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On lattice sums and Wigner limits

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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 [3], to integer lattices of arbitrary dimension. In doing so, we also resolve a problem posed in [6, 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. Appendix A is included to recall certain properties of Epstein zeta functions that are either used in the paper or serve to provide perspective.

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 [6, Chapter 7], we shall examine the behavior of

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

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

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

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

As usual, the summation in (1) is understood to avoid the term corresponding to $(n_1, \ldots, n_d) = (0, \ldots, 0)$. 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 [3, 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 [3, 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 this phenomenon 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 [6, 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 $Q(x) := x_1^2 + \cdots + x_d^2$, corresponding to the *cubic lattice* (also referred to as standard lattice or integer lattice), 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 [6, 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 centred at the lattice point.