Exponential Riemann Sums and "Near"-Quasicrystals

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Counting things is a great favorite of children, and mathematicians as well, whatever the things are

The primary aim of this short note[†] is, commemorating the 150th anniversary of Riemann's death, to explain how the idea of *Riemann sum* is linked to other branches of mathematics. The materials I treat are ones available to the "mathematician in the streets" except for a few. However one may still see interesting inter-connection and cohesiveness in mathematics.

1 Riemann sums

In December of 1853, Bernhard Riemann (1826–1866) presented the epochmaking paper "Über die Darstellbarkeit einer Function durch eine trigonometrische Reihe" (On the representability of a function by a trigonometric series) to the Council of Göttingen University as his Habilitationsschrift (Qualification to become an instructor), in which he gave a rigorous definition of integrals.

What plays a significant role in Riemann's definition of integrals is the notion of *Riemann sum*, which, if we use his notations, is expressed as

$$S = \delta_1 f(a + \epsilon_1 \delta_1) + \delta_2 f(x_1 + \epsilon_2 \delta_2) + \delta_3 f(x_3 + \epsilon_3 \delta_3) + \dots + \delta_n f(x_{n-1} + \epsilon_n \delta_n).$$

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Here f(x) is a function on the closed interval [a, b], $a = x_0 < x_1 < x_2 < \cdots < x_{n-1} < x_n = b$, and $\delta_i = x_i - x_{i-1}$ $(i = 1, 2, \dots, n)$. If S converges to A as $\max_i \delta_i$ goes to 0 whatever ϵ_i with $0 < \epsilon_i < 1$ $(i = 1, \dots, n)$ are chosen (thus $x_{k-1} + \epsilon_k \delta_k \in [x_{k-1}, x_k]$), then the value A is written as $\int_a^b f(x) dx$, and f(x) is called Riemann integrable. For example, every continuous function is Riemann integrable as we learn in calculus.

The notion of Riemann sum is immediately generalized to functions of several variables as follows.

Let $\Delta = \{D_{\alpha}\}_{\alpha \in A}$ be a partition of \mathbb{R}^d by a countable family of bounded domains D_{α} with piecewise smooth boundaries satisfying

(i) $\operatorname{mesh}(\Delta) := \sup_{\alpha \in A} d(D_{\alpha}) < \infty$, where $d(D_{\alpha})$ is the diameter of D_{α} ,

(ii) there are only finitely many α such that $K \cap D_{\alpha} \neq \emptyset$ for any compact set $K \subset \mathbb{R}^d$.

We select a point $\boldsymbol{\xi}_{\alpha}$ from each D_{α} , and put $\Gamma = \{\boldsymbol{\xi}_{\alpha} | \alpha \in A\}$. The Riemann sum $\sigma(f, \Delta, \Gamma)$ for a function f on \mathbb{R}^d with compact support is defined by

$$\sigma(f, \Delta, \Gamma) = \sum_{\alpha} f(\boldsymbol{\xi}_{\alpha}) \operatorname{vol}(D_{\alpha}),$$

where $\operatorname{vol}(D_{\alpha})$ is the volume of D_{α} . Note that $f(\boldsymbol{\xi}_{\alpha}) = 0$ for all but finitely many α because of Property (ii).

If the limit

$$\lim_{\text{mesh}(\Delta)\to 0} \sigma(f, \Delta, \Gamma) \tag{1}$$

exists, independently of the specific sequence of partitions and the choice of $\{\boldsymbol{\xi}_{\alpha}\}$, then f is said to be Riemannian integrable, and this limit is called the (*d*-tuple) Riemann integral of f, which we denote by $\int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x}$.

In particular, we take the sequence of partitions given by $\Delta_{\epsilon} = \{\epsilon D_{\alpha} \mid \alpha \in A\}$ ($\epsilon > 0$). Then for a Riemann integrable function f, we have

$$\lim_{\epsilon \to +0} \sum_{\alpha \in A} \epsilon^d f(\epsilon \boldsymbol{\xi}_{\alpha}) \operatorname{vol}(D_{\alpha}) = \int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x}.$$
 (2)

Here we look at Eq. (2) from a different angle. We think that $\omega(\boldsymbol{\xi}_{\alpha}) := \operatorname{vol}(D_{\alpha})$ is a *weight* of the point $\boldsymbol{\xi}_{\alpha}$, and that (2) is telling how the *weighted* discrete set (Γ, ω) are distributed in \mathbb{R}^d ; more specifically we may consider

that (2) implies *uniformity* of (Γ, ω) in \mathbb{R}^d . This view motivates us to propose the following definition.

In general, a weighted discrete subset (Γ, ω) in \mathbb{R}^d is a discrete set $\Gamma \subset \mathbb{R}^d$ with a map $\omega : \Gamma \to \mathbb{C} \setminus \{0\}$. Given a compactly supported function f on \mathbb{R}^d , define the *Riemann sum associated with* (Γ, ω) by setting

$$\sigma_{\epsilon}(f,\Gamma,\omega) = \sum_{\mathbf{z}\in\Gamma} \epsilon^d f(\epsilon \mathbf{z})\omega(\mathbf{z}).$$

We say that (Γ, ω) is uniformly arranged if there exists a constant $c(\Gamma, \omega) \neq 0$ such that

$$\lim_{\epsilon \to +0} \sigma_{\epsilon}(f, \Gamma, \omega) = c(\Gamma, \omega) \int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x}.$$

holds for any bounded Riemannian integrable function f on \mathbb{R}^d with compact support. In the case $\omega \equiv 1$, we simply say that Γ is uniformly arranged[‡], and write $c(\Gamma)$ for $c(\Gamma, \omega)$.

Well, what is the usability of the notion of uniform arrangement? Admittedly our formulation of uniformity is not profound. It may be, however, of great interest if we would focus our attention on the constant $c(\Gamma)$. In the subsequent sections, we give two "arithmetical" examples for which the constant $c(\Gamma)$ is explicitly computed.

2 Classical example 1

Let $\mathbb{Z}_{\text{prim}}^d$ is the set of *primitive lattice points* in the *d*-dimensional standard lattice \mathbb{Z}^d , i.e. the set of *lattice points visible from the origin* (note that $\mathbb{Z}_{\text{prim}}^2$ is the set of $(x, y) \in \mathbb{Z}^2$ such that |x| and |y| are coprime, together with $(\pm 1, 0)$ and $(0, \pm 1)$).

Theorem 1 $\mathbb{Z}^{d}_{\text{prim}}$ is uniformly arranged with $c(\mathbb{Z}^{d}_{\text{prim}}) = \zeta(d)^{-1}$; that is, $\lim_{\epsilon \to +0} \sum_{\mathbf{z} \in \mathbb{Z}^{d}_{\text{prim}}} \epsilon^{d} f(\epsilon \mathbf{z}) = \zeta(d)^{-1} \int_{\mathbb{R}^{d}} f(\mathbf{x}) d\mathbf{x}.$ (3)

 $^{^{\}ddagger}\mathrm{In}$ [7], the term "constant density" is used.

Here $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$ is the zeta function.

Noting $\zeta(2) = \pi^2/6$ and applying this theorem to the indicator function f for the square $\{(x, y) | 0 \le x, y \le 1\}$, we obtain the following well-known statement, which is equivalent to the 31st entry[§] dated 1796 September 6 in Gauss's Mathematisches Tagebuch, a record of the mathematical discoveries of C. F. Gauss from 1796 to 1814.

Corollary The probability that two randomly chosen positive integers are coprime is $6/\pi^2$. More precisely

$$\lim_{N \to \infty} \frac{1}{N^2} \left| \left\{ (a, b) \in \mathbb{N} \times \mathbb{N} \right| \operatorname{gcd}(a, b) = 1, \ a, b \le N \right\} \right| = \frac{6}{\pi^2}, \qquad (4)$$

where gcd(a, b) stands for the greatest common divisor of a, b.

3 Classical example 2

Primitive Pythagorean triples, the name stemming from the Pythagorean theorem for right triangles, have a long history since the Old Babilonian period in Mesopotamia nearly 4000 years ago [11].

A Pythagorean triple is a triple of positive integers (ℓ, m, n) satisfying the equation $\ell^2 + m^2 = n^2$. Since $(\ell/n)^2 + (m/n)^2 = 1$, a Pythagorean triple yields a it rational point $(\ell/n, m/n)$ on the unit circle $S^1 = \{(x, y) | x^2 + y^2 = 1\}$. Conversely any rational point on S^1 is derived from a Pythagorean triple. Furthermore the well-known parameterization of S^1 given by $x = (1-t^2)/(1+t^2)$, $y = 2t/(1+t^2)$ tells us that the set of rational points $S^1(\mathbb{Q}) = S^1 \cap \mathbb{Q}^2$ is dense in S^1 .

A Pythagorean triple (x, y, z) is called primitive if x, y, z are pair wise coprime. "Primitive" is so named because any Pythagorean triple is generated trivially from the primitive one, i. e., if (x, y, z) is Pythagorean, there are a positive integer ℓ and a primitive (x_0, y_0, z_0) such that (x, y, z) = $(\ell x_0, \ell y_0, \ell z_0)$.

The way to produce primitive Pythagorean triples (PPT) is described as follows: If (x, y, z) is a PPT, then there exist positive integer such that

[§]In Latin, it says "Numero fractionum inaequalium quorum denomonatores certum limitem non superant ad numerum fractionum omnium quarum num[eratores] aut denom[inatores] sint diversi infra limitem in infinito ut $6:\pi\pi$ "

- (i) m > n,
- (ii) m and n are coprime,
- (iii) m and n have different parity,

(iv) $(x, y, z) = (m^2 - n^2, 2mn, m^2 + n^2)$ or $(x, y, z) = (2mn, m^2 - n^2, m^2 + n^2)$.

Conversely, if m and n satisfy (i), (ii), (iii), then $(m^2 - n^2, 2mn, m^2 + n^2)$ and $(2mn, m^2 - n^2, m^2 + n^2)$ are PPTs.

We enumerate PPTs (x, y, z) in ascending order with respect to z, and let (x_N, y_N, z_N) be the N-th PPT (we do not discriminate between (x, y, z) and (y, x, z)). What we have interest in is the asymptotic behavior of z_N as N goes to infinity. The numerical observation tells us that the sequence $\{z_N\}$ almost linearly increase as N increases. Indeed $z_{100}/100 = 6.29$, $z_{1000}/1000 = 6.277$, $z_{1500}/1500 = 6.28333 \cdots$, which convinces us that $\lim_{N \to \infty} z_N/N$ exists (though the speed of convergence is very slow), and the limit is expected to be equal to $2\pi = 6.2831853 \cdots$. This is actually true (D. N. Lehmer [6], 1900), though the proof is by no means trivial. One can prove this by counting coprime pairs (m, n) satisfying the condition that m - n is odd.

A key of our proof is the following theorem.

Theorem 2 $\mathbb{Z}_{\text{prim}}^{2,*} = \{(m.n) \in \mathbb{Z}_{\text{prim}}^2 | m-n \text{ is odd}\}$ is uniformly arranged with $c(\mathbb{Z}_{\text{prim}}^{2,*}) = 4/\pi^2$; namely $\lim_{\epsilon \to +0} \sum_{\mathbf{z} \in \mathbb{Z}_{\text{prim}}^{2,*}} \epsilon^2 f(\epsilon \mathbf{z}) = \frac{2}{3} \zeta(2)^{-1} \int_{\mathbb{R}^2} f(\mathbf{x}) d\mathbf{x} = \frac{4}{\pi^2} \int_{\mathbb{R}^2} f(\mathbf{x}) d\mathbf{x}.$ (5)

We apply this to the indicator function f for the set $\{(x, y) | x \ge y, x^2 + y^2 \le 1\}$. Then

$$\sum_{\mathbf{z}\in\mathbb{Z}_{\text{prim}}^{2,*}} \epsilon^2 f(\epsilon \mathbf{z}) = \epsilon^2 \big| \big\{ (m,n)\in\mathbb{N}^2 | \gcd(m,n) = 1, \ m > n, \\ m^2 + n^2 \le \epsilon^{-2}, \ m - n \text{ is odd} \big\} \big|.$$

Therefore we obtain

$$\lim_{N \to \infty} \frac{1}{N} \left| \left\{ (m, n) \in \mathbb{N}^2 \right| \gcd(m, n) = 1, \ m > n, \ m^2 + n^2 \le N, m - n \text{ is odd} \right\} \right| = \frac{2}{3} \cdot \frac{6}{\pi^2} \cdot \frac{\pi}{8} = \frac{1}{2\pi}.$$

Note that $|\{(m,n) \in \mathbb{N}^2 | \gcd(m,n) = 1, m > n, m^2 + n^2 \leq N, m-n \text{ is odd}\}|$ coincides with the number of PPT (x, y, z) with $z \leq N$. This observation leads us to

Corollary (Lehmer)
$$\lim_{N \to \infty} \frac{z_N}{N} = 2\pi.$$

One may also establish

Corollary For a rational point $(p,q) \in S^1(\mathbb{Q}) (= S^1 \cap \mathbb{Q}^2)$, define the *height* h(p,q) to be the minimal positive integer h such that $(hp,hq) \in \mathbb{Z}^2$. Then for any arc A in S^1 , we have

$$\left|\left\{(p,q)\in A\cap\mathbb{Q}^2|\ h(p,q)\leq h\right\}\right|\sim\frac{2\cdot\operatorname{length}(A)}{\pi^2}h\quad(h\to\infty),$$

and hence rational points are *equidistributed* on the unit circle, i. e.

$$\lim_{h \to \infty} \frac{\left| \left\{ (p,q) \in A \cap \mathbb{Q}^2 \mid h(p,q) \le h \right\} \right|}{\left| \left\{ (p,q) \in S^1 \cap \mathbb{Q}^2 \mid h(p,q) \le h \right\} \right|} = \frac{\operatorname{length}(A)}{2\pi}.$$

This theorem is stated in Duke's paper [3]. He suggests that this can be proved by using tools from the theory of L-functions combined with Weyl's famous criterion for equidistribution on the circle [12].

4 How to prove the theorems

I gave two examples of uniform arrangement. The proof that these arrangements are uniform relies on the identities derived from the so-called *Inclusion-Exclusion Principle* (IEP), which is a generalization of the obvious equality $|A \cup B| = |A| + |B| - |A \cap B|$ for two finite sets A, B, and was, for the first time, used by Nicholas Bernoulli (1687–1759) to solve a combinatorial problem related to permutations. The IEP is a powerful tool to approach general *counting problems* involving aggregation of things that are not mutually exclusive [1].

For instance, it is an easy exercise of IEP (see [10] for instance) to prove

$$\sum_{\mathbf{z}\in\mathbb{Z}_{\text{prim}}^d} f(\mathbf{z}) = \sum_{k=1}^{\infty} \mu(k) \sum_{\mathbf{w}\in\mathbb{Z}^d\setminus\{\mathbf{0}\}} f(k\mathbf{w}),\tag{6}$$

where f is a function on \mathbb{R}^d with compact support (thus both sides are finite sums), and $\mu(k)$ is the *Möbius function*:

$$\mu(k) = \begin{cases} 1 & (k=1) \\ (-1)^r & (k=p_{i_1}\cdots p_{i_r}; \ i_1 < \cdots < i_r) \\ 0 & (\text{otherwise}), \end{cases}$$

where $p_1 < p_2 < \cdots$ are all primes enumerated into ascending order. Theorem 1 is easily derived from Eq. (6).

As for Theorem 2, we consider

$$\left(\mathbb{Z}^{\text{odd}}\right)^2_{\text{prim}} = \left\{ (m, n) \in \mathbb{Z}^{\text{odd}} \times \mathbb{Z}^{\text{odd}} | \gcd(m, n) = 1 \right\},\$$

where \mathbb{Z}^{odd} is the set of odd integers. Then

$$\mathbb{Z}^{2,*}_{\mathrm{prim}} = \mathbb{Z}^2_{\mathrm{prim}} \backslash \big(\mathbb{Z}^{\mathrm{odd}} \big)^2_{\mathrm{prim}}$$

Therefore it suffices to show that $(\mathbb{Z}^{\text{odd}})^2_{\text{prim}}$ is uniformly arranged with $c((\mathbb{Z}^{\text{odd}})^2_{\text{prim}}) = 2/\pi^2$. This is done by using the following formula for which we need a bit sophisticated use of the IEP.

$$\sum_{\mathbf{z} \in (\mathbb{Z}^{\mathrm{odd}})^2_{\mathrm{prim}}} f(\mathbf{z}) = \sum_{k=1}^{\infty} \mu(k) \sum_{i=0}^{\infty} \sum_{\mathbf{w} \in (\mathbb{Z}^{\mathrm{odd}})^2} f(k2^i \mathbf{w}).$$

It is interesting to treat a general "arithmetically defined" subset of $\mathbb{Z}^d_{\text{prim}}$ (i.e. the set of solutions of a congruence equation), and to ask whether it is uniformly arranged.

5 "Near"-quasicrystals

Our criterion of uniformity is rather weak in the sense that it does not say anything about a regular spacing of a uniformly arranged Γ . For instance, if Γ is uniformly arranged, then so is any bounded perturbation of Γ .

To give a more precise notion of uniformity, we shall introduce the notion of *exponential Riemann sum* defined by

$$\sigma_{\epsilon}(f, \Gamma, \boldsymbol{\xi}) = \sum_{\mathbf{z} \in \Gamma} \epsilon^d f(\epsilon \mathbf{z}) e^{2\pi i \langle \mathbf{z}, \boldsymbol{\xi} \rangle} \quad (\boldsymbol{\xi} \in \mathbb{R}^d).$$

Note that this is nothing but the Riemann sum associated with the weighted discrete set $(\Gamma, \omega_{\boldsymbol{\xi}})$ where $\omega_{\boldsymbol{\xi}}(\mathbf{z}) = e^{2\pi i \langle \mathbf{z}, \boldsymbol{\xi} \rangle}$.

Definition Γ is said to be "near"-quasicrystal (of Poisson type) if there exists a countable set $\Lambda \subset \mathbb{R}^d$ and $c(\Gamma, \boldsymbol{\xi}) \neq 0$ ($\boldsymbol{\xi} \in \Lambda$) such that $\lim_{\epsilon \to +0} \sigma_{\epsilon}(f, \Gamma, \boldsymbol{\xi}) = \begin{cases} c(\Gamma, \boldsymbol{\xi}) \int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x} & (\boldsymbol{\xi} \in \Lambda) \\ 0 & (\boldsymbol{\xi} \notin \Lambda) \end{cases}$ for every compactly supported smooth function f.

The reason why I named such Γ "near" quasicrystal will be given in the next section.

A typical example is given by a lattice (group) Γ , which is defined to be a subgroup of \mathbb{R}^d generated by a basis of \mathbb{R}^d . The *Poisson summation formula* tells us

$$\sum_{\mathbf{z}\in\Gamma} f(\mathbf{x}+\mathbf{z}) = \operatorname{vol}(D_{\Gamma})^{-1} \sum_{\boldsymbol{\xi}\in\Gamma^*} \hat{f}(\boldsymbol{\xi}) e^{2\pi\sqrt{-1}\langle \mathbf{x},\boldsymbol{\xi}\rangle}.$$
 (7)

Here Γ^* is the dual lattice of Γ , i. e. $\Gamma^* = \{ \boldsymbol{\xi} \in \mathbb{R}^d | \langle \boldsymbol{\xi}, \mathbf{z} \rangle \in \mathbb{Z} \text{ for every } \mathbf{z} \in \Gamma \}$, and \hat{f} is the *Fourier transform* of a rapidly decreasing smooth function f:

$$\hat{f}(\boldsymbol{\xi}) = \int_{\mathbb{R}^d} f(\mathbf{x}) e^{-2\pi\sqrt{-1}\langle \mathbf{x}, \boldsymbol{\xi} \rangle} d\mathbf{x}.$$

 D_{Γ} is a fundamental domain for Γ . Note that Eq. (7) is nothing but the Fourier series expansion of the periodic function $\sum_{\mathbf{z}\in L} f(\mathbf{x} + \mathbf{z})$. Applying

Eq. (7) to $\sum_{\mathbf{z}\in\Gamma} \epsilon^d f(\epsilon \mathbf{z}) e^{2\pi i \langle \mathbf{z}, \boldsymbol{\xi} \rangle}$, we get

$$\sigma_{\epsilon}(f,\Gamma,\boldsymbol{\xi}) = \operatorname{vol}(D_{\Gamma})^{-1} \sum_{\boldsymbol{\eta}\in\Gamma^*} \hat{f}\left(\frac{\boldsymbol{\eta}-\boldsymbol{\xi}}{\epsilon}\right),$$

from which it follows that

$$\lim_{\epsilon \to +0} \sigma_{\epsilon}(f, \Gamma, \boldsymbol{\xi}) = \begin{cases} \operatorname{vol}(D_{\Gamma})^{-1} \int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x} & (\boldsymbol{\xi} \in \Gamma^*) \\ 0 & (\boldsymbol{\xi} \notin \Gamma^*) \end{cases}.$$

Thus the lattice Γ is a "near"-quasicrystal.

Now what about $\mathbb{Z}^d_{\text{prim}}$?

For $\boldsymbol{\xi} \in \mathbb{Q}$, we write $\boldsymbol{\xi} = (b_1/a_1, \dots, b_d/a_d)$ with $a_i > 0, b_i \in \mathbb{Z}$, and $gcd(a_i, b_i) = 1$, and put $n_{\boldsymbol{\xi}} = lcm(a_1, \dots, a_d)$.

Theorem $\mathbb{Z}_{\text{prim}}^d$ is a "near"-quasicrystal with $\Lambda = \{ \boldsymbol{\xi} \in \mathbb{Q}^d | n_{\boldsymbol{\xi}} \text{ is square free} \}$, and $c(\Gamma, \boldsymbol{\xi}) = \frac{\mu(n_{\boldsymbol{\xi}})}{n_{\boldsymbol{\xi}}^d} \zeta(d)^{-1} \prod_{p \mid n_{\boldsymbol{\xi}}} (1 - p^{-d})^{-1}$.

This is a consequence of the following formula which is obtained by applying the Poisson formula to the right-hand side of Eq. (6).

$$\sum_{\mathbf{z}\in\mathbb{Z}_{\text{prime}}^{d}} f(\mathbf{x}+\mathbf{z}) = \sum_{k=1}^{N} \mu(k) k^{-d} \sum_{\substack{\boldsymbol{\xi}\in\mathbb{Q}^{d}\\ n_{\boldsymbol{\xi}}\mid k}} \hat{f}(\boldsymbol{\xi}) e^{2\pi i \langle \mathbf{x},\boldsymbol{\xi} \rangle} - \Big(\sum_{k=1}^{N} \mu(k)\Big) f(\mathbf{x}), \quad (8)$$

where supp f is supposed to be contained in $B_N(\mathbf{x})$, the ball of radius N with the center \mathbf{x} . Notice that if we ignore the last term, Eq. (8) looks like the Poisson formula.

6 Quasicrystals

A *quasicrystals* is a form of solid matter whose atoms are arranged like those of a crystal but assume patterns that do not exactly repeat themselves.

The interest in quasicrystals arose when in 1984 Schechtman and others [8] discovered materials whose X-ray diffraction spectra had sharp spots indicative of long range order. Soon after the announcement of their discovery, material scientists and mathematicians began intensive studies of quasicrystals from empirical and theoretical sides. On the other hand, the theoretical discovery of quasicrystal structures was already made by R. Penrose in 1973.

At the moment, there are several ways to define quasicrystals mathematically (see []sene). As a matter of fact, an official nomenclature has not yet been agreed upon. In many reference, however, the *Delone property* for the discrete set Γ representing the location of atoms is adopted as a minimum requirement for the characterization of quasicrystals.

A Delone set Γ is defined to be a discrete set satisfying the following two conditions [2].

(1) There exists R > 0 such that every ball $B_R(x)$ has a nonempty intersection with Γ , i. e. Γ is relatively dense,

(2) There is r > 0 such that each ball $B_r(x)$ contains at most one element of Γ , i. e. Γ is uniformly discrete.

In addition to the Delone property, many authors assume that a generalized Poisson summation formula holds for Γ , which embodies the patterns of X-ray diffractions for a real quasicrystal, namely there exist a countable subset $\Lambda \subset \mathbb{R}^d$ and a sequence $\{a(\boldsymbol{\xi})\}_{\boldsymbol{\xi} \in \Lambda}$ such that

$$\sum_{\mathbf{z}\in\Gamma} f(\mathbf{x}+\mathbf{z}) \sim \sum_{\boldsymbol{\xi}\in\Lambda} c(\boldsymbol{\xi}) \hat{f}(\boldsymbol{\xi}) e^{2\pi\sqrt{-1}\langle \mathbf{x}, \boldsymbol{\xi} \rangle}$$
(9)

for every compactly supported smooth function f.

What we have to point out is that Eq. (9) is not an equality in the ordinary sense, and that the series on the right-hand side is not supposed to be absolutely convergent in general, and hence the following calculation is formal, and is not really permitted:

$$\sum_{\mathbf{z}\in\Gamma} \epsilon^d f(\epsilon \mathbf{z}) e^{2\pi i \langle \mathbf{z}, \boldsymbol{\xi} \rangle} = \sum_{\boldsymbol{\eta}\in\Lambda} c(\boldsymbol{\eta}) \hat{f} \left(\frac{\boldsymbol{\eta} - \boldsymbol{\xi}}{\epsilon} \right) \to \begin{cases} c(\boldsymbol{\xi}) \int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x} & (\boldsymbol{\xi}\in\Lambda) \\ 0 & (\boldsymbol{\xi}\notin\Lambda) \end{cases}$$

But this gives us a formal justification for the naming "near-quasicrystal".

Another remark is that $\mathbb{Z}_{\text{prim}}^d$ is by no means a quasicrystal of Poisson type because of the extra term in Eq. (8).

7 Is the set of zeta-zeros a 1-dimensional quasicrystal?

An interesting problem related to quasicrystals comes up in the study of *non-trivial zeros* of the Riemann zeta function $\zeta(s)$, which is related to the *counting problem of prime numbers*. Thus we come across another Riemann's work which were to change the direction of mathematical research in a most significant way.

We take a look at the set of imaginary parts of non-trivial zeros of $\zeta(s)$, that is, we consider

$$\Gamma = \{ \operatorname{Im} s \in \mathbb{R} | \zeta(s) = 0, \ 0 < \operatorname{Re} s < 1 \}.$$

The Riemann Hypothesis (RH) says that all zeros are located on the critical line Re s = 1/2. Moreover all known zeros are simple, and it may well be that they are all simple (*the simple zero conjecture*).

Questions about how Γ is distributed in \mathbb{R} have a long history, and was renewed when the theory of quasicrystals was well developed. In his essay "Birds and Frogs" [4], famous physicist F. Dyson claimed that *if the RH is assumed, then the set* Γ *is a one-dimensional quasicrystal.* Actually a version of Riemann's explicit formula looks like a generalized Poisson formula (see [5]):

$$\begin{split} \sum_{\rho} f\left(\frac{\rho - 1/2}{\sqrt{-1}}\right) &= f\left(\frac{1}{2\sqrt{-1}}\right) + f\left(-\frac{1}{2\sqrt{-1}}\right) \\ &+ \frac{1}{2\pi} \int_{-\infty}^{\infty} f(u) \operatorname{Re} \frac{\Gamma'}{\Gamma} \left(\frac{1}{4} + \frac{\sqrt{-1}u}{2}\right) du \\ &- \frac{1}{2\pi} \widehat{f}(0) \log \pi - \frac{1}{2\pi} \sum_{m=1}^{\infty} \sum_{p} \frac{\log p}{p^{m/2}} \left(\widehat{f}\left(\frac{\log p^{m}}{2\pi}\right) + \widehat{f}\left(-\frac{\log p^{m}}{2\pi}\right)\right) \end{split}$$

where $\{\rho\}$ is the set of zeros of $\zeta(s)$ with $0 < \operatorname{Re} \rho < 1$, \sum_{p} is the sum over all primes, and Γ'/Γ is the logarithmic derivative of the gamma function. Under RH together with the simple zero conjecture, the sum in the left-hand side is written as $\sum_{\mathbf{z}\in\Gamma} f(\mathbf{z})$.

But it should be pointed out that the test function f(s) is not arbitrary, and is supposed to be analytic in the strip $|\text{Im } s| \leq 1/2 + \epsilon$ for some $\epsilon > 0$, and to satisfy $|f(s)| \leq (1 + |s|)^{-(1+\delta)}$ for some $\delta > 0$ when $|\text{Re } s| \to \infty$. This restriction on f together with the extra terms in the formula above says that Γ is not a quasicrystal of Poisson type. Furthermore Γ does not have the Delone property, and is not a near quasicrystal in our sense.

It is an interesting problem to find an appropriate formulation of quasicrystals which includes Γ .

References

- [1] L. Comtet, Advanced Combinatorics: The Art of Finite and Infinite Expansions, Springer, 1974.
- [2] B. N. Delone, Neue Darstellung der geometrischen Kristallographie, Z. Kristallographie 84(1932), 109–149.

- [3] W. Duke, Rational points on the sphere, Ramanujan Journal, 7(2003), 235–239.
- [4] F. Dyson, Birds and frogs, Notices of the AMS, 56(2009), 212–223
- [5] H. Iwaniec and E. Kowalski, *Analytic number theory*, Amer. Math. Soc. Colloq. Publ. 53 (American Mathematical Society, Providence, RI, 2004).
- [6] D. N. Lehmer, Asymptotic evaluation of certain totient sums, Amer. J. Math. 22(1900), 293–335.
- [7] J. Marklof and A. Strömbergsson, Visibility and directions in quasicrystals, Int. Math. Res. Not., first published online September 2, 2014 doi:10.1093/imrn/rnu140.
- [8] D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, Metallic phase with long-range orientational order and no translational symmetry, Phys. Rev. Lett. 53(1984), 1951–1953.
- M. Senechal and J. Taylor, Quasicrystals: The View from Les Houches, Math. Intel. 12(1990), 54–64.
- [10] I. M. Vinogradov, *Elements of Number Theory*, Mineola, NY: Dover Publications, 2003.
- [11] A. Weil, Number Theory, An approach through history from Hammurapi to Legendre, Birkhäuser, 1984.
- [12] H. Weyl, Uber die Gleichverteilung von Zahlen mod. Eins, Math. Ann. 77(1916), 313–352.