} \frac{Q_B(x)}{Q_A(x)^{s+1}}\mathrm{d}x &= \frac{\mathrm{tr}(C)}{\sqrt{\det(A)}} \int_{\|x\|_2^2\leqslant 1} \frac{x_1^2}{\|x\|_2^{2s+2}}\mathrm{d}x \\ &= \frac{\mathrm{tr}(C)}{d\sqrt{\det(A)}} \int_{\|x\|_2^2\leqslant 1} \frac{1}{\|x\|_2^{2s}}\mathrm{d}x \\ &= \frac{\mathrm{tr}(C)}{d\sqrt{\det(A)}} \frac{1}{d/2-s} \frac{\pi^{d/2}}{\Gamma(d/2)},\end{aligned}$$

with the final step as in (10). Since the trace is commutative,

$$\mathrm{tr}(C) = \mathrm{tr}(L^{-T} B L^{-1}) = \mathrm{tr}(B L^{-1} L^{-T}) = \mathrm{tr}(BA^{-1}).$$

We conclude that, for any compact region $D \subset \mathbb{R}^d$ containing a neighborhood of the origin,

$$\mathrm{res}_{d/2} \int_D \frac{Q_B(x)}{Q_A(x)^{s+1}}\mathrm{d}x = -\frac{\mathrm{tr}(BA^{-1})}{d\sqrt{\det(A)}} \frac{\pi^{d/2}}{\Gamma(d/2)}. \tag{15}$$

In light of the computation (11), we arrive at

$$\int_{\|x\|_\infty=1} \frac{Q_B(x)}{Q_A(x)^{1+d/2}}\mathrm{d}\lambda_{d-1} = -2\,\mathrm{res}_{d/2} \int_{\|x\|_\infty\leqslant 1} \frac{Q_B(x)}{Q_A(x)^{s+1}}\mathrm{d}x,$$

which, together with (15), implies (14). □

3. Convergence of Wigner limits

Our next goal is to show that $\sigma_N(s)$ indeed converges in the vertical strip suggested in Problem 1.1. As discussed in [BGM+13, Chapter 2 and 8], convergence over such hyper-cubes is more stable than that over Euclidean balls and similar shapes. Other limit procedures are compared in Section 5.

Proposition 3.1 (Convergence in a strip)**.** *Let Q be an arbitrary positive definite quadratic form on $\mathbb{R}^d$. Then the limit $\sigma(s) := \lim_{N\to\infty} \sigma_N(s)$ exists in the strip $d/2 - 1 < \mathrm{Re}\, s < d/2$ and coincides therein with the analytic continuation of $\alpha(s)$.*

Proof. For the first part of the claim, we follow the proof given in [BBS89] for binary forms Q. Fix $\sigma > 0$ as well as $R > 0$ and set $\Omega := \{s : \operatorname{Re} s > \sigma, \quad |s| < R\}$. All order terms below are uniform with respect to s in the bounded region Ω. For $N \geqslant 1$ let

$$\begin{aligned} \delta_N(s) &:= \sigma_N(s) - \sigma_{N-1}(s) \\ &= \sum_{\|n\|_\infty = N} \int_{\|x\|_\infty \leqslant 1/2} \left[\frac{1}{Q(n)^s} - \frac{1}{Q(n+x)^s} \right] \mathrm{d}x. \end{aligned}$$

Here and in the sequel, we let $f(x) := Q(n+x)^{-s}$ with $\|n\|_\infty = N$ and $\|x\|_\infty \leqslant 1/2$. Since we may assume $Q(x) = \sum_{i,j} a_{ij} x_i x_j$, with $a_{ij} = a_{ji}$, is positive definite, we have the estimate

$$\begin{aligned} f_{ij}(x) &= \frac{4s(s+1)}{Q(n+x)^{s+2}} \sum_k a_{ik}(n_k + x_k) \sum_\ell a_{j\ell}(n_\ell + x_\ell) - \frac{2a_{ij}s}{Q(n+x)^{s+1}} \\ &= O(N^{-2\sigma-2}). \end{aligned}$$

Here, the indices of f indicate partial derivatives with respect to the i-th or j-th variable. We thus have

$$f(x) - f(0) = \sum_i x_i f_i(0) + O(N^{-2\sigma-2}). \tag{16}$$

Consequently,

$$\begin{aligned} & \int_{\|x\|_\infty \leqslant 1/2} \left[\frac{1}{Q(n)^s} - \frac{1}{Q(n+x)^s} \right] \mathrm{d}x \\ = \; & - \int_{\|x\|_\infty \leqslant 1/2} \left[\sum_i x_i f_i(0) \right] \mathrm{d}x + O(N^{-2\sigma-2}) \\ = \; & O(N^{-2\sigma-2}), \end{aligned}$$

because the final integral, being odd, vanishes.

Hence,

$$\delta_N(s) = O(N^{d-2\sigma-3}),$$

and so, for all $s \in \Omega$, $|\delta_N(s)| \leqslant M N^{d-2\sigma-3}$ for some M, which is independent of N and s. Assume now that $\sigma > d/2 - 1$. Since $\delta_N(s)$ is an entire function, the Weierstrass M-test shows that

$$\delta(s) := \sum_{N=1}^{\infty} \delta_N(s)$$

is an analytic function in Ω. Since R was arbitrary, $\delta(s)$ is in fact analytic in the half-plane $\operatorname{Re} s > d/2 - 1$. By construction,

$$\delta(s) = \lim_{N\to\infty} \left[\sigma_N(s) - \sigma_0(s) \right] = \lim_{N\to\infty} \left[\sigma_N(s) + \beta_0(s) \right]. \tag{17}$$

It follows that the limit $\sigma(s)$ exists if, additionally, $\operatorname{Re} s < d/2$.

For the second part of the claim, we begin with the simple observation that, for $\operatorname{Re} s < d/2$,

$$\begin{aligned} \beta_N(s) &= \int_{\|x\|_\infty \leqslant N+1/2} \frac{1}{Q(x)^s} \mathrm{d}x \\ &= (2N+1)^{d-2s} \int_{\|x\|_\infty \leqslant 1/2} \frac{1}{Q(x)^s} \mathrm{d}x \\ &= (2N+1)^{d-2s} \beta_0(s). \end{aligned} \tag{18}$$

As shown in Proposition 2.1, both β_N and β_0 have meromorphic extensions to the entire complex plane, and the relation (18) continues to hold. In particular, this shows that, for $\operatorname{Re} s > d/2$, the meromorphic continuation of β_N satisfies

$$\lim_{N\to\infty} \beta_N(s) = \lim_{N\to\infty} (2N+1)^{d-2s} \beta_0(s) = 0.$$

Working from (17), we thus have, for $\operatorname{Re} s > d/2$,

$$\delta(s) = \lim_{N\to\infty} [\alpha_N(s) - \beta_N(s) + \beta_0(s)] = \alpha(s) + \beta_0(s). \tag{19}$$

On the other hand, we have shown via (17) that, for $\operatorname{Re} s < d/2$,

$$\delta(s) = \sigma(s) + \beta_0(s). \tag{20}$$

Since both $\delta(s)$ and $\beta_0(s)$ are meromorphic in the half-plane $\operatorname{Re} s > d/2 - 1$, comparing (19) and (20) proves that the analytic continuations of $\sigma(s)$ and $\alpha(s)$ agree. In particular, in the strip $d/2 - 1 < \operatorname{Re} s < d/2$, the limit $\sigma(s)$, which was shown to exist, equals the analytic continuation of $\alpha(s)$. □

We note that Proposition 3.1 agrees with the results known for $d = 2, 3$. In the $d = 2$ case, the limit $\sigma(s)$ exists for $0 < \operatorname{Re} s < 1$, in accordance with [BBS89, Theorem 1]. In the $d = 3$ case, the limit $\sigma(s)$ exists for $1/2 < \operatorname{Re} s < 3/2$, which is consistent with the special case of the cubic lattice discussed in [BBS89, Theorem 3].

4. Jump discontinuities in Wigner limits

In [BBS89, Theorem 3] it was shown that, in the case of the cubic lattice, the limit $\sigma(s)$ also exists for $s = 1/2$, but is discontinuous there. In fact, it was shown that

$$\sigma(1/2) - \pi/6 = \lim_{\varepsilon\to 0^+} \sigma(1/2 + \varepsilon).$$

We now extend this result to cubic lattices in arbitrary dimensions, in which case we can and do evaluate the jump discontinuity in simple terms. We then show that an analogous result is true for arbitrary positive definite quadratic forms, though the proof is more technical and no simple closed-form expression for the jumps is given.

Remark 4.1 ($\sigma(0)$)**.** Note that, for trivial reasons, the limit $\sigma(0)$ always exists and is given by $\sigma(0) = -1$, which agrees with the value $\alpha(0) = -1$, obtained by analytic continuation from (6) and (7). (The value $s = 0$ is missed in the statement of Theorem 3 in [BBS89].) ♢

Theorem 4.2 (Cubic jump discontinuity)**.** *Let $Q(x) = x_1^2 + \cdots + x_d^2$. Then the corresponding limit $\sigma(s) := \lim_{N\to\infty} \sigma_N(s)$ exists in the strip $d/2 - 1 < \operatorname{Re} s < d/2$ and for $s = d/2 - 1$. In the strip, $\sigma(s)$ coincides with the analytic continuation of $\alpha(s)$. On the other hand,*

$$\sigma(d/2-1) - \frac{1}{6}\frac{\pi^{d/2}}{\Gamma(d/2-1)} = \alpha(d/2-1) = \lim_{\varepsilon\to 0^+} \sigma(d/2-1+\varepsilon).$$

In particular, for $d \geqslant 3$, $\sigma(s)$ is discontinuous at $s = d/2 - 1$.

Proof. In light of Proposition 3.1, we only need to show the statement about the value of $\sigma(s)$ at $s = d/2 - 1$.

Let us adopt the notation used in Proposition 3.1, including, in particular, the definitions of δ_N and $f(x) := Q(n+x)^{-s}$ with $\|n\|_\infty = N$ and $\|x\|_\infty \leqslant 1/2$. Proceeding as for (16), we have that

$$f(x) - f(0) = \sum_i x_i f_i(0) + \frac{1}{2}\sum_{i,j} x_i x_j f_{ij}(0) + O(N^{-2\sigma-3}).$$

Since terms of odd order in the x_i are eliminated in the subsequent integration, we focus on the terms f_{ii}. In the present case of the cubic lattice,

$$\begin{aligned}\sum_i f_{ii}(0) &= \sum_i \left[\frac{4s(s+1)}{Q(n)^{s+2}} n_i^2 - \frac{2s}{Q(n)^{s+1}}\right] \\ &= \frac{4s(s+1) - 2ds}{Q(n)^{s+1}} \\ &= \frac{2s(2s-(d-2))}{Q(n)^{s+1}}. \end{aligned} \tag{21}$$

We thus find that

$$\begin{aligned}&\int_{\|x\|_\infty\leqslant 1/2} \left[\frac{1}{Q(n)^s} - \frac{1}{Q(n+x)^s}\right] \mathrm{d}x \\ &= -\frac{1}{2}\int_{\|x\|_\infty\leqslant 1/2} \left[\sum_i x_i^2 f_{ii}(0)\right] \mathrm{d}x + O(N^{-2\sigma-3}) \\ &= -\frac{1}{24}\sum_i f_{ii}(0) + O(N^{-2\sigma-3}),\end{aligned}$$

(on integrating term-by-term). Then, on appealing to (21),

$$\int_{\|x\|_\infty\leqslant 1/2} \left[\frac{1}{Q(n)^s} - \frac{1}{Q(n+x)^s}\right] \mathrm{d}x = \frac{1}{12}\frac{s(d-2-2s)}{Q(n)^{s+1}} + O(N^{-2\sigma-3}).$$

Hence,

$$\begin{aligned}\delta_N(s) &= \sum_{\|n\|_\infty=N} \int_{\|x\|_\infty \leqslant 1/2} \left[\frac{1}{Q(n)^s} - \frac{1}{Q(n+x)^s}\right] \mathrm{d}x \\ &= \frac{s(d-2-2s)}{12} \sum_{\|n\|_\infty=N} \frac{1}{Q(n)^{s+1}} + O(N^{d-2\sigma-4}) \\ &= \frac{s(d-2-2s)}{12N^{2s-d+3}} \frac{1}{N^{d-1}} \sum_{\|n\|_\infty=N} \frac{1}{Q(n/N)^{s+1}} + O(N^{d-2\sigma-4}).\end{aligned}$$

We now note that

$$\frac{1}{2dN^{d-1}} \sum_{\|n\|_\infty=N} \frac{1}{Q(n/N)^{s+1}} = V_N(s) + O(N^{-1}),$$

where

$$V_N(s) := \frac{1}{N^{d-1}} \sum_{-N \leqslant n_i < N} \frac{1}{(1 + (n_1/N)^2 + \cdots + (n_{d-1}/N)^2)^{s+1}}.$$

We first show that $V_N(s)$ approaches the integral

$$V(s) := \int_{[-1,1]^{d-1}} \frac{1}{(1 + x_1^2 + \cdots + x_{d-1}^2)^{s+1}} \mathrm{d}x.$$

Indeed, this follows since, for $\operatorname{Re} s \geqslant -2$,

$$\begin{aligned}|V(s) - V_N(s)| &= \left| \sum_{-N \leqslant n_i < N} \int_{n_i \leqslant N x_i \leqslant n_i+1} \left[\frac{1}{(1 + x_1^2 + \cdots + x_{d-1}^2)^{s+1}}\right.\right. \\ &\qquad \left.\left. - \frac{1}{(1 + (n_1/N)^2 + \cdots + (n_{d-1}/N)^2)^{s+1}}\right] \mathrm{d}x \right| \\ &\leqslant \sum_{-N \leqslant n_i < N} \int_{n_i \leqslant N x_i \leqslant n_i+1} (d-1) \frac{2|s+1|}{N} \, \mathrm{d}x \\ &= \frac{2^d (d-1)|s+1|}{N}.\end{aligned}$$

To bound the above integrand, we used that $|x^\lambda - y^\lambda| \leqslant |\lambda||x-y|$ when $\operatorname{Re} \lambda \leqslant 1$ and $x, y \geqslant 1$ (as follows from the mean value theorem).

Combining these estimates, we can thus write

$$\delta_N(s) = \frac{d}{6} \frac{s(d-2-2s)}{N^{2s-d+3}} V(s) + W_N(s), \tag{22}$$

where $W_N(s) = O(N^{d-2\sigma-4})$. For $\sigma > d/2 - 3/2$, the sum

$$W(s) := \sum_{N=1}^{\infty} W_N(s)$$

converges and, by the Weierstrass M-test, defines an analytic function. If, further, $\operatorname{Re} s > d/2-1$ then, from (22), the sum $\delta(s) := \sum_{N=1}^{\infty} \delta_N(s)$ converges and we have

$$\delta(s) = \frac{d}{6} s(d-2-2s)\zeta(2s-d+3)V(s) + W(s).$$

In particular, since $\zeta(s)$ has a simple pole at $s=1$ of residue 1, we find

$$\lim_{\varepsilon \to 0^+} \delta(d/2-1+\varepsilon) = -\frac{d}{6}(d/2-1)V(d/2-1) + W(d/2-1). \tag{23}$$

On the other hand, it follows from (22) that $\delta_N(d/2-1) = W_N(d/2-1)$.

Hence, the defining series for $\delta(s)$ also converges when $s = d/2-1$ and we obtain

$$\delta(d/2-1) = W(d/2-1). \tag{24}$$

Using the consequence (13) of Lemma 2.3, we have

$$\frac{d}{6}(d/2-1)V(d/2-1) = \frac{1}{6}\frac{\pi^{d/2}}{\Gamma(d/2-1)}.$$

Since, by construction, $\delta(s) = \sigma(s) - \sigma_0(s) = \sigma(s)$, on comparing (23) and (24) we are done. □

Example 4.3 (Explicit evaluations in even dimensions)**.** In the case of cubic lattice sums and small even dimension, the value $\sigma(d/2-1)$, at the jump discontinuity, can be given explicitly by combining Theorem 4.2 and the closed forms for the corresponding Epstein zeta function, recalled in Example A.2 below. Let $Q_d(x) = x_1^2 + \ldots + x_d^2$.

$$\begin{aligned}
\sigma_{Q_2}(0) &= \alpha_{Q_2}(0) = -1, \\
\sigma_{Q_4}(1) &= \frac{\pi^2}{6} + \alpha_{Q_4}(1) = \frac{\pi^2}{6} - 8\log 2, \\
\sigma_{Q_6}(2) &= \frac{\pi^3}{6} + \alpha_{Q_6}(2) = \frac{\pi^3}{6} - \frac{\pi^2}{3} - 8G, \\
\sigma_{Q_8}(3) &= \frac{\pi^4}{12} + \alpha_{Q_8}(3) = \frac{\pi^4}{12} - 8\zeta(3), \\
\sigma_{Q_{24}}(11) &= \frac{\pi^{12}}{6\cdot 10!} + \alpha_{Q_{24}}(11) = \frac{\pi^{12}}{6\cdot 10!} - \frac{8}{691}\zeta(11) + \frac{271435}{5528} L_\Delta(11).
\end{aligned}$$

Here, $G = \sum_{n=1}^{\infty} \chi_{-4}(n)/n^2$ denotes Catalan's constant, and L_Δ is (the analytic continuation of) $L_\Delta(s) = \sum_{n=1}^{\infty} \tau(n)/n^s$ with $\tau(n)$ Ramanujan's τ-function. A few properties of this remarkable function are commented on in Example A.2. We note that we have used the appropriate reflection formulas to simplify these evaluations.

We note that the above values mix numbers of different 'order', such as π^4 and $\zeta(3)$ which have order 4 and 3, respectively. This may be another argument

to use $\alpha(d/2-1)$ as the 'value' of the Wigner limit even when the limit $\sigma(d/2-1)$ itself converges. $\Diamond$

We now extend Theorem 4.2 to arbitrary definite quadratic forms. For the most part, the proof is a natural extension of the proof of Theorem 4.2. For the convenience of the reader, we duplicate some parts, as well as the overall structure, of the previous proof.

As in (4), let $Q = Q_A$ be the positive definite quadratic form associated to the symmetric matrix A. Set also $B(s) := \mathrm{tr}(A)A - 2(s+1)A^2$. Finally, define

$$V(s) := V_Q(s) := \int_{\|x\|_\infty = 1} \frac{Q_{B(s)}(x)}{Q_A(x)^{s+2}} \mathrm{d}\lambda_{d-1}, \tag{25}$$

with λ_{d-1} the induced $(d-1)$-dimensional measure as in (11).

Theorem 4.4 (General jump discontinuity)**.** *Let Q be an arbitrary positive definite quadratic form. Then the corresponding limit $\sigma(s) := \lim_{N\to\infty} \sigma_N(s)$ exists in the strip $d/2 - 1 < \mathrm{Re}\, s < d/2$ and for $s = d/2 - 1$. In the strip, $\sigma(s)$ coincides with the analytic continuation of $\alpha(s)$. On the other hand,*

$$\sigma(d/2-1) + \frac{d/2-1}{24} V_Q'(d/2-1) = \alpha(d/2-1) = \lim_{\varepsilon\to 0^+} \sigma(d/2-1+\varepsilon), \tag{26}$$

with V_Q as introduced in equation (25).

Proof. In light of Proposition 3.1, we only need to show the statement about the value of $\sigma(s)$ at $s = d/2 - 1$.

Let us adopt the notation used in Proposition 3.1, including, in particular, the definitions of δ_N and $f(x) := Q(n+x)^{-s}$ with $\|n\|_\infty = N$ and $\|x\|_\infty \leqslant 1/2$. Proceeding as for (16), we have that

$$f(x) - f(0) = \sum_i x_i f_i(0) + \frac{1}{2} \sum_{i,j} x_i x_j f_{ij}(0) + O(N^{-2\sigma-3}).$$

Since terms of odd order in the x_i are eliminated in the subsequent integration, we focus on the terms $f_{ii}(0)$, which are given by

$$f_{ii}(0) = \frac{4s(s+1)}{Q(n)^{s+2}} \left[\sum_{k=1}^d a_{ik} n_k\right]^2 - \frac{2a_{ii}s}{Q(n)^{s+1}}.$$

Hence, equation (21) generalizes to

$$\begin{aligned}
\sum_{i=1}^d f_{ii}(0) &= \frac{4s(s+1)}{Q(n)^{s+2}} \sum_{1\leqslant k,l\leqslant d} \left(\sum_{i=1}^d a_{ki}a_{il}\right) n_k n_l - 2s\frac{\mathrm{tr}(A)}{Q(n)^{s+1}} \\
&= \frac{4s(s+1)}{Q(n)^{s+2}} Q_{A^2}(n) - 2s\frac{\mathrm{tr}(A)}{Q(n)^{s+1}} \\
&= \frac{2s}{Q(n)^{s+2}} \left[2(s+1)Q_{A^2}(n) - \mathrm{tr}(A)Q(n)\right].
\end{aligned} \tag{27}$$

We thus find, on integrating term-by-term, that

$$\begin{aligned}
&\int_{\|x\|_\infty \leqslant 1/2} \left[\frac{1}{Q(n)^s} - \frac{1}{Q(n+x)^s}\right] \mathrm{d}x \\
&= -\frac{1}{2} \int_{\|x\|_\infty \leqslant 1/2} \left[\sum_{i=1}^{d} x_i^2 f_{ii}(0)\right] \mathrm{d}x + O(N^{-2\sigma-3}) \\
&= -\frac{1}{24} \sum_{i=1}^{d} f_{ii}(0) + O(N^{-2\sigma-3}) \\
&= \frac{s}{12} \frac{\mathrm{tr}(A) Q(n) - 2(s+1) Q_{A^2}(n)}{Q(n)^{s+2}} + O(N^{-2\sigma-3}).
\end{aligned}$$

In the final step, we appealed to (27). Hence,

$$\begin{aligned}
\delta_N(s) &= \sum_{\|n\|_\infty = N} \int_{\|x\|_\infty \leqslant 1/2} \left[\frac{1}{Q(n)^s} - \frac{1}{Q(n+x)^s}\right] \mathrm{d}x \\
&= \frac{s}{12} \sum_{\|n\|_\infty = N} \frac{\mathrm{tr}(A) Q(n) - 2(s+1) Q_{A^2}(n)}{Q(n)^{s+2}} + O(N^{d-2\sigma-4}) \\
&= \frac{s}{12 N^{2s+2}} \sum_{\|n\|_\infty = N} \frac{\mathrm{tr}(A) Q(n/N) - 2(s+1) Q_{A^2}(n/N)}{Q(n/N)^{s+2}} + O(N^{d-2\sigma-4}).
\end{aligned}$$

Consider, as defined above, $B(s) = \mathrm{tr}(A)A - 2(s+1)A^2$. As in the proof of Theorem 4.2, one obtains that, for $\mathrm{Re}\, s \geqslant -2$,

$$V(s) = \int_{\|x\|_\infty = 1} \frac{Q_{B(s)}(x)}{Q_A(x)^{s+2}} \mathrm{d}\lambda_{d-1} = \frac{1}{N^{d-1}} \sum_{\|n\|_\infty = N} \frac{Q_{B(s)}(n/N)}{Q_A(n/N)^{s+2}} + O(N^{-1}),$$

with λ_{d-1} as in (11). Combining these, we can thus write

$$\delta_N(s) = s \frac{V(s)}{12 N^{2s-d+3}} + W_N(s), \tag{28}$$

where $W_N(s) = O(N^{d-2\sigma-4})$. For $\sigma > d/2 - 3/2$, the sum

$$W(s) := \sum_{N=1}^{\infty} W_N(s)$$

converges and, by the Weierstrass M-test, defines an analytic function. If, further, $\mathrm{Re}\, s > d/2 - 1$ then, from (28), the sum $\delta(s) := \sum_{N=1}^{\infty} \delta_N(s)$ converges and we have

$$\delta(s) = \frac{s V(s)}{12} \zeta(2s - d + 3) + W(s). \tag{29}$$

Since

$$\mathrm{tr}(B(s)A^{-1}) = \mathrm{tr}(\mathrm{tr}(A) I - 2(s+1)A) = (d - 2(s+1)) \,\mathrm{tr}(A),$$

Lemma 2.5 shows that

$$V(d/2-1)=0. \tag{30}$$

Using that $\zeta(s)$ has a simple pole at $s=1$ of residue 1, we thus deduce from (29) that

$$\lim_{\varepsilon\to 0^+}\delta(d/2-1+\varepsilon)=\frac{d/2-1}{24}V'(d/2-1)+W(d/2-1). \tag{31}$$

On the other hand, (28) together with (30) implies $\delta_N(d/2-1)=W_N(d/2-1)$. Hence, the defining series for $\delta(s)$ also converges when $s=d/2-1$ and we obtain

$$\delta(d/2-1)=W(d/2-1).$$

The claim follows on comparison with (31). □

4.1. The behaviour of $V_Q'(d/2-1)$

We now examine the nature of $V_Q'(d/2-1)$ in somewhat more detail. Specifically, we are interested in the following question:

Problem 4.5. Let $d>1$. Are there positive definite quadratic forms Q on $\mathbb{R}^d$ such that $V_Q'(d/2-1)=0$?

Recall that, in light of Theorem 4.4, if $V_Q'(d/2-1)\neq 0$ for a quadratic form Q on $\mathbb{R}^d$, with $d>2$, then the corresponding Wigner limit $\sigma_Q(s)$ exhibits a jump discontinuity at $s=d/2-1$. In fact, in all the cases of Q, that we consider in this section, including the cubic lattice case, we find that $V_Q'(d/2-1)<0$, which leads us to speculate whether this inequality holds in general.

From the definition (25) we obtain that

$$\begin{aligned} V_Q'(d/2-1) &= \int_{\|x\|_\infty=1}\frac{-2Q_{A^2}(x)}{Q_A(x)^{d/2+1}}\mathrm{d}\lambda_{d-1} \\ &\quad -\int_{\|x\|_\infty=1}\frac{\operatorname{tr}(A)Q_A(x)-dQ_{A^2}(x)}{Q_A(x)^{d/2+1}}\log Q_A(x)\mathrm{d}\lambda_{d-1} \qquad (32)\\ &= -\frac{4\operatorname{tr}(A)}{d\sqrt{\det(A)}}\frac{\pi^{d/2}}{\Gamma(d/2)} \\ &\quad -\int_{\|x\|_\infty=1}\frac{\operatorname{tr}(A)Q_A(x)-dQ_{A^2}(x)}{Q_A(x)^{d/2+1}}\log Q_A(x)\mathrm{d}\lambda_{d-1}. \qquad (33)\end{aligned}$$

The last equality is a useful consequence of Lemma 2.5.

We also have that

$$V_{\lambda Q}'(d/2-1)=\lambda^{-(d/2-1)}V_Q'(d/2-1). \tag{34}$$

Indeed, it follows directly from the definition (25) that, for $\lambda>0$, $V_{\lambda Q}(s)=\lambda^{-s}V_Q(s)$ and hence, by (30), that (34) holds. The rescaling result (34) shows that scaling Q does not change the sign of $V_Q'(d/2-1)$. Also note that both

integrals in (32) scale in the same way; that this is true for the integral involving the logarithm is equivalent to

$$\int_{\|x\|_\infty=1} \frac{\operatorname{tr}(A)Q_A(x) - dQ_{A^2}(x)}{Q_A(x)^{d/2+1}} \mathrm{d}\lambda_{d-1} = 0,$$

which follows from Lemma 2.5.

Example 4.6 (Recovery of cubic jump)**.** Let us demonstrate that Theorem 4.4 reduces to Theorem 4.2 in the cubic lattice case. In that case, $A = I$ and $\operatorname{tr}(A) = d$, so that the integral in (33), involving the logarithm, vanishes. Hence,

$$V'(d/2-1) = -4\frac{\pi^{d/2}}{\Gamma(d/2)},$$

in agreement with the value given in Theorem 4.2. ◊

We now give a simple criterion that $V_Q'(d/2-1) < 0$ for certain $Q = Q_A$. Suppose that there is some $\lambda > 0$ such that, for all x with $\|x\|_\infty = 1$,

$$2Q_{A^2}(x) \geqslant [dQ_{A^2}(x) - \operatorname{tr}(A)Q_A(x)] \log Q_{\lambda A}(x). \tag{35}$$

It then follows from (32) that $V_Q'(d/2-1) \leqslant 0$. To see that, in fact, $V_Q'(d/2-1) < 0$, we note that (35) cannot be an equality for all x, because $dQ_{A^2}(x) - \operatorname{tr}(A)Q_A(x)$ does not vanish identically unless A is a multiple of the identity matrix (which corresponds to the cubic case, for which we know the explicit values from Theorem 4.2). In the non-cubic case, the right-hand side thus is a nonzero polynomial times the logarithm of a nonconstant polynomial, while the left-hand side is a polynomial.

Since $\log Q_{\lambda A}(x) = \log\lambda + \log Q_A(x)$, a $\lambda > 0$ satisfying (35) certainly exists if the sign of $dQ_{A^2}(x) - \operatorname{tr}(A)Q_A(x)$ is constant for all x with $\|x\|_\infty = 1$. We have thus proved the following result.

Proposition 4.7. *Let Q be a positive definite quadratic form on $\mathbb{R}^d$ such that*

$$d\,Q_{A^2}(x) \leqslant \operatorname{tr}(A)Q_A(x) \tag{36}$$

for all x with $\|x\|_\infty = 1$. Then $V_Q'(d/2-1) < 0$. The same conclusion holds if '$\leqslant$' is replaced with '$\geqslant$' in (36).

Example 4.8 (Some non-cubic lattices)**.** Consider the case when A is given by $A_p := I - pE$, where E is the matrix with all entries equal to 1. One easily checks that A_p is positive definite if and only if $p < 1/d$. Hence, we assume $p < 1/d$. We further observe that

$$Q_{A_p}(x) = \|x\|_2^2 - p\left(\sum_{j=1}^d x_j\right)^2,$$

as well as $A_p^2 = A_{p(2-dp)}$. Thus equipped, a brief calculation reveals that

$$dQ_{A_p^2}(x) - \mathrm{tr}(A_p)Q_{A_p}(x) = pd\|x\|_2^2 - p\left[1-(d-1)p\right]\left(\sum_{j=1}^d x_j\right)^2.$$

Notice that, by Hölder's inequality,

$$\left(\sum_{j=1}^d x_j\right)^2 \leqslant \|x\|_1^2 \leqslant d\|x\|_\infty\|x\|_2^2.$$

Assume further that $p \geqslant 0$, so that $p\left[1-(d-1)p\right] > 0$. We then find that, for all x with $\|x\|_\infty = 1$,

$$dQ_{A_p^2}(x) - \mathrm{tr}(A_p)Q_{A_p}(x) \geqslant p^2 d(d-1)\|x\|_2^2 \geqslant 0.$$

By Proposition 4.7, we have thus shown that $V_Q'(d/2-1) < 0$, with $Q = Q_{A_p}$, for all $0 \leqslant p < 1/d$. ♢

Continuing in this vein, we explicitly determine $V_Q'(d/2-1)$ for some very simple binary forms.

Example 4.9. To indicate the nature of the quantities $V_Q(s)$ and, in consequence, $V_Q'(d/2-1)$, let us consider the very basic case of $Q(x_1,x_2) := ax_1^2 + bx_2^2$, with $a, b > 0$, (of course, the factor $d/2-1$ in (26) vanishes in this case, so the contribution of $V_Q'(d/2-1)$ is not, in the end, brought to bear). We have

$$\begin{aligned} V_Q(s) &= \int_{\|x\|_\infty=1} \frac{(ab-(2s+1)a^2)x_1^2 + (ab-(2s+1)b^2)x_2^2}{(ax_1^2+bx_2^2)^{s+2}}\mathrm{d}\lambda_1 \\ &= 4\int_0^1 \frac{(ab-(2s+1)a^2)x_1^2 + (ab-(2s+1)b^2)}{(ax_1^2+b)^{s+2}}\mathrm{d}x_1 \\ &\quad +4\int_0^1 \frac{(ab-(2s+1)a^2) + (ab-(2s+1)b^2)x_2^2}{(a+bx_2^2)^{s+2}}\mathrm{d}x_2. \end{aligned}$$

Using the basic integral

$$\int_0^1 \frac{1}{(ax^2+b)^s}\mathrm{d}x = {}_2F_1\left(\begin{matrix}1/2, s\\ 3/2\end{matrix}\middle| -a\right), \tag{37}$$

and some standard hypergeometric manipulations, we thus find

$$V_Q(s) = \frac{-8s}{(a+b)^s}\left[{}_2F_1\left(\begin{matrix}1, 1/2-s\\ 3/2\end{matrix}\middle| -\frac{a}{b}\right) + {}_2F_1\left(\begin{matrix}1, 1/2-s\\ 3/2\end{matrix}\middle| -\frac{b}{a}\right)\right]. \tag{38}$$

The factor of s in $V_Q(s)$, together with the elementary special case $s = 1$ of (37), allows us to conclude that

$$V_Q'(0) = -8\left[\sqrt{\frac{b}{a}}\arctan\sqrt{\frac{a}{b}} + \sqrt{\frac{a}{b}}\arctan\sqrt{\frac{b}{a}}\right].$$

In particular, we observe that $V_Q'(d/2-1) < 0$, though Proposition 4.7 does not apply in the present case. ◊

Sadly, as illustrated by this example, Proposition 4.7 is not always accessible. Indeed, it can fail quite comprehensively.

Example 4.10 (Some scaled cubic lattices)**.** Consider the case when A is given by $A_p := I + pD(a)$, where $D(a) = D(a_1, \ldots, a_d)$ is a diagonal matrix and, without loss, $p \geqslant 0$. The matrix A_p is positive definite if and only if $pa_k + 1 > 0$ for all $1 \leqslant k \leqslant d$.

Suppose that $\operatorname{tr}(D(a)) = 0$, so that $\operatorname{tr}(A_p) = d$. Also $A_p^2 = I + 2pD(a) + p^2 D(a_1^2, \ldots, a_k^2)$. Thence,

$$dQ_{A_p^2}(x) - \operatorname{tr}(A_p) Q_{A_p}(x) = pd \sum_{k=1}^{d} a_k(1 + pa_k)x_k^2,$$

which must change signs on the sphere, since the a_k vary in sign, and so Proposition 4.7 does not apply. ◊

We conclude this section with a comment on the behaviour of $\sigma(s)$ at the other side of the strip of convergence, that is, as $s \to d/2$.

Remark 4.11 ($\sigma(s)$ as $s \to d/2$)**.** From Proposition 2.1 and the fact that $\alpha_N(s)$ is an entire function, we know that $\sigma_N(s)$ has a simple pole at $s = d/2$ with the same residue as $\alpha(s)$ (which, by Proposition 3.1, is the analytic continuation of the limit $\sigma(s)$). ◊

5. Alternative procedures for Wigner limits

The limit $\sigma(s) = \lim_{N\to\infty} [\alpha_N(s) - \beta_N(s)]$, considered in the preceding sections, is built from the sum $\alpha_N(s)$, which sums over the lattice points in the hypercube $\{x \in \mathbb{R}^d : \|x\|_\infty \leqslant N\}$. In this section, we will show that some of the previous discussion carries over to the case when the hypercubes get replaced by more general sets. For simplicity, we restrict to the case of general hyperballs $\{x \in \mathbb{R}^d : \|x\| \leqslant N\}$ where $\|\cdot\|$ is any norm in $\mathbb{R}^d$, and consider

$$\widehat{\alpha}_N(s) := \sum_{0<\|n\|\leqslant N} \frac{1}{Q(n)^s}, \tag{39}$$

$$\widehat{\beta}_N(s) := \int_{\|x\|\leqslant N} \frac{1}{Q(x)^s} \mathrm{d}x, \tag{40}$$

as well as $\widehat{\sigma}_N := \widehat{\alpha}_N - \widehat{\beta}_N$. Again, if $\operatorname{Re} s > d/2$, then $\widehat{\alpha}_N(s)$ converges to the Epstein zeta function $\alpha(s) = Z_Q(s)$ as $N \to \infty$.

Of particular interest is the case $\|\cdot\| = \|\cdot\|_2$, in which the lattice sum extends over the usual Euclidean d-balls of radius N. This case was considered

in [BBS89, Theorem 2] when $d = 2$ and it was shown that the limit $\widehat{\sigma}(s) := \lim_{N\to\infty} \widehat{\sigma}_N(s)$ exists in the strip $1/3 < \operatorname{Re} s < 1$ and coincides therein with the analytic continuation of $\alpha(s)$. As we will see below, this strip can be extended on the left-hand side, though not below $1/4$.

In contrast to Remark 4.1, we note that $\widehat{\sigma}_N(0)$ usually does not converge. We therefore let λ be the infimum of all values $\ell \geqslant 0$ such that

$$\widehat{\sigma}_N(0) = \#\{n \in \mathbb{Z}^d : \|n\| \leqslant N\} - \operatorname{vol}\{x \in \mathbb{R}^d : \|x\| \leqslant N\} - 1 = O(N^\ell). \quad (41)$$

The determination of λ, especially for the p-norms $\|\cdot\|_p$, is a famous problem and in several cases still open. In particular, when $d = 2$ and $\|\cdot\| = \|\cdot\|_2$, this is Gauss's circle problem. For a recent survey, we refer to [IKKN06]. A number of results on the values of λ are discussed in the proof of Corollary 5.2 and the remarks thereafter. We also recall the well-known fact, due to Weierstrass, that the balls in the p-norm have volume

$$\operatorname{vol}\{x \in \mathbb{R}^d : \|x\|_p \leqslant N\} = \frac{2^d \Gamma^d(1 + 1/p)}{\Gamma(1 + d/p)} N^d.$$

We prove the following analog of Proposition 3.1, which includes [BBS89, Theorem 2] as the special case $d = 2$ and $\|\cdot\| = \|\cdot\|_2$.

Proposition 5.1. *Let $\|\cdot\|$ be a norm on $\mathbb{R}^d$, and assume that λ is the infimum of all values $\ell \geqslant 0$ such that (41) holds. Further, let Q be a positive definite quadratic form. Then the limit $\widehat{\sigma}(s) := \lim_{N\to\infty} \widehat{\sigma}_N(s)$ exists in the strip $\max(d/2 - 1, \lambda/2) < \operatorname{Re} s < d/2$ and coincides therein with the analytic continuation of $\alpha(s)$.*

Proof. As before, we fix $\sigma > 0$ as well as $R > 0$ and set $\Omega = \{s : \operatorname{Re} s > \sigma, \quad |s| < R\}$. All order terms below are uniform with respect to s in the bounded region Ω. In order to proceed along the lines of Proposition 3.1, we introduce

$$\tilde{\beta}_N(s) := \sum_{\|n\| \leqslant N} \int_{\|x\|_\infty \leqslant 1/2} \frac{1}{Q(n + x)^s} \mathrm{d}x,$$

and observe that, by (41) and the fact that all norms on $\mathbb{R}^d$ are equivalent,

$$\widehat{\beta}_N(s) - \tilde{\beta}_N(s) = O(N^{-2s+\ell}) \quad (42)$$

for all values $\ell > \lambda$. On the other hand, set $\tilde{\sigma}_N(s) := \widehat{\alpha}_N(s) - \tilde{\beta}_N(s)$ and let

$$\begin{aligned}
\delta_N(s) &:= \tilde{\sigma}_N(s) - \tilde{\sigma}_{N-1}(s) \\
&= \sum_{N-1 < \|n\| \leqslant N} \int_{\|x\|_\infty \leqslant 1/2} \left[\frac{1}{Q(n)^s} - \frac{1}{Q(n + x)^s} \right] \mathrm{d}x. \\
&= O(N^{-2\sigma-2}) \sum_{N-1 < \|n\| \leqslant N} 1 \\
&= O(N^{d-2\sigma-3}),
\end{aligned}$$

where the estimates follow as in the proof of Proposition 3.1.

Again, we conclude that the series $\delta(s) := \sum_{N=1}^{\infty} \delta_N(s)$ converges in the half-plane $\operatorname{Re} s > d/2 - 1$ and defines an analytic function therein. By construction,

$$\delta(s) = \lim_{N\to\infty} \left[\tilde{\sigma}_N(s) + \tilde{\beta}_0(s)\right]. \tag{43}$$

Since $\tilde{\beta}_0(s)$ is analytic for $\operatorname{Re} s < d/2$, it follows that the limit $\tilde{\sigma}(s) := \lim_{N\to\infty} \tilde{\sigma}_N(s)$ exists in the strip $d/2 - 1 < \operatorname{Re} s < d/2$. In combination with (42), this shows that the limit $\widehat{\sigma}(s)$ exists in the strip $\max(d/2-1, \lambda/2) < \operatorname{Re} s < d/2$ and equals $\tilde{\sigma}(s)$ therein.

For the second part of the claim, we proceed as in the proof of Proposition 3.1 and observe that, for $\operatorname{Re} s < d/2$,

$$\widehat{\beta}_N(s) = N^{d-2s} \int_{\|x\|\leqslant 1} \frac{1}{Q(x)^s} \mathrm{d}x = N^{d-2s} \widehat{\beta}_1(s). \tag{44}$$

We note that Proposition 2.1, with the same proof, also applies to $\widehat{\beta}_N$ in place of β_N. In particular, $\widehat{\beta}_N$ and $\widehat{\beta}_0$ have meromorphic continuations to the entire complex plane, and the relation induced by (44) continues to hold. For $\operatorname{Re} s > d/2$,

$$\lim_{N\to\infty} \widehat{\beta}_N(s) = \lim_{N\to\infty} N^{d-2s} \widehat{\beta}_1(s) = 0.$$

We therefore have, for $\operatorname{Re} s > d/2$,

$$\delta(s) = \lim_{N\to\infty} \left[\widehat{\alpha}_N(s) - \widehat{\beta}_N(s) + \tilde{\beta}_0(s)\right] = \alpha(s) + \tilde{\beta}_0(s). \tag{45}$$

On the other hand, it follows from (42) and (43) that, for $\operatorname{Re} s < d/2$,

$$\delta(s) = \widehat{\sigma}(s) + \tilde{\beta}_0(s). \tag{46}$$

Since both $\delta(s)$ and $\tilde{\beta}_0(s)$ are meromorphic in the half-plane $\operatorname{Re} s > d/2 - 1$, comparing (45) and (46) proves that the analytic continuations of $\widehat{\sigma}(s)$ and $\alpha(s)$ agree. □

Corollary 5.2 (Four and higher dimensions)**.** *Let Q be a positive definite quadratic form on $\mathbb{R}^d$ for $d \geqslant 4$. Then the limit*

$$\widehat{\sigma}(s) = \lim_{N\to\infty} \left[\sum_{0<\|n\|_2\leqslant N} \frac{1}{Q(n)^s} - \int_{\|x\|_2\leqslant N} \frac{1}{Q(x)^s} \mathrm{d}x \right]$$

exists in the strip $d/2 - 1 < \operatorname{Re} s < d/2$ and coincides therein with the analytic continuation of $\alpha(s)$.

Proof. We recall, see [IKKN06], the fact that, for all $d \geqslant 5$,

$$\#\{n \in \mathbb{Z}^d : \|n\|_2 \leqslant N\} - \mathrm{vol}\{x \in \mathbb{R}^d : \|x\|_2 \leqslant N\} = O(N^{d-2}),$$

while, for $d = 4$, the right-hand side needs to be replaced with, for instance, the rather classical $O(N^2(\log N))$, or the improved $O(N^2(\log N)^{2/3})$ shown in [Wal59]. In any case, we conclude that, for all $d \geqslant 4$, the infimum λ_d of all values $\ell \geqslant 0$ such that (41) holds, is $\lambda_d = d - 2$. The claim therefore follows from Proposition 5.1. □

Remark 5.3 (Two and three dimensions)**.** Thorough reports on the current status of the cases $d = 2$ and $d = 3$, missing in Corollary 5.2, can be found in [IKKN06]. In the case $d = 2$, it was shown by Hardy as well as Landau that $\lambda_2 \geqslant 1/2$. While it is believed that in fact $\lambda_2 = 1/2$, the best currently known bound is $\lambda \leqslant 131/208 \approx 0.6298$, obtained in [Hux03]. For $d = 3$, it is known that $\lambda_3 \geqslant 1$ and it is believed that $\lambda_3 = 1$, in which case the conclusion of Corollary 5.2 would also hold for $d = 3$. The smallest currently fully proven upper bound is $\lambda_3 \leqslant 21/16 = 1.3125$ from [HB99]. ♢

Remark 5.4 (more general p-norms)**.** Let us briefly note some results and their consequences for more general p-norms, again referring to [IKKN06] for further details and missing cases. Let $d \geqslant 2$. For integers $p > d + 1$ it is known that

$$\#\{n \in \mathbb{Z}^d : \|n\|_p \leqslant N\} - \mathrm{vol}\{x \in \mathbb{R}^d : \|x\|_p \leqslant N\} = O\left(N^{(d-1)(1-1/p)}\right),$$

and that the exponent in this estimate cannot be improved. This result was obtained in [Ran66] for even p, and in [Krä73] for odd p. In light of Proposition 5.1, we conclude that the limit

$$\widehat{\sigma}(s) = \lim_{N\to\infty} \left[\sum_{0<\|n\|_p\leqslant N} \frac{1}{Q(n)^s} - \int_{\|x\|_p\leqslant N} \frac{1}{Q(x)^s} \mathrm{d}x \right]$$

exists in the strip $(d-1)(1-1/p)/2 < \mathrm{Re}\, s < d/2$ and coincides therein with the analytic continuation of $\alpha(s)$. We note that this strip shrinks to $d/2 - 1/2 < \mathrm{Re}\, s < d/2$ as $p \to \infty$. In particular, for $d = 2$, the physically interesting value $\widehat{\sigma}(1/2)$ always exists and equals $\alpha\,(1/2)$. ♢

A. Brief review of cubic lattice sums

The d-dimensional cubic lattice sum

$$Z_d(s) := {\sum_{n_1,\ldots,n_d}}' \frac{1}{(n_1^2 + n_2^2 + \cdots + n_d^2)^s}, \tag{A.1}$$

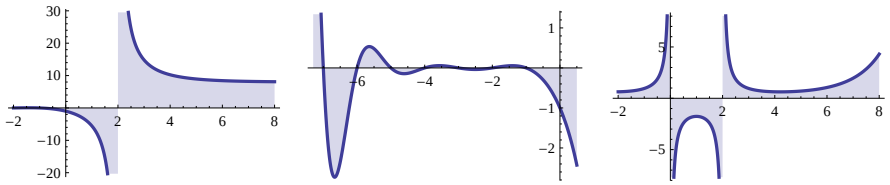
which converges for $s > d/2$, is a special case of an Epstein zeta function as introduced in (5). As such, the sum $Z_d(s)$ has a meromorphic continuation to the entire complex plane and satisfies the functional equation

$$\frac{Z_d(s)\Gamma(s)}{\pi^s} = \frac{Z_d(d/2-s)\Gamma(d/2-s)}{\pi^{d/2-s}}. \tag{A.2}$$

The sum $Z_d(s)$ has a simple pole at $s = d/2$ with residue $\pi^{d/2}/\Gamma(d/2)$. We record that the values of $\pi^{d/2}/\Gamma(d/2)$, for $d = 1, 2, \ldots, 6$, are

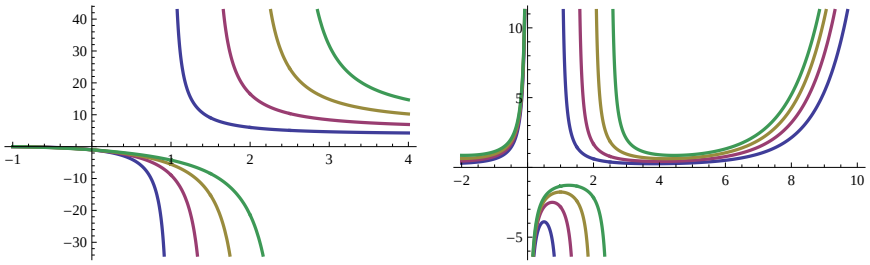
$$1, \quad \pi, \quad 2\pi, \quad \pi^2, \quad \frac{4}{3}\pi^2, \quad \frac{1}{2}\pi^3.$$

The plots in Figures A.1 and A.2 illustrate these functions and their properties in small dimensions. Observe the symmetries around the poles in Figure 1(c) and Figure 2(b).



(a) $Z_4(s)$ on $[-2, 8]$ (b) $Z_4(s)$ on $[-7, 0]$ (c) $Z_4(s)\Gamma(s)\pi^{-s}$

Figure A.1: Different views on $Z_4(s)$ on the real line.



(a) $Z_d(s)$ for $d = 2, 3, 4, 5$ (b) $Z_d(s)\Gamma(s)\pi^{-s}$ for $d = 2, 3, 4, 5$

Figure A.2: The functions $Z_d(s)$ on the real line for various values of d.

Remark A.1 (Lattice sums and integer representations)**.** Let $r_d(n)$ denote the number of integer solutions (counting permutations and signs) of $n_1^2 + n_2^2 + \cdots + n_d^2 = n$. Clearly, by definition (A.1), the lattice sum $Z_d(s)$ is precisely the Dirichlet series for the sum-of-d-squares counting function $r_d(n)$, that is,

$$Z_d(s) = \sum_{n=1}^{\infty} \frac{r_d(n)}{n^s}.$$

In particular, Lagrange's theorem on the sum of four squares [BGM+13] shows that, if $d > 3$, then $r_d(n) > 0$ for all $n > 0$. ♢

The defining lattice sum (5) only converges when $\mathrm{Re}\, s > d/2$. Our next goal is to make the analytic continuation of $Z_d(s)$ explicit, in particular in the critical strip $0 \leqslant \mathrm{Re}\, s \leqslant d/2$. To this end, let us, for $\mathrm{Re}\, s > 0$, define the normalized Mellin transform $M_s[f]$ of a function f on the positive real line by

$$M_s[f] := \frac{1}{\Gamma(s)} \int_0^\infty f(x) x^{s-1} \mathrm{d}x.$$

The point of this normalization is that, for $\lambda > 0$,

$$M_s[e^{-\lambda x}] = \frac{1}{\lambda^s}.$$

This allows many classes of lattice sum to be interpreted as the Mellin transform of combinations of Jacobi theta functions. In the present case of cubic lattice sums, one finds

$$\begin{aligned} Z_d(s) &= M_s \left[{\sum_{n_1,\ldots,n_d}}' e^{-(n_1^2+n_2^2+\cdots+n_d^2)x} \right] \\ &= M_s \left[\left(\sum_{n=-\infty}^{\infty} e^{-n^2 x} \right)^d - 1 \right] \\ &= \pi^s M_s \left[\theta_3^d(ix) - 1 \right], \end{aligned}$$

where

$$\theta_3(z) := \sum_{n=-\infty}^{\infty} e^{\pi i n^2 z}$$

is the third Jacobi special theta function. In order to obtain the analytic continuation of $Z_d(s)$, we proceed in the classical fashion and use the modular transformation

$$\theta_3(i/x) = x^{1/2} \theta_3(ix)$$

to write, assuming $\mathrm{Re}\, s > d/2$,

$$\int_0^1 \left(\theta_3^d(ix) - 1 \right) x^{s-1} \mathrm{d}x = \frac{1}{s - d/2} - \frac{1}{s} + \int_1^\infty \left(\theta_3^d(ix) - 1 \right) x^{d/2-s-1} \mathrm{d}x.$$

It follows that

$$Z_d(s) = \frac{\pi^s}{\Gamma(s)} \left[\frac{1}{s - d/2} - \frac{1}{s} + \int_1^\infty \left(\theta_3^d(ix) - 1 \right) \left(x^{s-1} + x^{d/2-s-1} \right) \mathrm{d}x \right]. \tag{A.3}$$

We note that the integral in (A.3) converges and is analytic for all s. Since the zero of the gamma function cancels the $1/s$ term, it is clear from (A.3) that $Z_d(s)$ is indeed analytic except for a simple pole at $s = d/2$ with residue $\pi^{d/2}/\Gamma(d/2)$. Moreover, the functional equation (A.2) is another nearly immediate consequence of (A.3). Equation (A.3) is well-suited to numerically compute $Z_d(s)$ as well as its analytic continuation.

Example A.2. (Exact evaluations) In small even dimensions, the cubic lattice sums can be evaluated in terms of $\zeta(s)$ and $\beta(s)$, the Dirichlet series for the primitive character χ_{-4} modulo 4. By realizing the lattice sum Z_d as, essentially, the Mellin transform of the power $\theta_3^d - 1$, where θ_3 is as before the Jacobi theta function, one finds, for instance, the evaluations

$$\begin{aligned} Z_2(s) &= 4\zeta(s)\beta(s), \\ Z_4(s) &= 8(1-2^{2-2s})\zeta(s-1)\zeta(s), \\ Z_6(s) &= 16\zeta(s-2)\beta(s) - 4\zeta(s)\beta(s-2), \\ Z_8(s) &= 16\left(1-2^{1-s}+4^{2-s}\right)\zeta(s)\zeta(s-3). \end{aligned}$$

See [Zuc74] for these and many further exact evaluations of lattice sums. In higher even dimensions, exact evaluations involve further L-functions. A more direct, but equivalent, approach to these evaluations is presented in [BC03], where the discussion is based on explicit formulas for $r_{2d}(n)$. For instance, [BC03, Sec. 6.2],

$$\begin{aligned} Z_{24}(s) &= \frac{16}{691}\left(2^{12-2s}-2^{1-s}+1\right)\zeta(s)\zeta(s-11) \\ &\quad + \frac{128}{691}\left(259+745\cdot 2^{4-s}+259\cdot 2^{12-2s}\right)L_\Delta(s), \end{aligned}$$

where $L_\Delta(s) = \sum \tau(n)/n^s$ and $\tau(n)$ is Ramanujan's τ-function (here, $\Delta = \eta^{24}$ in terms of the Dedekind η-function). We remark that the critical values of L_Δ are known to be *periods*, that is, values of an integral of an algebraic function over an algebraic domain [KZ01]. Moreover, up to the usual powers of π, all odd (respectively, even) critical values are rational multiples of each other. (More generally, all values $L_\Delta(m)$ for integers $m > 0$ are *periods*.) Ramanujan's τ satisfies many wonderful congruences. Moreover, Lehmer conjectured [Leh47] that $\tau(n)$ (while taking both signs) is never zero, as has been verified for more than the first $2\cdot 10^{19}$ terms [Bos07]. Lehmer's conjecture is also known to be implied by the alleged irrationality of the coefficients of the holomorphic part of a certain Maass-Poincaré series, see [Ono09, Example 12.6].

The case of odd d is much harder and no simple exact evaluations are known. We refer to, for instance, [BC03, Sec. 6] and [BGM+13]. It transpires in [BC03] that, when considering $r_d(2n)$, the smallest odd cases $d = 3, 5$ are in many ways the hardest in terms of estimating asymptotic behavior. ◊

Remark A.3 (A curious but useful Bessel series)**.** We recall from [BC03, Sec. 6] a modified Bessel function series for Z_d.

(a) For all integers $d \geqslant 2$,

$$\begin{aligned} Z_d(s) &= 2d\,\frac{\Gamma\left((2s-d+3)/2\right)}{\Gamma(s+1)}\pi^{(d-1)/2}\,\zeta(2s-d+1) \\ &\quad + \frac{4d\pi^{s+1}}{\Gamma(s+1)}\sum_{m\geqslant 1}\frac{r_{d-1}(m)}{m^{(d-2s-3)/4}}\sum_{n\geqslant 1}\frac{K_{(2s-d+3)/2}\left(2\pi n\sqrt{m}\right)}{n^{(2s-d-1)/2}}. \end{aligned} \tag{A.4}$$

(b) We note that the first summand of (A.4), just like the sum $Z_d(s)$ itself, is analytic except for a simple pole at $s = d/2$ with residue $\pi^{d/2}/\Gamma(d/2)$. Consequently, the double sum involving the Bessel terms defines an entire function. Indeed, this easily follows directly from the asymptotic fact, see [DLMF, Chapter 10, §10.40], that, for positive real argument, the Bessel function behaves as

$$K_s(x) \sim \sqrt{\frac{\pi}{2x}} e^{-x}$$

when $x \to \infty$. One thus finds that the double sum converges for all values of s and defines an analytic function. In particular, (A.4) is another explicit representation of the analytic continuation of $Z_d(s)$ to the entire complex plane.

(c) When $r := 2s - d + 3$ is an odd integer we need compute only Bessel function values at half-integers which become elementary [DLMF, §10.47(ii) and §10.49(ii)]. When $s = d/2 - 1$, the value of the jump discontinuity, then $r = 1$ and we need consider only $K_{1/2}\left(2\pi n\sqrt{m}\right)$ for integers $m, n > 0$. We then have [DLMF, §10.39 (ii)] that

$$K_{1/2}(z) = K_{-1/2}(z) = \sqrt{\frac{\pi}{2z}} e^{-z}.$$

This reduces (A.4) to a rapidly convergent exponential double series. Summing the second series, for each positive integer $d > 1$, we obtain

$$\begin{aligned} Z_d(d/2-1) &= \frac{2d\pi^{d/2}}{\Gamma(d/2)} \left[-\frac{1}{12} + \sum_{m \geqslant 1} \frac{r_{d-1}(m) e^{-2\pi\sqrt{m}}}{(1 - e^{-2\pi\sqrt{m}})^2} \right] \\ &= \frac{2d\pi^{d/2}}{\Gamma(d/2)} \left[-\frac{1}{12} + \frac{1}{2} \sum_{m \geqslant 1} \frac{r_{d-1}(m)}{\cosh(2\pi\sqrt{m}) - 1} \right] \end{aligned} \tag{A.5}$$

for the value corresponding to the jump in Theorem 4.2. Amongst odd integers, (A.5) is most rapid for $d = 3$ since $r_2(m)$ is the smallest coefficient set. For even integers, (A.5) combines with Example A.2 to provide evaluations of the hyperbolic sum. With $d = 2$, this recovers

$$\sum_{m=1}^{\infty} \frac{1}{\cosh(2\pi m) - 1} = \frac{1}{12} - \frac{1}{4\pi},$$

as the simplest evaluation. ◊

Conclusion

We have been able to analyse the behaviour of Wigner limits for electron sums in arbitrary dimensions quite extensively. The analysis sheds light on

the remarkable interplay between the physical and analytic properties of lattice sums. We also observe that physicists typically proceed by taking Laplace and related transforms quite formally. This suggests that the subtle boundary behaviour of the limit $\sigma(s)$ would never be noticed without careful mathematical analysis. Finally, it remains to conclusively answer Problem 4.5 in order to decide whether, for $d > 2$, every quadratic form indeed exhibits a jump at $d/2 - 1$ in the corresponding Wigner limit.

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