Combinatorial aspects of colour symmetries

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Abstract

The problem of colour symmetries of crystals and quasicrystals is investigated from its combinatorial point of view. For various lattices and modules in two and three dimensions, the number of colourings compatible with point and translation symmetry is given in terms of Dirichlet series generating functions.

Introduction

The concept of colour symmetry is a useful tool to investigate the structure of discrete point sets (or related patterns) with additional (scalar) degrees of freedom on top of each point, called colours. To make this a bit more precise, let us consider a discrete point set $\mathcal{P}$ in Euclidean space $\mathbb{E}^n$. Let us assume that each point shows one of finitely many colours. Finally, define the local isomorphism class $\mathrm{LI}(\mathcal{P})$ as the class of coloured point sets that are patch-equivalent with $\mathcal{P}$, i.e. the class of point sets $\mathcal{P}'$ with the property that arbitrarily large patches of $\mathcal{P}'$ occur in $\mathcal{P}$ and vice versa.

Now, a Euclidean motion combined with a (global) permutation of colours is called a (generalized) colour symmetry of $\mathrm{LI}(\mathcal{P})$ iff it maps $\mathrm{LI}(\mathcal{P})$ into itself. The classification of these symmetries is a rather difficult task, and has been studied extensively in two and three dimensions, see [6, 16, 17] and references therein. While being incomplete even in this crystallographic case, things are much worse with non-crystallographic symmetries which are of considerable interest in the theory of quasicrystals.

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There are attempts to find the colour symmetries with a small number of colours explicitly [9], and an approach via the Fourier transform can be used algorithmically to calculate all possibilities up to a given number of colours [8], but neither of these can give full answers. There is another approach to colourings, based on the algebraic structure of crystals and quasicrystals [12], which can be used to count the different possibilities to colour such structures in a way that is compatible with its natural symmetry.

To expand on that, we will now consider the slightly more special case of colour point symmetries where one colour occupies an object of the same kind as the original, uncoloured one (e.g. it occupies a square sublattice of the square lattice etc.) and all the other colours are translates (i.e. they code the cosets or residue classes). Admittedly, this is only a subclass of the colouring problem (compare with the discussion in [6]), but we will restrict our attention even further to irreducible symmetries, such as n-fold symmetry in the plane ($n \geq 3$) or cubic and icosahedral symmetry in 3-space. Nevertheless, this problem should be of some interest because it can be solved completely in 2D and to a large extent in 3D.

In the latter case, one has to extend the setup to the situation that one colour occupies a sublattice (or submodule) with the same point symmetry (which actually only means that the point symmetry groups under consideration are conjugates of one another in $O(3)$). This is necessary because the black-and-white colouring of $\mathbb{Z}^3$ (i.e. the 3D checkerboard lattice) results in a face-centred Bravais type, but, obviously, should not be excluded.

In this article, we start with the analysis of possibilities to achieve such a colouring (which is a combinatorial problem) and postpone the determination of the corresponding colour groups (which is a group theoretic problem), together with some more general results, compare [2], to a forthcoming publication. The first part deals with the plane, where we explain the setting with the familiar case of the square lattice and later present other cases of interest. As we focus on applicability to quasicrystals, we will actually have to talk about the colouring of modules rather than of lattices in general.

The second part derives similar results for cubic lattices as well as icosahedral modules, with additional material being presented in the Appendix. In both cases, we also discuss in some detail the relation between the three different Bravais classes that can sit inside each other and give rise to colourings compatible with cubic resp. icosahedral symmetry.

A warm-up exercise: the square lattice $\mathbb{Z}^2$

Let us illustrate the problem and its solutions with a simple 2D example. The only lattice in the Euclidean plane that shows fourfold symmetry (described by the cyclic group C_4) is the square lattice resp. its Bravais class, i.e. up to scaling and Euclidean motions, only

$$\mathbb{Z}^2 \;=\; \{(m,n) \mid m,n \in \mathbb{Z}\} \tag{1}$$

has C_4-symmetry. Due to invariance under reflection in the x-axis, the full symmetry group is actually D_4, the dihedral group of order 8.

We now want to colour the lattice sites with finitely many pairwise different colours in such a way that the coloured version is still crystallographic (i.e. its periods span the plane over the reals), one of the colours occupies a sublattice which is still invariant under fourfold rotation (and hence of square lattice type), while the other colours label the cosets. To classify all possibilities, we thus have to know how many square sublattices of $\mathbb{Z}^2$ of a given index m exist (the cosets are unique). Let us call this number $a_4(m)$.

Clearly, $\mathbb{Z}^2$ contains many more sublattices than those we are presently interested in: there are e.g. three sublattices of index 2, only one of which is square while the other two have rectangular symmetry only. Consequently, our numbers $a_4(m)$ are smaller than the number $f^{(2)}(m)$ of *all* sublattices of index m, given by [1]

$$f^{(2)}(m) \;=\; \sum_{d|m} d \tag{2}$$

where $d|m$ means d divides m. Its Dirichlet series generating function is $\zeta(s)\zeta(s-1)$ where $\zeta(s)$ is Riemann's ζ-function, see [5] or the Appendix. This type of generating function is more appropriate than the usual power series because $f^{(2)}(m)$ is a multiplicative function, i.e. $f^{(2)}(1) = 1$ and $f^{(2)}(mn) = f^{(2)}(m)f^{(2)}(n)$ whenever m,n are coprime. This type of structure will also show up in all other cases discussed in this article.

How can we select, from the sublattices of index m, those that are square lattices? An efficient way, which also generalizes to other planar symmetries, is through the observation that $\mathbb{Z}^2$ can be seen as a ring of algebraic integers. In this case, we have

$$\mathbb{Z}^2 \;=\; \mathbb{Z}[i] \;=\; \{m+ni \mid m,n \in \mathbb{Z}\} \tag{3}$$

which are the so-called Gaussian integers [5], the algebraic integers in the quadratic field $\mathbb{Q}(i) \;=\; \{p+qi \mid p,q \in \mathbb{Q}\}$ (a field extension of the rationals $\mathbb{Q}$ of degree 2).

Sublattices now correspond to subgroups of finite index, and those invariant under fourfold rotation (i.e. under multiplication by i) correspond to *ideals*. They are the subgroups $\mathfrak{a} \subset \mathbb{Z}[i]$ with $\gamma\mathfrak{a} \subset \mathfrak{a}$ for all $\gamma \in \mathbb{Z}[i]$, for background material on the concepts and results used we refer to [7, 5, 18].

Consequently, counting all square sublattices of $\mathbb{Z}^2$ of index m is the same as counting all ideals of the ring $\mathbb{Z}[i]$ of finite index m, where $m = \mathrm{norm}(\mathfrak{a})$ is the (number theoretic) norm of $\mathfrak{a}$ (which equals the number of residue classes of $\mathfrak{a}$ in $\mathbb{Z}[i]$). As the ring $\mathbb{Z}[i]$ is a principal ideal domain and commutative, each ideal $\mathfrak{a}$ is two-sided and generated by an element $\alpha \in \mathbb{Z}[i]$, i.e.

$$\mathfrak{a} \;=\; \alpha\mathbb{Z}[i] \tag{4}$$

for some $\alpha = k + \ell i$. But then, the norm of $\mathfrak{a}$ simply reads

$$\mathrm{norm}(\mathfrak{a}) \;=\; |\alpha|^2 \;=\; k^2 + \ell^2 \tag{5}$$

which is the area of the fundamental domain of the sublattice defined by α.

The number of these ideals of index m is our number $a_4(m)$, and it is a multiplicative function which is a consequence of unique prime factorization (up to units) [5] in the ring $\mathbb{Z}[i]$. Its generating function (of Dirichlet series type) is the Dedekind ζ-function of the field $K = \mathbb{Q}(i)$

$$\zeta_K(s) \;=\; \sum_{\mathfrak{a}} \frac{1}{\mathrm{norm}(\mathfrak{a})^s} \;=\; \sum_{m=1}^{\infty} \frac{a_4(m)}{m^s} \tag{6}$$

where the first sum runs over all ideals $\mathfrak{a} \neq \{0\}$. It reads explicitly

$$\begin{aligned}
\zeta_K(s) \;&=\; \sum_{m=1}^{\infty} \frac{a_4(m)}{m^s} \;=\; \frac{1}{1-2^{-s}} \cdot \prod_{p\equiv 1\ (4)} \frac{1}{(1-p^{-s})^2} \cdot \prod_{p\equiv 3\ (4)} \frac{1}{1-p^{-2s}} \\
&=\; 1 + \tfrac{1}{2^s} + \tfrac{1}{4^s} + \tfrac{2}{5^s} + \tfrac{1}{8^s} + \tfrac{1}{9^s} + \tfrac{2}{10^s} + \tfrac{2}{13^s} + \tfrac{1}{16^s} + \tfrac{2}{17^s} + \tfrac{1}{18^s} + \tfrac{2}{20^s} + \tfrac{3}{25^s} + \tfrac{2}{26^s} + \cdots
\end{aligned} \tag{7}$$

One can easily derive an explicit expression for the coefficients. The result is $a_4(1) = 1$, $a_4(2^r) = 1$, $a_4(mn) = a_4(m)a_4(n)$ for m,n coprime (multiplicativity of $a_4(m)$), $a_4(p^r) = r+1$ for $p \equiv 1\ (4)$, and, finally, $a_4(p^{2r}) = 1$ and $a_4(p^{2r-1}) = 0$ for $p \equiv 3\ (4)$.

A Dirichlet series generating function allows for the determination of the asymptotic behaviour of the coefficients through the residue of the ζ-function at its rightmost pole in the complex s-plane ($s = 1$ in this case). The result is that the *average* value of $a_4(m)$ is constant, namely $\pi/4$. In other words, the number of possibilities to colour the square lattice with less than N colours (and with our general restrictions discussed above) is asymptotically $\pi N/4$.

More generality: other planar cases

Having desribed the square lattice in detail, we shall now generalize our approach to other $\mathbb{Z}$-modules of the plane, namely those with n-fold rotational symmetry, $n > 2$. Though many things are similar here, the number theoretic background is a lot more involved, see [18].

Let us nevertheless consider the $\mathbb{Z}$-span of a regular n-star,

$$\mathcal{M}_n \;:=\; \mathbb{Z}\cdot 1 + \mathbb{Z}\cdot\xi + \ldots + \mathbb{Z}\cdot\xi^{n-1}\,, \tag{8}$$

where $\xi = \exp(2\pi i/n)$. This is called the standard n-fold symmetric module of the plane [11]. It is a $\mathbb{Z}$-module of rank $\phi(n)$, where ϕ denotes Euler's totient function [5], and it is discrete (i.e. a lattice) only for $n = 3, 4, 6$. Note that $\mathcal{M}_3 = \mathcal{M}_6$, and, in general, $\mathcal{M}_n = \mathcal{M}_N$ where N is defined as n resp. $2n$ for n even resp. odd. So, the module $\mathcal{M}_n$ has N-fold rotational symmetry.

The cases with $n = 5$ and $n \geq 7$ correspond to 2D quasicrystals or other nonperiodic Delone sets, where they show up as the so-called limit translation modules [4] of the discrete structures. Consequently, as discussed in detail in [14], these modules are the universal objects, and the colouring problem has to be solved for them. The results then apply to each translation class of points of the corresponding Delone set separately.

Now, how does the definition (8) help? The first observation is that $\mathcal{M}_n = \mathbb{Z}[\xi]$ is the ring of cyclotomic integers in the cyclotomic field $\mathbb{Q}(\xi)$ (see [18] for details), and the second is that the subgroups we need (i.e. those with N-fold symmetry) are again *ideals* of $\mathbb{Z}[\xi]$. So, it is helpful to know the Dedekind ζ-function of $\mathbb{Q}(\xi)$ which is the Dirichlet series generating function of the numbers of ideals of a given index.

In what follows, we will list some examples, including all those related to 2D quasicrystals found so far. They share another special property with other cases of small n, namely the uniqueness of the ideal class. This means that, for fixed n, all ideals are equal up to a similarity transformation, or, in other words, there is only one Bravais-type of n-fold symmetric modules of the plane [11] of rank $\phi(n)$. This is true of precisely 29 planar modules, namely those with

$$\begin{gathered} n = 3, 4, 5, 7, 8, 9, 11, 12, 13, 15, 16, 17, 19, 20, 21, \\ 24, 25, 27, 28, 32, 33, 35, 36, 40, 44, 45, 48, 60, 84 \end{gathered}$$

(where $n \not\equiv 2 \bmod 4$ to avoid double counting), see theorem 11.1 of [18].

The necessary material for the actual calculation of the ζ-functions can be found in section III of [14] and will not be repeated here. In what follows, we just summarize the results for several important 2D lattices and modules.

The triangular lattice

The triangular lattice (with sixfold symmetry) is a scaled down version of the root lattice A_2 and coincides with the ring of Eisenstein integers [5]. They are the algebraic integers in the quadratic field $K = \mathbb{Q}(\sqrt{-3}\,)$. The corresponding ζ-function reads

$$\begin{aligned} \zeta_K(s) &= \sum_{m=1}^{\infty} \frac{a_6(m)}{m^s} = \frac{1}{1-3^{-s}} \cdot \prod_{p\equiv 1\ (3)} \frac{1}{(1-p^{-s})^2} \cdot \prod_{p\equiv 2\ (3)} \frac{1}{1-p^{-2s}} \qquad (9) \\ &= 1 + \tfrac{1}{3^s} + \tfrac{1}{4^s} + \tfrac{2}{7^s} + \tfrac{1}{9^s} + \tfrac{1}{12^s} + \tfrac{2}{13^s} + \tfrac{1}{16^s} + \tfrac{2}{19^s} + \tfrac{2}{21^s} + \tfrac{1}{25^s} + \tfrac{1}{27^s} + \tfrac{2}{28^s} + \cdots \end{aligned}$$

The explicit expressions for the coefficients are $a_6(1) = 1$, $a_6(3^r) = 1$, $a_6(mn) = a_6(m)a_6(n)$ for m, n coprime, $a_6(p^r) = r + 1$ for $p \equiv 1\ (3)$, and finally, for $p \equiv 2\ (3)$, one has $a_6(p^{2r}) = 1$ and $a_6(p^{2r-1}) = 0$. The average value of $a_6(m)$ is asymptotically $\pi/3\sqrt{3}$.

Fivefold symmetry

The fivefold module in the plane, $\mathcal{M}_5$, is the ring of algebraic integers in the field $K = \mathbb{Q}(\xi)$, with $\xi = e^{2\pi i/5}$. Its ζ-function reads

$$\begin{aligned} \zeta_K(s) &= \sum_{m=1}^{\infty} \frac{a_{10}(m)}{m^s} = \qquad (10) \\ &= \frac{1}{1-5^{-s}} \cdot \prod_{p\equiv 1\ (5)} \frac{1}{(1-p^{-s})^4} \cdot \prod_{p\equiv -1\ (5)} \frac{1}{(1-p^{-2s})^2} \cdot \prod_{p\equiv \pm 2\ (5)} \frac{1}{1-p^{-4s}} \\ &= 1 + \tfrac{1}{5^s} + \tfrac{4}{11^s} + \tfrac{1}{16^s} + \tfrac{1}{25^s} + \tfrac{4}{31^s} + \tfrac{4}{41^s} + \tfrac{4}{55^s} + \tfrac{4}{61^s} + \tfrac{4}{71^s} + \tfrac{1}{80^s} + \tfrac{1}{81^s} + \tfrac{4}{101^s} + \cdots \end{aligned}$$

As before, the coefficients $a_{10}(m)$ can be given explicitly. Due to their multiplicativity, it is sufficient to know them for prime powers. The result is $a_{10}(1) = 1$; $a_{10}(5^r) = 1$; $a_{10}(p^r) = (r+1)(r+2)(r+3)/6$ for $p \equiv 1\ (5)$; $a_{10}(p^{2r+1}) = 0$ and $a_{10}(p^{2r}) = r + 1$ for $p \equiv 4\ (5)$; finally, $a_{10}(p^{4r}) = 1$ and $a_{10}(p^{4r-\ell}) = 0$ (with $\ell = 1, 2, 3$) for $p \equiv \pm 2\ (5)$. The average value of $a_{10}(m)$ is asymptotically $4\pi^2 \log(\tau)/25\sqrt{5} \simeq 0.339837$.

Sevenfold symmetry

Before we complete the examples related to quadratic irrationalities, let us give at least one example of a more complicated structure, namely that of sevenfold (and hence also fourteenfold) symmetry. Here, $K = \mathbb{Q}(e^{2\pi i/7})$, and the ζ-function reads:

$$\zeta_K(s) = \sum_{m=1}^{\infty} \frac{a_{14}(m)}{m^s}$$

$$
\begin{aligned}
&= \frac{1}{1-7^{-s}} \cdot \prod_{p\equiv 1\ (7)} \frac{1}{(1-p^{-s})^6} \cdot \prod_{p\equiv 3 \text{ or } 5\ (7)} \frac{1}{1-p^{-6s}} \cdot \\
&\quad \prod_{p\equiv 2 \text{ or } 4\ (7)} \frac{1}{(1-p^{-3s})^2} \cdot \prod_{p\equiv 6\ (7)} \frac{1}{(1-p^{-2s})^3} \cdot \\
&= 1 + \tfrac{1}{7^s} + \tfrac{2}{8^s} + \tfrac{6}{29^s} + \tfrac{6}{43^s} + \tfrac{1}{49^s} + \tfrac{2}{56^s} + \tfrac{3}{64^s} + \tfrac{6}{71^s} + \tfrac{6}{113^s} + \tfrac{6}{127^s} + \tfrac{3}{169^s} + \tfrac{6}{197^s} + \cdots
\end{aligned}
\tag{11}
$$

Since it is clear how to derive explicit formulas for the coefficients by suitable manipulations with geometric series, we suppress such details from now on. Also, the asymptotic behaviour can be calculated along the lines mentioned above, see [14] for details.

Eightfold symmetry

Here, we obtain, with $K = \mathbb{Q}(e^{2\pi i/8})$:

$$
\begin{aligned}
\zeta_K(s) &= \sum_{m=1}^{\infty} \frac{a_8(m)}{m^s} \\
&= \frac{1}{1-2^{-s}} \cdot \prod_{p\equiv 1\ (8)} \frac{1}{(1-p^{-s})^4} \cdot \prod_{p\equiv -1\ (8)} \frac{1}{(1-p^{-2s})^2} \cdot \prod_{p\equiv \pm 3\ (8)} \frac{1}{(1-p^{-2s})^2} \\
&= 1 + \tfrac{1}{2^s} + \tfrac{1}{4^s} + \tfrac{1}{8^s} + \tfrac{2}{9^s} + \tfrac{1}{16^s} + \tfrac{4}{17^s} + \tfrac{2}{18^s} + \tfrac{2}{25^s} + \tfrac{1}{32^s} + \tfrac{4}{34^s} + \tfrac{2}{36^s} + \tfrac{4}{41^s} + \tfrac{2}{49^s} + \cdots
\end{aligned}
\tag{12}
$$

Twelvefold symmetry

The cyclotomic field is now $K = \mathbb{Q}(e^{2\pi i/12})$, and the ζ-function reads

$$
\begin{aligned}
\zeta_K(s) &= \sum_{m=1}^{\infty} \frac{a_{12}(m)}{m^s} \\
&= \frac{1}{1-4^{-s}} \cdot \frac{1}{1-9^{-s}} \prod_{p\equiv 1\ (12)} \frac{1}{(1-p^{-s})^4} \cdot \prod_{p\equiv -1\ (12)} \frac{1}{(1-p^{-2s})^2} \cdot \prod_{p\equiv \pm 5\ (12)} \frac{1}{(1-p^{-2s})^2} \\
&= 1 + \tfrac{1}{4^s} + \tfrac{1}{9^s} + \tfrac{4}{13^s} + \tfrac{1}{16^s} + \tfrac{2}{25^s} + \tfrac{1}{36^s} + \tfrac{4}{37^s} + \tfrac{2}{49^s} + \tfrac{4}{52^s} + \tfrac{4}{61^s} + \tfrac{1}{64^s} + \tfrac{4}{73^s} + \tfrac{1}{81^s} + \cdots
\end{aligned}
\tag{13}
$$

At this point, we close the section on 2D examples. More can be worked out explicitly with the material of section III of [14] and the general theory as explained in sections 1-4 and 11 of [18]. In Table 1, the numbers $a_N(m)$ up to $m = 30$ are summarized for various N.

m	$a_4(m)$	$a_6(m)$	$a_8(m)$	$a_{10}(m)$	$a_{12}(m)$	$a_{14}(m)$
1	1	1	1	1	1	1
2	1	0	1	0	0	0
3	0	1	0	0	0	0
4	1	1	1	0	1	0
5	2	0	0	1	0	0
6	0	0	0	0	0	0
7	0	2	0	0	0	1
8	1	0	1	0	0	2
9	1	1	2	0	1	0
10	2	0	0	0	0	0
11	0	0	0	4	0	0
12	0	1	0	0	0	0
13	2	2	0	0	4	0
14	0	0	0	0	0	0
15	0	0	0	0	0	0
16	1	1	1	1	1	0
17	2	0	4	0	0	0
18	1	0	2	0	0	0
19	0	2	0	0	0	0
20	2	0	0	0	0	0
21	0	2	0	0	0	0
22	0	0	0	0	0	0
23	0	0	0	0	0	0
24	0	0	0	0	0	0
25	3	1	2	1	2	0
26	2	0	0	0	0	0
27	0	1	0	0	0	0
28	0	2	0	0	0	0
29	2	0	0	0	0	6
30	0	0	0	0	0	0

Table 1: Number of colourings for various planar symmetries

3D: The cubic Bravais classes

Let us consider the so-called primitive cubic lattice, represented by $\mathbb{Z}^3$. This is also called P-type for short. It is only one of three possible Bravais classes with cubic symmetry O_h, the other two being the face-centred cubic (*fcc* or F-type) and the body-centred cubic (*bcc* or B-type) ones. This shows one immediate complication: sublattices with cubic symmetry may be of different Bravais type! In fact, inside $\mathbb{Z}^3$ there is one F-type sublattice of index 2 ($\Gamma_F = \{(m_1, m_2, m_3) \mid m_1 + m_2 + m_3 \text{ even}\}$) and one B-type sublattice of index 4 ($\Gamma_B = \{(m_1, m_2, m_3) \mid m_1 \equiv m_2 \equiv m_3 \ (2)\}$). Consequently, it is natural to attack our problem in two steps, first focusing on a single Bravais class and later extending to all of them.

Again, the focus is on those cases where one colour occupies a sublattice (compare [6] for the more general situation). Let us thus first ask for sublattices of P-type, i.e. we ask for rotations R, followed by a homothety $\alpha > 0$, such that

$$\alpha R \mathbb{Z}^3 \ \subset \ \mathbb{Z}^3 \, . \tag{14}$$

Note that we need neither consider reflections, as they can always be written as $-R$ and inversion is a lattice symmetry, nor negative α, for the same reason. Also, $\alpha = 0$ would not give us a 3D lattice. If we now use the standard basis $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ and write $\mathbb{Z}^3 = \mathbb{Z}\boldsymbol{e}_1 \oplus \mathbb{Z}\boldsymbol{e}_2 \oplus \mathbb{Z}\boldsymbol{e}_3$, we are actually asking for all $R \in SO(3)$ and $\alpha > 0$ such that αR has integer entries only.

Now, if αR is integral, so is its transpose, and $\alpha R (\alpha R)^t = \alpha^2 \mathbb{1}$ implies $\alpha^2 \in \mathbb{N}$. On the other hand, $\det(\alpha R) = \alpha^3$ is also in integer. Therefore, $\alpha = \alpha^3/\alpha^2$ must be rational. But, as its square is an integer, α itself must be an integer, and then the rotation matrix R can only have rational entries, i.e. $R \in SO(3, \mathbb{Q})$. Then, α must actually be an integer multiple of the denominator of R (being the smallest integer m such that mR is integral), see [2] for a more detailed discussion.

Let us pause to remark that the same type of argument can be used for $\mathbb{Z}^n$ with arbitrary n. If n is *odd*, one finds that αR maps to a P-type sublattice if and only if $R \in SO(n, \mathbb{Q})$ and α is an integer multiple of the denominator of R. If, however, n is *even*, we can also get solutions where α is a quadratic irrationality (and only $R^2 \in SO(n, \mathbb{Q})$), as happened above in the case of the square lattice.

Our combinatorial problem in 3D can now be solved it we know the number of $SO(3, \mathbb{Q})$-matrices with a given denominator. This number is known from the solution of a different, but closely related problem, namely that of the coincidence rotations of the cubic lattice, compare [3] and references therein. The corresponding Dirichlet series generating function $\Phi_{cub}(s)$ is repeated in the Appendix for convenience.

Let us now derive the generating function for the number of cubic sublattices of $\mathbb{Z}^3$. There are three different sources for them. First, for each $R \in SO(3,\mathbb{Q})$, we have one solution of the form $\Gamma = \mathrm{den}(R) \cdot R\mathbb{Z}^3$ (with $\mathrm{den}(R)^3$ different colours, namely one for Γ and each of its cosets). This same solution is obtained by altogether 24 pairwise different $SO(3,\mathbb{Q})$-matrices, because $SO(3,\mathbb{Z})$ (the rotation symmetry group of $\mathbb{Z}^3$) contains 24 elements. The generating function for these cases is obviously $\Phi_{cub}(3s)$.

Next, for each such Γ, we also have the sublattice $m\Gamma$ for each $m \in \mathbb{N}$, and none of those, except Γ itself, has been counted yet. Since the number of colours for $m\Gamma$ is m^3 times as large as that for Γ, our generating function gets multiplied by $\zeta(3s)$ to account for these possibilities. This exhausts the P-type sublattices of $\mathbb{Z}^3$ wherefore

$$\begin{aligned} F(s) &= \zeta(3s)\Phi_{cub}(3s) \qquad (15)\\ &= 1 + \tfrac{1}{8^s} + \tfrac{5}{27^s} + \tfrac{1}{64^s} + \tfrac{7}{125^s} + \tfrac{5}{216^s} + \tfrac{9}{343^s} + \tfrac{1}{512^s} + \tfrac{17}{729^s} + \tfrac{7}{1000^s} + \tfrac{13}{1331^s} + \cdots \end{aligned}$$

is the proper generating function for them.

Finally, one can also find, as explained earlier, an F-type and a B-type sublattice in each of the P-type cubic ones, which results in an overall factor $1 + 2^{-s} + 4^{-s}$. Altogether this gives the generating function

$$\begin{aligned} F_{cub}(s) &= (1 + 2^{-s} + 4^{-s}) \cdot \zeta(3s) \cdot \Phi_{cub}(3s) \qquad (16)\\ &= 1 + \tfrac{1}{2^s} + \tfrac{1}{4^s} + \tfrac{1}{8^s} + \tfrac{1}{16^s} + \tfrac{5}{27^s} + \tfrac{1}{32^s} + \tfrac{5}{54^s} + \tfrac{1}{64^s} + \tfrac{5}{108^s} + \tfrac{7}{125^s} + \tfrac{1}{128^s} + \cdots \end{aligned}$$

The Bravais type can be determined as follows. If m is a possible number of colours (i.e. the denominator of a fraction with non-zero numerator), and if s is the largest integer such that $2^s | m$, then the colouring is based on P-, F- or B-type if s is congruent (mod 3) to 0, 1 or 2, respectively. The answer for the other cubic lattices is similar, with the roles of P, F and B and the prefactor in (16) appropriately changed (note that Γ_B as defined above is not a sublattice of Γ_F).

3D: The icosahedral modules of rank 6

It is well known that there are three different icosahedral modules in 3-space, which can be obtained as projections of the three types of hypercubic lattices in 6-space. They are thus called B-, P- and F-type for body-centred, primitive and face-centred, respectively. It is convenient to describe them in an orthogonal basis $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ of twofold axes of the icosahedron. With $\alpha_i \in \mathbb{Z}[\tau]$, $\tau = (1+\sqrt{5})/2$ the golden ratio, the B- and F-type modules then read

$$\mathcal{M}_B = \{\textstyle\sum_{i=1}^{3} \alpha_i \boldsymbol{e}_i \mid \tau^2\alpha_1 + \tau\alpha_2 + \alpha_3 \equiv 0 \ (2)\},$$

$$\mathcal{M}_F \;=\; \{\, \boldsymbol{x} \in \mathcal{M}_B \mid \alpha_1 + \alpha_2 + \alpha_3 \equiv 0 \ (2) \} \,.$$

Clearly, $\mathcal{M}_F$ is a submodule of $\mathcal{M}_B$ of index 4, and both are $\mathbb{Z}$-modules of rank 6, but also $\mathbb{Z}[\tau]$-modules of rank 3. In particular, they are both invariant under multiplication by τ.

In between these two modules, there is also a P-type module, or in fact there are three different ones of this type (all three on different scales), namely

$$\begin{aligned}
\mathcal{M}_P^{(1)} &= \{\, \boldsymbol{x} \in \mathcal{M}_B \mid \alpha_1 + \alpha_2 + \alpha_3 \equiv 0 \text{ or } 1 \ (2) \} \,, \\
\mathcal{M}_P^{(2)} &= \{\, \boldsymbol{x} \in \mathcal{M}_B \mid \alpha_1 + \alpha_2 + \alpha_3 \equiv 0 \text{ or } \tau \ (2) \} \,, \\
\mathcal{M}_P^{(3)} &= \{\, \boldsymbol{x} \in \mathcal{M}_B \mid \alpha_1 + \alpha_2 + \alpha_3 \equiv 0 \text{ or } \tau^2 \ (2) \} \,.
\end{aligned} \tag{17}$$

They are again $\mathbb{Z}$-modules of rank 6, but not $\mathbb{Z}[\tau]$-modules because they are not invariant under multiplication by τ. In fact, as $\tau \mathcal{M}_P^{(1)} = \mathcal{M}_P^{(2)}$ etc., they form a 3-cycle under multiplication by τ. Nevertheless, together with $\mathbb{Z}[\tau]^3 = \mathbb{Z}[\tau]\boldsymbol{e}_1 + \mathbb{Z}[\tau]\boldsymbol{e}_2 + \mathbb{Z}[\tau]\boldsymbol{e}_3$, we have the inclusion

$$2\mathbb{Z}[\tau]^3 \overset{4}{\subset} \mathcal{M}_F \overset{2}{\subset} \mathcal{M}_P^{(i)} \overset{2}{\subset} \mathcal{M}_B \overset{4}{\subset} \mathbb{Z}[\tau]^3 \tag{18}$$

for $i = 1, 2, 3$, where the integer on top of the inclusion symbol denotes the corresponding index, e.g. $\mathcal{M}_B$ is a submodule of $\mathbb{Z}[\tau]^3$ of index 4 which means that $\mathbb{Z}[\tau]^3$ is a disjoint union of $\mathcal{M}_B$ and three cosets of it.

Let us now consider the colouring problem for the module $\mathcal{M}_B$ and let us assume that we know all submodules Λ of the same Bravais type which are maximal in the sense that $\alpha\Lambda \subset \mathcal{M}_B$ implies $\alpha \in \mathbb{Z}[\tau]$. But then, as Λ itself must be a $\mathbb{Z}[\tau]$-module, each $\alpha \in \mathbb{Z}[\tau]$ is possible, and the corresponding group-subgroup index is

$$[\Lambda : \alpha\Lambda] \;=\; |\mathrm{N}(\alpha)^3| \tag{19}$$

where $\mathrm{N}(\gamma)$ denotes the (number theoretic) norm in the quadratic field $\mathbb{Q}(\tau)$. For $\gamma = p + q\tau$ it reads

$$\mathrm{N}(\gamma) \;:=\; \gamma\gamma' \;=\; p^2 + pq - q^2 \tag{20}$$

where $\gamma' = p + q\tau'$ is the algebraic conjugate of γ defined through $\tau' = -1/\tau = 1 - \tau$.

In particular, Eq. (19) says that $\alpha\Lambda$ requires $|\mathrm{N}(\alpha)^3|$ times as many colours as Λ. The number of *different* solutions obtained this way is in one-to-one correspondence with the ideals of $\mathbb{Z}[\tau]$, which are counted by the ζ-function $\zeta_{\mathbb{Q}(\tau)}(s)$, see the Appendix. So, this contributes a factor $\zeta_{\mathbb{Q}(\tau)}(3s)$ to the generating function of the colouring problem.

Now, we have to determine the maximal submodules Λ of B-type. Before we do that, let us briefly look at the related colouring problem for the (modulated cubic) module $\mathbb{Z}[\tau]^3 = \mathbb{Z}^3 \oplus \tau\mathbb{Z}^3$. Consider a rotation R and a stretching factor α such that

$$\alpha R \mathbb{Z}[\tau]^3 \subset \mathbb{Z}[\tau]^3 . \tag{21}$$

Then, by an analogous argument to that of the cubic case, we may conclude that both α^2 and α^3 are in $\mathbb{Z}[\tau]$, and hence $\alpha \in \mathbb{Q}(\tau)$. But, from (20), $\mathrm{N}(\alpha) \in \mathbb{Q}$ and $\mathrm{N}(\alpha^2) = \mathrm{N}(\alpha)^2 \in \mathbb{Z}$, hence $\mathrm{N}(\alpha) \in \mathbb{Z}$ which implies $\alpha \in \mathbb{Z}[\tau]$. Consequently, $R \in SO(3, \mathbb{Q}(\tau))$, and we then conclude, very much as in the case of the cubic lattice $\mathbb{Z}^3$, that the only (linear) similarity transformations that map $\mathbb{Z}[\tau]^3$ into itself are $\mathbb{Z}[\tau]$-multiples of $\mathrm{den}(R)R$, where $\mathrm{den}(R)$ is the greatest common divisor of all $\beta \in \mathbb{Z}[\tau]$ with βR integral. Note that $SO(3, \mathbb{Q}(\tau))$ is the group of coincidence rotations of $\mathbb{Z}[\tau]^3$ (and simultaneously of the icosahedral module $\mathcal{M}_B$), see [3, 1] for details. From here, one can calculate the generating function of the different colourings [2], using explicit results from [1].

Instead of going into details there, let us now consider the icosahedral module $\mathcal{M}_B$, and a similarity transformation αR such that

$$\alpha R \mathcal{M}_B \subset \mathcal{M}_B . \tag{22}$$

From (18) it follows that then also $\alpha R \mathcal{M}_B \subset \mathbb{Z}[\tau]^3$ and hence $\alpha R(2\mathbb{Z}[\tau]^3) \subset \mathbb{Z}[\tau]^3$, which means that $2\alpha R$ must have $\mathbb{Z}[\tau]$ entries only. This is a necessary (but not sufficient) condition, while αR integral is certainly sufficient, but not necessary. In any case, we can conclude that $2\alpha \in \mathbb{Z}[\tau]$ and $R \in SO(3, \mathbb{Q}(\tau))$ is a rational matrix.

For each $R \in SO(3, \mathbb{Q}(\tau))$ we thus obtain one maximal $\mathcal{M}_B$-submodule Λ, and precisely 60 different R's will result in the same Λ as there are 60 rotation symmetries of the icosahedron that map Λ onto itself. To get Λ, we have to multiply R by a suitable number, and, in contrast to the cubic case above, this number is not always the denominator of R, but sometimes a divisor of it (then coinciding with $\mathrm{den}(R)/2$ up to units in $\mathbb{Z}[\tau]$). In any case, it can be chosen as a totally positive number in $\mathbb{Z}[\tau]$ whose norm is the so-called *coincidence index* $\Sigma(R)$, defined through [3, 1]

$$\Sigma(R) \;:=\; [\mathcal{M}_B : (\mathcal{M}_B \cap R\mathcal{M}_B)] . \tag{23}$$

The corresponding similarity transformation maps $\mathcal{M}_B$ to a maximal submodule Λ which then requires $\Sigma(R)^3$ different colours. So, with $\Phi_{ico}(s)$ being the generating function for the icosahedral coincidence problem, see [3, 1] and the Appendix, the contribution to the colouring problem is given by the factor $\Phi_{ico}(3s)$, in complete analogy to the cubic case.

The same kind of reasoning also applies to the module $\mathcal{M}_F$. Therefore,

$$\begin{aligned} F(s) &= \zeta_{\mathbb{Q}(\tau)}(3s)\Phi_{ico}(3s) && (24) \\ &= 1 + \tfrac{6}{64^s} + \tfrac{7}{125^s} + \tfrac{11}{729^s} + \tfrac{26}{1331^s} + \tfrac{26}{4096^s} + \tfrac{42}{6859^s} + \tfrac{42}{8000^s} + \tfrac{37}{15625^s} + \tfrac{62}{24389^s} + \cdots \end{aligned}$$

is, at the same time, the generating function for the B-type submodules of $\mathcal{M}_B$ and for the F-type submodules of $\mathcal{M}_F$. In order to include the P-type modules in a natural way, we observe that the triple $(\mathcal{M}_P^{(1)}, \mathcal{M}_P^{(2)}, \mathcal{M}_P^{(3)})$ considered as a set is mapped onto itself under multiplication with *any* $\mathbb{Z}[\tau]$-number, while each member of the set has its own coincidence site submodules (with the same index formula as for the B- and F-type modules). Furthermore, two such triples (which are 3-cycles under multiplication by τ) are either equal or disjoint. So, it is easiest to count triples rather than single modules because $F(s)$ is then also the generating function for this case, and a separate counting just requires multiplication of the corresponding numerator by 3.

If we want to know the number of icosahedral submodules of either type, we obtain three different solutions, depending on the module we start from:

$$\begin{aligned} F_{ico}^{(B)}(s) &= (1 + 2^{-s} + 4^{-s}) \cdot \zeta_{\mathbb{Q}(\tau)}(3s) \cdot \Phi_{ico}(3s) \\ F_{ico}^{(P)}(s) &= (1 + 2^{-s} + 32^{-s}) \cdot \zeta_{\mathbb{Q}(\tau)}(3s) \cdot \Phi_{ico}(3s) && (25) \\ F_{ico}^{(F)}(s) &= (1 + 16^{-s} + 32^{-s}) \cdot \zeta_{\mathbb{Q}(\tau)}(3s) \cdot \Phi_{ico}(3s) \end{aligned}$$

This is slightly more complicated than the cubic case as a consequence of Eq. (18). In particular, both B- and P-type allow for a 2-colouring (then being of P- and F-type, respectively) while 16 is the smallest number of colours for the F-type module.

Concluding Remarks

In this article, a subclass of the colouring problem of lattices and modules with irreducible symmetries was considered. The combinatorial part was explicitly solved by means of Dirichlet series generating functions for various planar modules with n-fold symmetry as well as for cubic lattices and icosahedral modules in 3-space. A similar analysis is possible in 4D, as well as for certain series of lattices in higher dimension.

Clearly, one is not only interested in the number of colouring possibilities but in the actual colour symmetry groups. In the planar case, a more complete answer is possible through the unique factorization property in rings of cyclotomic integers, which will be reported separately. In 3-space, due to non-commutativity of the ring of integer quaternions resp. the ring of icosian numbers, things are more complicated and will require a more detailed analysis.

Concerning the generality of our findings, it is clear that there are relevant cases of colourings already with 4-fold symmetry that do *not* belong to the restricted class investigated here, compare [17]. They can be found systematically by the method of [8] which also allows for an algorithmic version that can be used on a computer. Whether the generating function approach allows for a generalization to cover this, e.g. along the lines of [6, 17, 15], is presently under investigation.

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Appendix

It is the purpose of this Appendix to provide some details on the generating functions and the ζ-functions used above. The simplest case is Riemann's ζ-function itself,

$$\zeta(s) \;=\; \sum_{m=1}^{\infty} \frac{1}{m^s} \;=\; \prod_{p} \frac{1}{1-p^{-s}}\,, \tag{26}$$

which allows a representation as an Euler product because all numerators of the sum are 1 and thus define a multiplicative function.

Similarly, the ζ-function of $\mathbb{Q}(\tau)$ (which counts the ideals in $\mathbb{Z}[\tau]$) is the Dirichlet series of a multiplicative function and reads

$$\begin{aligned} \zeta_{\mathbb{Q}(\tau)}(s) \;&=\; \frac{1}{1-5^{-s}} \cdot \prod_{p\equiv\pm 1\;(5)} \frac{1}{(1-p^{-s})^2} \cdot \prod_{p\equiv\pm 2\;(5)} \frac{1}{1-p^{-2s}} \\ &=\; 1 + \tfrac{1}{4^s} + \tfrac{1}{5^s} + \tfrac{1}{9^s} + \tfrac{2}{11^s} + \tfrac{1}{16^s} + \tfrac{2}{19^s} + \tfrac{1}{20^s} + \tfrac{1}{25^s} + \tfrac{2}{29^s} + \tfrac{2}{31^s} + \tfrac{1}{36^s} + \tfrac{2}{41^s} + \tfrac{2}{44^s} + \cdots \end{aligned} \tag{27}$$

The various other ζ-functions that appear in the text are described in detail in [14] and need not be repeated here.

Finally, let us give the generating functions of the coincidence problem, for details on how to calculate them we refer to [1].

$$\Phi_{cub}(s) \;=\; \prod_{p\neq 2} \frac{1+p^{-s}}{1-p^{1-s}} \;=\; \frac{1-2^{1-s}}{1+2^{-s}} \cdot \frac{\zeta(s)\zeta(s-1)}{\zeta(2s)} \tag{28}$$
$$= 1 + \tfrac{4}{3^s} + \tfrac{6}{5^s} + \tfrac{8}{7^s} + \tfrac{12}{9^s} + \tfrac{12}{11^s} + \tfrac{14}{13^s} + \tfrac{24}{15^s} + \tfrac{18}{17^s} + \tfrac{20}{19^s} + \tfrac{32}{21^s} + \tfrac{24}{23^s} + \tfrac{30}{25^s} + \tfrac{36}{27^s} + \cdots$$

$$\Phi_{ico}(s) \;=\; \frac{1+5^{-s}}{1-5^{1-s}} \prod_{p\equiv\pm 2\ (5)} \frac{1+p^{-2s}}{1-p^{2(1-s)}} \prod_{p\equiv\pm 1\ (5)} \left(\frac{1+p^{-s}}{1-p^{1-s}}\right)^2 \tag{29}$$
$$= 1 + \tfrac{5}{4^s} + \tfrac{6}{5^s} + \tfrac{10}{9^s} + \tfrac{24}{11^s} + \tfrac{20}{16^s} + \tfrac{40}{19^s} + \tfrac{30}{20^s} + \tfrac{30}{25^s} + \tfrac{60}{29^s} + \tfrac{64}{31^s} + \tfrac{50}{36^s} + \tfrac{84}{41^s} + \tfrac{120}{44^s} + \cdots$$

The latter function can be expressed in terms of the ζ-function of Eq. (27)

$$\Phi_{ico}(s) \;=\; \frac{\zeta_{\mathbb{Q}(\tau)}(s)\zeta_{\mathbb{Q}(\tau)}(s-1)}{\zeta_{\mathbb{Q}(\tau)}(2s)} \tag{30}$$

which shows again the close analogy between the cubic and the icosahedral case.

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