Octagonal quasicrystals and a formula for shelling

1998 J. Phys. A: Math. Gen. 31 9321

(http://iopscience.iop.org/0305-4470/31/46/021)

J. Phys. A: Math. Gen. **31** (1998) 9321–9325. Printed in the UK PII: S0305-4470(98)95173-3

Octagonal quasicrystals and a formula for shelling

Jun Morita and Kuniko Sakamoto
Institute of Mathematics, University of Tsukuba, Tsukuba, Ibaraki, 305-8571, Japan

Received 17 June 1998

Abstract. Octagonal quasicrystals will be realized in a cyclotomic field, and a formula for shelling will be given using number theory.

Let $V = \oplus_{i=1}^{4}\mathbb{R}\varepsilon_i$ be a Euclidean space with an orthonormal basis $\{\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4\}$, and $Q = \oplus_{i=1}^{4}\mathbb{Z}\varepsilon_i$ the lattice in V spanned by this basis. We take a primitive eighth root of unity $\zeta = (\sqrt{2}+\sqrt{-2})/2$, and a cyclotomic field $\mathbb{F} = \mathbb{Q}(\zeta)$. Put $\mathbb{E} = \mathbb{R}\cap\mathbb{F} = \mathbb{Q}(\sqrt{2})$. Let $\mathfrak{O}_{\mathbb{F}} = \mathbb{Z}[\zeta]$, the ring of integers of $\mathbb{F}$, and $\mathfrak{O}_{\mathbb{E}} = \mathbb{Z}[\sqrt{2}]$, the ring of integers of $\mathbb{E}$. We put $\tau = 1+\sqrt{2}$ and $\sigma = 1-\sqrt{2}$. We choose a generator δ of $\mathrm{Gal}(\mathbb{F}/\mathbb{Q}(\sqrt{-1})) \simeq \mathrm{Gal}(\mathbb{E}/\mathbb{Q})$ with $\delta(\sqrt{2}) = -\sqrt{2}$. We use $\bar{x}$ for the complex conjugate of x. Now we define a $\mathbb{Z}$-linear map, called $\pi_\parallel$, of Q onto $\mathfrak{O}_{\mathbb{F}}$ with

$$\pi_\parallel(\varepsilon_1) = \zeta^0 = 1 \qquad \pi_\parallel(\varepsilon_2) = \zeta = (\sqrt{2}+\sqrt{-2})/2$$
$$\pi_\parallel(\varepsilon_3) = \zeta^{-1} = (\sqrt{2}-\sqrt{-2})/2 \qquad \pi_\parallel(\varepsilon_4) = \zeta^2 = \sqrt{-1}.$$

For a positive real number r, we define a quasicrystal

$$\Sigma^r = \{x \in \mathfrak{O}_{\mathbb{F}} \mid |\delta(x)| < r\}.$$

This definition is equivalent to the following construction using $p_\parallel$ and $p_\perp$. (For quasiperiodic patterns, quasicrystals and related alloys, we refer to [1–14] and so on.) Let

$$v_1 = \varepsilon_1 - \varepsilon_2 + (1+\sqrt{2})\varepsilon_3 - (1+\sqrt{2})\varepsilon_4 \qquad v_2 = \varepsilon_2 - \varepsilon_3 + \sqrt{2}\varepsilon_4$$
$$v_1' = \varepsilon_1 - \varepsilon_2 + (1-\sqrt{2})\varepsilon_3 - (1-\sqrt{2})\varepsilon_4 \qquad v_2' = \varepsilon_2 - \varepsilon_3 - \sqrt{2}\varepsilon_4.$$

We put $V_\parallel = \mathbb{R}v_1 \oplus \mathbb{R}v_2$ and $V_\perp = \mathbb{R}v_1' \oplus \mathbb{R}v_2'$. Then $V = V_\parallel \oplus V_\perp$. We take a canonical orthogonal projection, $p_\parallel$, of V onto $V_\parallel$, and a canonical orthogonal projection, $p_\perp$, of V onto $V_\perp$. Then we see that Σ^r is isomorphic to

$$\Sigma_Q^r = \{p_\parallel(x) \mid x \in Q, |p_\perp(x)| < r\}$$

under $\pi_\parallel$ (up to some scaling). Here, we will discuss a shelling of a particular quasicrystal. We will follow the idea of Moody and Patera [9], and we will establish a formula for shelling, which is analogous to Moody and Weiss [10].

For each $N = 0, 1, 2, \ldots,$ we define

$$Q_N = \{x \in Q \mid (x, x) = N\}.$$

0305-4470/98/469321+05\$19.50

Then the lattice Q decomposes into a set of concentric shells Q_N. We now introduce a shelling on each quasicrystal Σ^r. We put $\mathfrak{O}_{\mathbb{F},N} = \pi_{\|}(Q_N)$ and

$$\begin{aligned}\Sigma_N^r &= \Sigma^r \cap \mathfrak{O}_{\mathbb{F},N} \\ &= \{x \in \mathfrak{O}_{\mathbb{F},N} \mid |\delta(x)| < r\}.\end{aligned}$$

Let $x = \sum_{i=1}^4 a_i\varepsilon_i \in Q_N$. Then

$$\begin{aligned}|\pi_{\|}(x)|^2 &= |a_1 + a_2(\sqrt{2}+\sqrt{-2})/2 + a_3(\sqrt{2}-\sqrt{-2})/2 + a_4\sqrt{-1}|^2 \\ &= (a_1 + a_2/\sqrt{2} + a_3/\sqrt{2})^2 + (a_2/\sqrt{2} - a_3/\sqrt{2} + a_4)^2 \\ &= (a_1^2 + a_2^2 + a_3^2 + a_4^2) + (a_1a_2 + a_1a_3 + a_2a_4 - a_3a_4)\sqrt{2}.\end{aligned}$$

Hence, for each $x \in \mathfrak{O}_{\mathbb{F}}$, we see that $x \in \Sigma_N^r$ if and only if

$$\begin{aligned}&|x|^2 = N + m\sqrt{2} \\ &0 \leqslant |\delta(x)|^2 = N - m\sqrt{2} < r^2\end{aligned}$$

for some $m \in \mathbb{Z}$, which implies

$$N/\sqrt{2} \geqslant m > (N - r^2)/\sqrt{2}.$$

In particular, it is an interesting situation when $N/\sqrt{2} = (N - r^2)/\sqrt{2} + 1$. Such an r will be denoted by ρ. That is,

$$\rho = (2)^{1/4}.$$

In this case, we obtain

$$\Sigma_N^\rho = \{x \in \mathfrak{O}_{\mathbb{F}} \mid |x|^2 = N + [N/\sqrt{2}]\sqrt{2}\}$$

for $N = 0, 1, 2, \dots,$ where [ ] is the Gauss symbol. Now we consider the inflation

$$x \longmapsto \tau x$$

which maps Σ^ρ bijectively onto $\Sigma^{\rho/\tau}$ contained in Σ^ρ. Then we obtain

$$\begin{aligned}x \in \Sigma_N^\rho \Longrightarrow |x|^2 &= N + [N/\sqrt{2}]\sqrt{2} \\ \Longrightarrow |\tau x|^2 &= (1+\sqrt{2})^2(N + [N/\sqrt{2}]\sqrt{2}) \\ &= (3 + 2\sqrt{2})(N + [N/\sqrt{2}]\sqrt{2}) \\ &= (3N + 4[N/\sqrt{2}]) + (2N + 3[N/\sqrt{2}])\sqrt{2}.\end{aligned}$$

Since $\tau x \in \Sigma^\rho$, we see that $|\tau x|^2 = M + [M/\sqrt{2}]\sqrt{2}$ and $\tau x \in \Sigma_M^\rho$ for some M by the choice of our ρ, which automatically means $M = 3N + 4[N/\sqrt{2}]$. Hence,

$$\begin{aligned}&\tau\Sigma_N^\rho \subset \Sigma_{3N+4[N/\sqrt{2}]}^\rho \\ &[(3N + 4[N/\sqrt{2}])/\sqrt{2}] = 2N + 3[N/\sqrt{2}].\end{aligned}$$

For each N, we define a sequence $\{L_n(N)\}_{n=1}^\infty$ by

$$\begin{aligned}&L_1(N) = N \\ &L_2(N) = [N/\sqrt{2}] \\ &L_{2\ell+1}(N) = 3L_{2\ell-1}(N) + 4L_{2\ell}(N) \\ &L_{2\ell+2}(N) = 2L_{2\ell-1}(N) + 3L_{2\ell}(N).\end{aligned}$$

Then, we can see, for all odd n,

$$\tau\Sigma^{\rho}_{L_n(N)} \subset \Sigma^{\rho}_{L_{n+2}(N)}$$
$$x \in \Sigma^{\rho}_{L_n(N)} \Rightarrow |x|^2 = L_n(N) + L_{n+1}(N)\sqrt{2}$$
$$L_{n+1}(N) = [L_n(N)/\sqrt{2}].$$

Now we suppose $x \in \Sigma^{\rho}_{L_{n+2}(N)}$ with n odd. Then

$$|x|^2 = L_{n+2}(N) + L_{n+3}(N)\sqrt{2}$$

and

$$\begin{aligned}|\sigma x|^2 &= (3-2\sqrt{2})(L_{n+2}(N) + L_{n+3}(N)\sqrt{2})\\ &= (3L_{n+2}(N) - 4L_{n+3}(N)) + (3L_{n+3}(N) - 2L_{n+2}(N))\sqrt{2}\\ &= L_n(N) + L_{n+1}(N)\sqrt{2}.\end{aligned}$$

Hence, $\sigma x \in \Sigma^{\rho}_{L_n(N)}$, and so $x = -\tau(\sigma x) \in \tau\Sigma^{\rho}_{L_n(N)}$. Therefore,

$$\tau\Sigma^{\rho}_{L_n(N)} = \Sigma^{\rho}_{L_{n+2}(N)}.$$

We define

$$s_N = \mathrm{card}\,\Sigma^{\rho}_N$$

for $N = 0, 1, 2, \ldots$. Then we see

$$s_N = s_{3N+4[N/\sqrt{2}]}.$$

We also observe that each shell Σ^{ρ}_N has complete $\mathrm{I}_2(8)$-symmetry. That is, $\zeta\Sigma^{\rho}_N = \Sigma^{\rho}_N$. Hence, $8|s_N$ for all $N = 1, 2, 3, \ldots$. Furthermore, using a field extension $\mathbb{F}/\mathbb{E}$ (cf [15]), it is easily seen that s_N has the following formula:

$$s_N = 8 \cdot \prod_{\mathfrak{p}\in X}(v_{\mathfrak{p}}(N^*) + 1)$$

if $v_{\mathfrak{p}}(N^*) \equiv 0 \pmod 2$ for all $\mathfrak{p} \in Z$ and $N > 0$, where

$$X = \{\mathfrak{p} \in \mathrm{Spec}\,\mathfrak{O}_{\mathbb{E}} \mid \exists P \in \mathrm{Spec}\,\mathfrak{O}_{\mathbb{F}}, \mathfrak{p}\mathfrak{O}_{\mathbb{F}} = P\bar{P}, P \neq \bar{P}\}$$
$$Y = \{\mathfrak{p} \in \mathrm{Spec}\,\mathfrak{O}_{\mathbb{E}} \mid \exists P \in \mathrm{Spec}\,\mathfrak{O}_{\mathbb{F}}, \mathfrak{p}\mathfrak{O}_{\mathbb{F}} = P^2, P = \bar{P}\}$$
$$Z = \{\mathfrak{p} \in \mathrm{Spec}\,\mathfrak{O}_{\mathbb{E}} \mid \mathfrak{p}\mathfrak{O}_{\mathbb{F}} \in \mathrm{Spec}\,\mathfrak{O}_{\mathbb{F}}\}$$

where Spec is the spectrum of prime ideals, $v_{\mathfrak{p}}$ is the discrete valuation of $\mathfrak{O}_{\mathbb{E}}$ with respect to $\mathfrak{p}$ and $N^* = N + [N/\sqrt{2}]\sqrt{2}$. If $v_{\mathfrak{p}}(N^*) \not\equiv 0 \pmod 2$ for some $\mathfrak{p} \in Z$, then $s_N = 0$.

We will explain in more detail. Let ϕ be a map of

$$\Sigma^{\rho}_N = \{x \in \mathfrak{O}_{\mathbb{F}} \mid |x|^2 = N^*\}$$

into

$$\Lambda_N = \{I \subset \mathfrak{O}_{\mathbb{F}} \mid I = \text{ideal}, I\bar{I} = N^*\mathfrak{O}_{\mathbb{F}}\}$$

defined by $\phi(x) = x\mathfrak{O}_{\mathbb{F}}$. If $\phi(x) = \phi(y)$ with $x, y \in \Sigma^{\rho}_N$, then $x\mathfrak{O}_{\mathbb{F}} = y\mathfrak{O}_{\mathbb{F}}$ and $x = yu$ for some $u \in \mathfrak{O}^{\times}_{\mathbb{F}}$. This implies $|x|^2 = |y|^2 \cdot |u|^2$ and $|u|^2 = 1$. Hence, $u = \zeta^i$ for some i. Conversely we see that $\phi(x) = \phi(\zeta^i x)$. Therefore, ϕ is an eight-to-one map. On the other hand, let take an ideal $I \in \Lambda_N$. We write $I = z\mathfrak{O}_{\mathbb{F}}$ with $z \in \mathfrak{O}_{\mathbb{F}}$. Then $I\bar{I} = z\bar{z}\mathfrak{O}_{\mathbb{F}} = N^*\mathfrak{O}_{\mathbb{F}}$. Hence, there is $t \in \mathfrak{O}^{\times}_{\mathbb{F}}$ such that $z\bar{z}t = N^*$, which implies that $t \in \mathfrak{O}^{\times}_{\mathbb{F}} \cap \mathbb{E} = \mathfrak{O}^{\times}_{\mathbb{E}}$. Thus, $t = \pm(1+\sqrt{2})^k$ for some k. Since $z\bar{z}t = N^*$, $t > 0$ and $t = (1+\sqrt{2})^k$. Then, $\delta(z\bar{z}t) = \delta(N^*)$ and $|\delta(z)|^2\delta(t) = \delta(N^*) > 0$. Hence, $\delta(t) > 0$, which means that $t = (1+\sqrt{2})^{2k}$ for some k. Therefore, if we put $x = z(1+\sqrt{2})^k \in \Sigma_N^\rho$, then $\phi(x) = x\mathfrak{O}_{\mathbb{F}} = z(1+\sqrt{2})^k\mathfrak{O}_{\mathbb{F}} = z\mathfrak{O}_{\mathbb{F}} = I$. Hence, we see that ϕ is surjective. We now established the following:

$$s_N = 8 \cdot \mathrm{card}\,\Lambda_N.$$

If $N^*\mathfrak{O}_{\mathbb{E}} = \mathfrak{p}_1^{e_1}\ldots\mathfrak{p}_k^{e_k}\mathfrak{p}_1'^{f_1}\ldots\mathfrak{p}_\ell'^{f_\ell}\mathfrak{p}_1''^{g_1}\ldots\mathfrak{p}_m''^{g_m}$ with $\mathfrak{p}_i \in X$, $\mathfrak{p}_i' \in Y$ and $\mathfrak{p}_i'' \in Z$, then

$$N^*\mathfrak{O}_{\mathbb{F}} = (P_1\bar{P}_1)^{e_1}\ldots(P_k\bar{P}_k)^{e_k}P_1'^{2f_1}\ldots P_\ell'^{2f_\ell}P_1''^{g_1}\ldots P_m''^{g_m}$$

where $\mathfrak{p}_i\mathfrak{O}_{\mathbb{F}} = P_i\bar{P}_i$, $\mathfrak{p}_i'\mathfrak{O}_{\mathbb{F}} = P_i'^2$ and $\mathfrak{p}_i''\mathfrak{O}_{\mathbb{F}} = P_i''$ with $P_i, P_i', P_i'' \in \mathrm{Spec}(\mathfrak{O}_{\mathbb{F}})$. Then we must find all possible choices for I satisfying $I\bar{I} = N^*\mathfrak{O}_{\mathbb{F}}$. If all g_i are even, say $g_i = 2h_i$, then we can choose

$$I = P_1^{v_1}\bar{P}_1^{w_1}\ldots P_k^{v_k}\bar{P}_k^{w_k}P_1'^{f_1}\ldots P_\ell'^{f_\ell}P_1''^{h_1}\ldots P_m''^{h_m}$$

with $v_i + w_i = e_i$. In this case, we have $(e_1+1)\ldots(e_k+1)$ possibilities. If one of the g_i is odd, then there is no I satisfying $I\bar{I} = N^*\mathfrak{O}_{\mathbb{F}}$. Here we should note that $v_{\mathfrak{p}_i}(N^*) = e_i$. Hence, it is now easy to obtain the above formula for s_N. However, there is some redundancy in this formula. That is, the cardinality of Y is just one. Also we can obtain the following explicit description:

$$X = X_1 \cup X_2$$
$$X_1 = \{(a+b\sqrt{2}) \in \mathrm{Spec}\,\mathfrak{O}_{\mathbb{E}} \mid a, b \in \mathbb{Z}, (a^2-2b^2) \in \mathrm{Spec}\,\mathbb{Z}, |a^2-2b^2| \equiv 1 \pmod 8\}$$
$$X_2 = \{(p) \in \mathrm{Spec}\,\mathfrak{O}_{\mathbb{E}} \mid p \in \mathbb{Z}, (p) \in \mathrm{Spec}\,\mathbb{Z}, p \equiv \pm 3 \pmod 8\}$$
$$Y = \{(\sqrt{2}) \in \mathrm{Spec}\,\mathfrak{O}_{\mathbb{E}}\}$$
$$Z = \{(a+b\sqrt{2}) \in \mathrm{Spec}\,\mathfrak{O}_{\mathbb{E}} \mid a, b \in \mathbb{Z}, (a^2-2b^2) \in \mathrm{Spec}\,\mathbb{Z}, |a^2-2b^2| \equiv -1 (\mathrm{mod} 8)\}.$$

Furthermore, we can rewrite the formula as follows:

$$s_N = 8 \cdot \prod_{i=1}^{\ell}(a_i+1) \cdot \prod_{j=1}^{m}(b_j+1)$$

if $c_k \equiv 0 \pmod 2$ for all $1 \leqslant k \leqslant n$, and $s_N = 0$ otherwise, where

$$N^{**} = N^2 - 2[N/\sqrt{2}]^2 = 2^d p_1^{a_1}\ldots p_\ell^{a_\ell} q_1^{2b_1}\ldots q_m^{2b_m} r_1^{c_1}\ldots r_n^{c_n}$$

is a factorization of N^{**} into prime numbers satisfying $p_i \in A$, $q_j \in B$, $r_k \in C$ with $1 \leqslant i \leqslant \ell$, $1 \leqslant j \leqslant m$, $1 \leqslant k \leqslant n$,

$$A = \{p \mid p \text{ is a prime number}, p \equiv 1 \pmod 8\}$$
$$B = \{p \mid p \text{ is a prime number}, p \equiv \pm 3 \pmod 8\}$$
$$C = \{p \mid p \text{ is a prime number}, p \equiv -1 \pmod 8\}.$$

This means that we need only the factorization of N^{**} to get the value s_N, which characterizes our shelling. A table of the first few non-trivial s_N is given below:

N	1	2	3	4	6	7	9	10	12	14	15	17	18	20	21	...	69	...	90
s_N	8	8	8	8	8	16	16	8	8	16	16	8	16	8	8	...	32	...	24

It should be interesting to have information about the average shelling, which might be more difficult.

References

[1] Baake M, Joseph D, Kramer P and Schlottmann 1990 Root lattices and quasicrystals *J. Phys. A: Math. Gen.* **23** L1037–41
[2] De Bruijin N G 1981 Sequences of zeros and ones generated by special production rules *Math. Proc.* A **84** 27–37
[3] De Bruijin N G 1981 Algebraic theory of Penrose's non-periodic tilings of the plane *Math. Proc.* A **84** 39–66
[4] Elser V 1986 The diffraction pattern of projected structures *Acta Crystallogr.* A **42** 36–43
[5] Elser V and Sloane N J A 1987 A highly symmetric four-dimensional quasicrystal *J. Phys. A: Math. Gen.* **20** 6161–8
[6] Janot C 1994 *Quasicrystals—A primer* 2nd edn (Oxford: Oxford Science)
[7] Katz A and Deneau M 1985 Quasiperiodic patterns *Phys. Rev. Lett.* **54** 2688–91
[8] Kalugin P A, Kitayev A Yu and Levitov L S 1985 6-dimensional properties of $Al_{0.86}Mn_{0.14}$ alloy *J. Physique Lett.* **46** L601–7
[9] Moody R V and Patera J 1993 Quasicrystals and icosians *J. Phys. A: Math. Gen.* **26** 2829–53
[10] Moody R V and Weiss A 1994 On shelling E_8 quasicrystals *J. Number Theory* **47** 405–12
[11] Shechtman D, Blech I, Gratias D and Cahn J W 1984 Metallic phase with long-range orientational order and no translational symmetry *Phys. Rev. Lett.* **53** 1951–3
[12] Sadoc J-F and Mosseri R 1993 The E_8 lattice and quasicrystals: geometry, number theory, and quasicrystals *J. Phys. A: Math. Gen.* **26** 1789–809
[13] Wang N, Chen H and Kuo K H 1987 Two dimensional quasicrystal with eightfold rotational symmetry *Phys. Rev. Lett.* **59** 1010–13
[14] Wang Z M and Kuo K H 1988 The octagonal quasilattice and electron diffraction patterns of the octagonal phase *Acta Crystallogr.* A **44** 857–63
[15] Washington L C 1997 *Introduction to Cyclotomic Fields (Graduate Texts in Mathematics 83)* 2nd edn (New York: Springer)