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CUBES IN $\{0, 1, \ldots, N\}^3$

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Abstract

The main aim of this paper is to describe a procedure for calculating the number of cubes that have coordinates in the set $\{0, 1, \ldots, n\}$. For this purpose we continue and, at the same time, revise some of the work begun in a sequence of papers about equilateral triangles and regular tetrahedra all having integer coordinates for their vertices. We adapt the code that was included in a paper by the first author and was used to calculate the number of regular tetrahedra with vertices in $\{0, 1, \ldots, n\}^3$. The idea is based on the theoretical results obtained by the first author with A. Markov. We then extend the sequence A098928 in the Online Encyclopedia of Integer Sequences to the first one hundred terms.

1. Introduction

In this paper we consider cubes in $\mathbb{R}^3$ whose vertices have only integer coordinates. Very often we will refer to this property by saying that the various objects are in $\mathbb{Z}^3$. Strictly speaking these geometric objects are defined as being more than the set of their vertices that determines them. However, we are simply going to think of these objects as sets of vertices. So, for instance, an equilateral triangle is going to be a set of three points in $\mathbb{Z}^3$ for which the Euclidean distances between every two of these points are the same. The main purpose of our paper is to take a close look at the cubes in $\mathbb{Z}^3$. One can easily imagine such cubes by taking the faces parallel to the planes of coordinates. However, it is less obvious that there exist many more other cubes sitting in space as in Figure 1 (a). As a curiosity, our counting shows

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that there are precisely 242,483,634 cubes with vertices in $\{0, 1, \ldots, 100\}^3$. One non-trivial example of these cubes is given by the points

$$\mathcal{C} := \{[0, 56, 59], [21, 68, 3], [24, 0, 56], [45, 12, 0], [52, 77, 83], [73, 89, 27], [76, 21, 80], [97, 33, 24]\}.$$

In [14] we proved the following theorem.

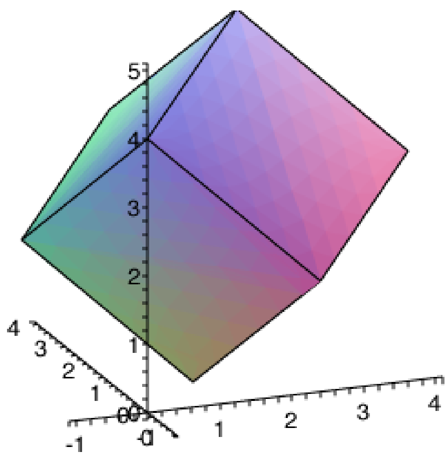

Figure 1(a): Non−trivial cube

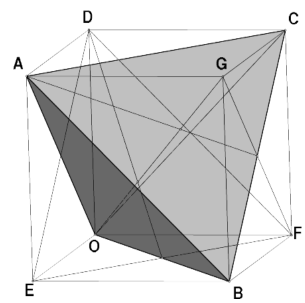

Figure 1(b): Regular tetrahedron inscribed: OABC

Theorem 1 *Every regular tetrahedron in $\mathbb{Z}^3$ can always be completed to a cube in $\mathbb{Z}^3$ (See Figure 1 (b)).*

This theorem implies that there is a one-to-two correspondence between the cubes and the regular tetrahedra in $\mathbb{Z}^3$. In [11] we developed a Maple code to compute the number of regular tetrahedra in $\{0, 1, 2, \ldots, n\}^3$. Here, we basically use the same idea and introduce some updates based on important theoretical observations. The problem of finding the number of cubes in space with coordinates in $\{0, 1, 2, \ldots, n\}$ has also been studied in [17]. We list here a few more terms in the sequence A098928.

n	1	2	3	4	5	6	7	8	9	10	11
A098928	1	9	36	100	229	473	910	1648	2795	4469	6818

n	12	13	14	15	16	17	18
A098928	10032	14315	19907	27190	36502	48233	62803

.

It is clear that $A098928 \leq A103158$. For $n \geq 4$ we actually have a strict inequality, $A098928 < A103158$, and this is due to the fact that some of the tetrahedra inside of the grid $\{0, 1, .., n\}^3$ extend beyond the grid's boundaries to the unique cube containing it described above. In Figure 2 we are including the graphs of the sequences A098928 and A103158 up to $n = 100$.

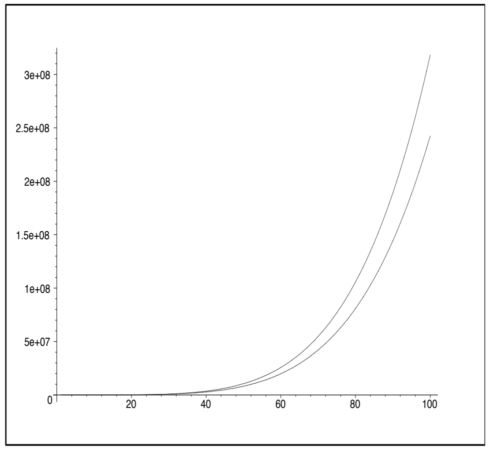

Figure 2: Tetrahedra versus cubes

2. Theoretical Background

Let us review some of the facts that we are using. Regular tetrahedra are going to be obtained from equilateral triangles. Equilateral triangles in $\mathbb{Z}^3$ are obtained in the following way. Given an odd integer d there is a precise number of primitive solutions for the Diophantine equation (see [11])

$$a^2+b^2+c^2=3d^2,\ with\ 0<a\le b\le c\ and\ gcd(a,b,c)=1, \tag{1}$$

which is given by

$$\pi\epsilon(d)=\frac{\Lambda(d)+24\Gamma_2(d)}{48}, \tag{2}$$

where

$$\Gamma_2(d)=\begin{cases} 0 & \text{if } d \text{ is divisible by a prime factor of the form } 8s+5 \text{ or } 8s+7,\ s\ge 0\\ 1 & \text{if } d \text{ is } 3\\ 2^k & \begin{cases}\text{where } k \text{ is the number of distinct prime factors of } d\\ \text{of } d \text{ of the form } 8s+1 \text{ or } 8s+3\ (s>0),\end{cases}\end{cases} \tag{3}$$

$$\Lambda(d):=8d\prod_{p|d,p\ prime}\left(1-\frac{(\frac{-3}{p})}{p}\right), \tag{4}$$

and $(\frac{-3}{p})$ is the Legendre symbol. We remind the reader that, if p is an odd prime then

$$(\frac{-3}{p}) = \begin{cases} 0 \ \text{ if } p = 3 \\ \\ 1 \ \text{ if } p \equiv 1 \text{ or } 7 \pmod{12} \\ \\ -1 \ \text{ if } p \equiv 5 \text{ or } 11 \pmod{12} \end{cases} . \tag{5}$$

In particular, this counting shows that the equation (1) has primitive solutions for every odd $d \geq 1$. We took advantage of this simple way of calculating $\pi\epsilon(n)$, and we found experimentally (see Figure 3) that

$$\lim_{k\to\infty} \frac{\sum_i^k \pi\epsilon(2i+1)}{k} \approx 0.34131 \quad .$$

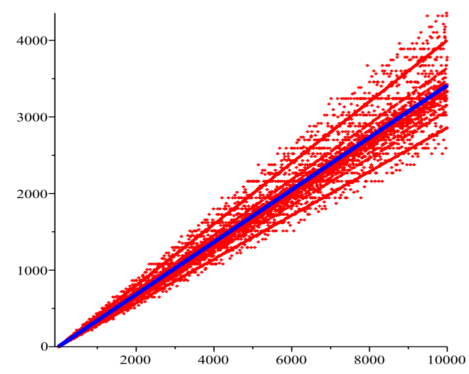

Figure 3: Graph of $k \to \pi\epsilon(2k+1), k = 1, 2, \ldots, 10000$

As an example, for the prime $d = 2011 = 251(8) + 3 = 167(12) + 7$, we get $\Lambda(d) = 16080$ and $\Gamma_2(d) = 48$, and so $\pi\epsilon(2011) = \frac{16080+48}{48} = 336$. There is only one primitive solution, in this case, for which the three values of a, b, and c are not all distinct: $a = 139$ and $b = c = 2461$.

For each solution of (1) we have the following lattice of points in $\mathbb{Z}^3$:

$$\begin{aligned} \mathcal{P}_{a,b,c} := \{(\alpha, \beta, \gamma) \in \mathbb{Z}^3 | \ \ a\alpha + b\beta + c\gamma = 0, \quad a^2 + b^2 + c^2 = 3d^2, \\ gcd(a, b, c) = 1, a, b, c, d \in \mathbb{Z}\}. \end{aligned} \tag{6}$$

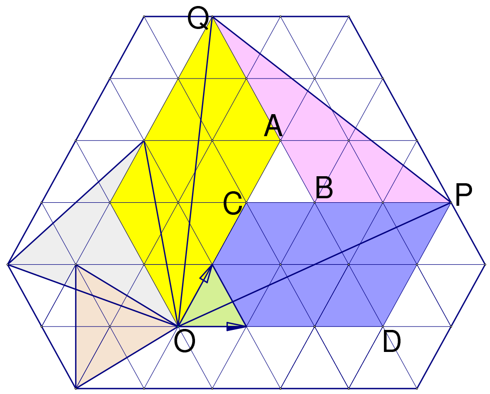

Figure 4: The sub-lattice $\mathcal{P}^{eq}{}_{a,b,c}$

This lattice is in general much richer than the sub-lattice, $\mathcal{P}^{eq}{}_{a,b,c}$, of all points which are vertices of equilateral triangles with one of the vertices being the origin (see Figure 4). Such an equilateral triangle, say $\triangle OPQ$, can be given in terms of two vectors $\overrightarrow{\zeta}$ and $\overrightarrow{\eta}$ described by the next formulae:

$$\overrightarrow{OP} = m\overrightarrow{\zeta} - n\overrightarrow{\eta}, \quad \overrightarrow{OQ} = n\overrightarrow{\zeta} - (n-m)\overrightarrow{\eta}, \tag{7}$$

with $\overrightarrow{\zeta} = (\zeta_1, \zeta_1, \zeta_2)$, and $\overrightarrow{\eta} = (\eta_1, \eta_2, \eta_3)$ given by

$$\begin{cases} \zeta_1 = -\dfrac{rac+dbs}{q}, \\ \\ \zeta_2 = \dfrac{das-bcr}{q}, \\ \\ \zeta_3 = r, \end{cases} \quad , \quad \begin{cases} \eta_1 = -\dfrac{db(s-3r)+ac(r+s)}{2q}, \\ \\ \eta_2 = \dfrac{da(s-3r)-bc(r+s)}{2q}, \\ \\ \eta_3 = \dfrac{r+s}{2}, \end{cases} \tag{8}$$

where $q = a^2+b^2$ and (r, s) is a suitable solution of $2q = s^2+3r^2$ that makes all the numbers in (8) integers. The sides-lengths of $\triangle OPQ$ are equal to $d\sqrt{2(m^2-mn+n^2)}$.

One way to give a more precise construction of a good choice of (r, s) is to compute the greatest common divisor, $s + i\sqrt{3}r$, of $A - i\sqrt{3}B$ and $2q$ in the ring $\mathbb{Z}[i\sqrt{3}]$, where $A = ac$ and $B = bd$. Indeed, let us observe that

$$A^2 + 3B^2 = (ac)^2 + 3(bd)^2 = a^2c^2 + b^2(a^2 + b^2 + c^2) = (a^2 + b^2)(c^2 + b^2)$$

which shows that $2q$ divides $A^2+3B^2 = (A+i\sqrt{3}B)(A-i\sqrt{3}B)$. Since $2q = 4(4k+1)$ for some integer k, we are thinking of 4 as $(1 + i\sqrt{3})(1 - i\sqrt{3})$, so the prime factors of $2q$ here are given by $1 + i\sqrt{3}$, $1 - i\sqrt{3}$ and all the others which are either primes of the form $6k-1$ or of the form $6k+1$. The factors of the form $6k-1$ must appear to even power and those of the form $6k+1$ can be decomposed into prime factors

$u + i\sqrt{3}v$ and $u - i\sqrt{3}v$ (by Fermat's Theorem, see [4] and [16]). As a result, each of these factors can be found either in the factorization of $A + i\sqrt{3}B$ or in the one for $A - i\sqrt{3}B$. The product of these common factors with $A - i\sqrt{3}B$ gives, say, $s + i\sqrt{3}r$. By construction $A - i\sqrt{3}B = (s + i\sqrt{3}r)(u + i\sqrt{3}v)$ and it turns out that $2q = (s+i\sqrt{3}r)(s-i\sqrt{3}r)$. This implies that $(A-i\sqrt{3}B)(s-i\sqrt{3}r) = 2q(u+i\sqrt{3}v)$.

Hence we get the relations

$$2q = s^2 + 3r^2, \quad As - 3Br = 2qu \quad and \quad Ar + Bs = -2qv.$$

These relations show that ζ_1 and η_1 in (8) are integers. Lagrange's identity shows that

$$\zeta_1^2 + \zeta_2^2 = \frac{(a^2+b^2)((rc)^2 + (ds)^2)}{q^2} = \frac{(rc)^2 + (ds)^2}{a^2+b^2},$$

which in turn gives

$$\zeta_1^2 + \zeta_2^2 + \zeta_3^2 = \frac{r^2(a^2+b^2) + r^2c^2 + d^2s^2}{a^2+b^2} = \frac{d^2(s^2+3r^2)}{q} = 2d^2.$$

This implies in particular that ζ_2 must be an integer and that $|\overrightarrow{\zeta}| = d\sqrt{2}$.
It is clear that r and s must be either both odd or both even. This implies that η_3 is an integer. Using again Lagrange's identity we get

$$\eta_1^2 + \eta_2^2 = \frac{(a^2+b^2)[c^2(r+s)^2 + d^2(s-3r)^2]}{4q^2} = \frac{c^2(r+s)^2 + d^2(s-3r)^2}{4(a^2+b^2)},$$

which implies

$$\eta_1^2+\eta_2^2+\eta_3^2 = \frac{(r+s)^2(a^2+b^2+c^2) + d^2(s-3r)^2}{4(a^2+b^2)} = \frac{d^2[3(r+s)^2 + (s-3r)^2]}{4q} = 2d^2.$$

As before, this proves that η_2 is an integer and $|\overrightarrow{\eta}| = d\sqrt{2}$. In order to find the dot product of $\overrightarrow{\zeta}$, $\overrightarrow{\eta}$ we observe that

$$\zeta_1\eta_1 + \zeta_2\eta_2 = \frac{(a^2+b^2)[c^2(r^2+rs) + d^2(s^2-3rs)]}{2q^2}$$

which implies

$$\overrightarrow{\zeta} \cdot \overrightarrow{\eta} = \frac{c^2(r^2+rs) + d^2(s^2-3rs)}{2q} + \frac{r^2+rs}{2} = \frac{d^2(3r^2+3rs+s^2-3rs)}{2q} = d^2.$$

Hence the angle between the vectors $\overrightarrow{\zeta}$, $\overrightarrow{\eta}$ is $\arccos(\frac{\overrightarrow{\zeta}\cdot\overrightarrow{\eta}}{|\overrightarrow{\zeta}||\overrightarrow{\eta}|}) = 60°$.

Using these relations, we can easily calculate

$$|\overrightarrow{OP}|^2 = m^2|\overrightarrow{\zeta}|^2 - 2\overrightarrow{\zeta}\cdot\overrightarrow{\eta}mn + n^2|\overrightarrow{\eta}|^2 = 2d^2(m^2 - mn + n^2), \quad \text{and}$$

$$|\overrightarrow{OQ}|^2 = n^2|\overrightarrow{\zeta}|^2 - 2\overrightarrow{\zeta}\cdot\overrightarrow{\eta}n(n-m) + (n-m)^2|\overrightarrow{\eta}|^2 =$$

$$2d^2[n^2 - n(n-m) + (n-m)^2] = 2d^2(m^2 - mn + n^2).$$

The dot product of $\overrightarrow{OP}$ and $\overrightarrow{OQ}$ is then equal to

$$\overrightarrow{OP}\cdot\overrightarrow{OQ} = mn|\overrightarrow{\zeta}|^2 - [m(n-m) + n^2]\overrightarrow{\zeta}\cdot\overrightarrow{\eta} + n(n-m)|\overrightarrow{\eta}|^2 =$$

$$d^2(2mn - mn + m^2 - n^2 + 2n^2 - 2mn) = d^2(m^2 - mn + n^2).$$

These relations show that the triangle $\triangle OPQ$ is indeed equilateral and its side lengths are equal to $d\sqrt{2(m^2 - mn + n^2)}$.

Next, one can easily check that

$$a\zeta_1 + b\zeta_2 + c\zeta_3 = a\eta_1 + b\eta_2 + c\eta_3 = 0,$$

which implies that $\triangle OPQ$ is indeed contained in the plane of normal $\overrightarrow{n} = \frac{(a,b,c)}{d\sqrt{3}}$. The natural question now is, whether or not there are other equilateral triangles with integer coordinates contained in this same plane, or in other words, is the parametrization given by (7) and (8) exhaustive ? The answer to the first question is negative and we showed this in [2]. However, we include here a new and relatively simpler argument which has a geometric flavor. Let us assume, by way of contradiction, that there exists one triangle, say $\triangle OAB$, which is not covered by the parametrization. We may assume that O is the origin (otherwise we use a translation with integer coordinates to accomplish that). Because the vectors $\overrightarrow{\zeta}$ and $\overrightarrow{\eta}$ form a basis for the space of vectors perpendicular to $\overrightarrow{n}$, the equation $\overrightarrow{OA} = m\overrightarrow{\zeta} - n\overrightarrow{\eta}$ can be solved uniquely for real numbers m and n. Let us then consider the vectors

$$\overrightarrow{OB'} = n\overrightarrow{\zeta} - (n-m)\overrightarrow{\eta}, \quad \overrightarrow{OB''} = (m-n)\overrightarrow{\zeta} - m\overrightarrow{\eta}.$$

With the same computations as before, we obtain that $\triangle OAB'$ and $\triangle OAB''$ are equilateral in the same plane of normal $\overrightarrow{n}$. Because there are only two equilateral triangles sharing the side OA in the given plane, we must have either $B' = B$ or $B'' = B$. Without loss of generality, let us assume that $B' = B$. From the formulae in (8) we get that

$$mr - \frac{r+s}{2}n = u \in \mathbb{Z}, \quad \textit{and} \quad nr - \frac{r+s}{2}(n-m) = \frac{r+s}{2}m + \frac{r-s}{2}n = v \in \mathbb{Z}.$$

If we look at these two relations as a system of equations in m and n, we get by Cramer's formula, a unique solution in terms of u and v, which are rational numbers. Hence, m and n are fractions with denominators equal to

$$r\frac{r-s}{2}+\frac{r+s}{2}\frac{r+s}{2}=\frac{s^2+3r^2}{4}=\frac{q}{2}=\frac{a^2+b^2}{2}\geq 1.$$

Similar calculations as before show that the side lengths of $\triangle OAB$ are equal to $\ell = d\sqrt{2(m^2-mn+n^2)}$. We consider similar constructions for b and c, and for a and c, instead of a and b. We get that

$$\ell^2 = 2d^2(m^2-mn+n^2) = 2d^2(m_1^2-m_1n_1+n_1^2) = 2d^2(m_2^2-m_2n_2+n_2^2) \quad (9)$$

with m_1, n_1, m_2, n_2 rational numbers having $\frac{b^2+c^2}{2}$ and $\frac{a^2+c^2}{2}$ as denominators, respectively. Since $\gcd(a,b,c)=1$, it is easy to see that $\gcd(\frac{a^2+b^2}{2},\frac{b^2+c^2}{2},\frac{a^2+c^2}{2})=1$. Hence, in (9) the number $m^2-mn+n^2=m_1^2-m_1n_1+n_1^2=m_2^2-m_2n_2+n_2^2$ as a fraction in the reduced form, cannot have a denominator greater than one since any prime dividing it, divides $\gcd(\frac{a^2+b^2}{2},\frac{b^2+c^2}{2},\frac{a^2+c^2}{2})=1$. So, we proved that the triangle $\triangle OAB$ (or any other triangle with integer coordinates in the plane of normal $\overrightarrow{n}$ passing through the origin) has sides at least $d\sqrt{2}$.

Now, if m and n are not integers, then A and B fall strictly inside of the tessellation with equilateral triangles generated by the two vectors $\overrightarrow{\zeta}$ and $\overrightarrow{\eta}$ (see Figure 5). Because the tessellation is invariant to 60° rotations, the position of B in the interior of one of the equilateral triangles is perfectly similar to the position of A inside of the corresponding equilateral triangle containing it. This creates two vectors of the same length, one being the rotation of the other by 60°. Using translations with integer coordinates the two vectors show the existence of an equilateral triangle with the origin as one of its vertices, $\triangle OCD$, having integer coordinates and side lengths strictly less than $d\sqrt{2}$. This contradiction shows that A and B must be vertices of the tessellation generated by $\overrightarrow{\zeta}$ and $\overrightarrow{\eta}$, and so the parametrization (8) is exhaustive.

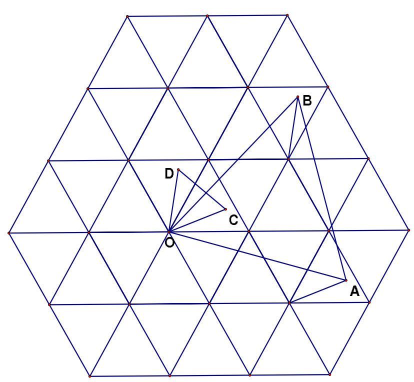

Figure 5: Two distinct tessellations

We have given then another proof of Theorem 1 in [10].

Let us illustrate how this parametrization works in a particular situation. For $d = 2011$ we have seen the particular solution of (1) in which $b = c$: $a = 139$ and $b = c = 2461$. If we do the parametrization with $q = a^2 + b^2 = (2)(3037921)$ (3037921 is prime), since $A = ac = (23)(107)(139)$ and $B = (23)(107)(2011)$, we get

$$A - iB = (23)(107)(1 - \sqrt{3}i)(1543 - 468\sqrt{3}i)$$

and

$$2q = (1 - \sqrt{3}i)(1543 - 468\sqrt{3}i)(1 + \sqrt{3}i)(1543 + 468\sqrt{3}i)$$

which gives $s + r\sqrt{3}i = (1 - \sqrt{3}i)(1543 - 468\sqrt{3}i) = 139 - 2011\sqrt{3}i$. Therefore, we have

$$\begin{cases} \zeta_1 = 0 \\ \zeta_2 = 2011 \\ \zeta_3 = -2011 \end{cases} \quad \text{and} \quad \begin{cases} \eta_1 = -2461 \\ \zeta_2 = 1075 \\ \zeta_3 = -936. \end{cases}$$

One can check that, in fact, in the case $b = c$ we may always take

$$\begin{cases} \zeta_1 = 0 \\ \zeta_2 = d \\ \zeta_3 = -d \end{cases} \quad \text{and} \quad \begin{cases} \eta_1 = -b \\ \eta_2 = \frac{a+d}{2} \\ \eta_3 = \frac{a-d}{2}. \end{cases} \tag{10}$$

We summarize all these facts that we have shown so far.

Theorem 2 *The sub-lattice $\mathcal{P}^{eq}{}_{a,b,c}$ is generated by two vectors $\overrightarrow{\zeta}$ and $\overrightarrow{\eta}$ in the following sense: $\mathcal{T}^{m,n}_{a,b,c} := \triangle OPQ$ with P, Q in $\mathcal{P}_{a,b,c}$, is equilateral if and only if for some integers m, n*

$$\begin{gathered} \overrightarrow{OP} = m\overrightarrow{\zeta} - n\overrightarrow{\eta}, \quad \overrightarrow{OQ} = n\overrightarrow{\zeta} + (m-n)\overrightarrow{\eta}, \text{ with} \\ \overrightarrow{\zeta} = (\zeta_1, \zeta_1, \zeta_2), \overrightarrow{\varsigma} = (\varsigma_1, \varsigma_2, \varsigma_3), \overrightarrow{\eta} = \frac{\overrightarrow{\zeta} + \overrightarrow{\varsigma}}{2}, \end{gathered} \tag{11}$$

$$\begin{cases} \zeta_1 = -\dfrac{rac + dbs}{q} \\ \\ \zeta_2 = \dfrac{das - bcr}{q} \\ \\ \zeta_3 = r \end{cases}, \quad \begin{cases} \varsigma_1 = \dfrac{3dbr - acs}{q} \\ \\ \varsigma_2 = -\dfrac{3dar + bcs}{q} \\ \\ \varsigma_3 = s \end{cases}, \tag{12}$$

where $q = a^2 + b^2$ and r, s can be chosen so that all six numbers in (12) are integers. The sides-lengths of $\triangle OPQ$ are equal to $d\sqrt{2(m^2 - mn + n^2)}$. Moreover, r and s can be constructed in such a way that the following properties are also verified:

(i) r and s satisfy $2q = s^2 + 3r^2$ and similarly $2(b^2 + c^2) = \varsigma_1^2 + 3\zeta_1^2$ and $2(a^2 + c^2) = \varsigma_2^2 + 3\zeta_2^2$
(ii) $r = r'\omega\chi$, $s = s'\omega\chi$ where $\omega = gcd(a, b)$, $gcd(r', s') = 1$ and χ is the product of the prime factors of the form $6k - 1$ of $(a^2 + b^2)/\omega^2$
(iii) $|\overrightarrow{\zeta}| = d\sqrt{2}$, $|\overrightarrow{\varsigma}| = d\sqrt{6}$, and $\overrightarrow{\zeta} \cdot \overrightarrow{\varsigma} = 0$
(iv) $s + i\sqrt{3}r = gcd(A - i\sqrt{3}B, 2q)$, in the ring $\mathbb{Z}[i\sqrt{3}]$, where $A = ac$ and $B = bd$.

In [13], we have shown that the only equilateral triangles, in $\mathbb{Z}^3$, which can be completed to a regular tetrahedron in $\mathbb{Z}^3$, are the ones (given as in (11) and (12)) for which $m^2 - mn + n^2 = k^2$ for some $k \in \mathbb{Z}$. More precisely, if k is divisible by 3 then one can accomplish this on either side of the plane containing the triangle and if k is not divisible by 3 then this can be done on only one side. By the way, this is saying in particular that, there are a lot more equilateral triangles than regular tetrahedra in $\mathbb{Z}^3$.

The coordinates for the fourth vertex, assuming the equilateral triangle's vertices are as in (7) and (12), are given by

$$\left(\frac{(2\zeta_1 - \eta_1)m - (\zeta_1 + \eta_1)n \pm 2ak}{3}, \frac{(2\zeta_2 - \eta_2)m - (\zeta_2 + \eta_2)n \pm 2bk}{3}, \frac{(2\zeta_3 - \eta_3)m - (\zeta_3 + \eta_3)n \pm 2ck}{3}\right). \tag{13}$$

As we already mentioned in Theorem 1, as long as the coordinates in (13) are integers then the tetrahedron can be completed to a cube in $\mathbb{Z}^3$. We are using this formula mostly for $k = 1$ (let us choose $m = 1$ and $n = 0$) although there is a need for the general case for big values of d because, as pointed out in [11], there are irreducible regular tetrahedra which cannot be constructed from a face as above, by simply taking $k = 1$. However for small ℓ ($\ell < 5187 = 3(7)(13)(19)$) one can find a face of a given regular tetrahedron of sides equal to $\ell\sqrt{2}$ which has the corresponding k as in (13) equal to 1.

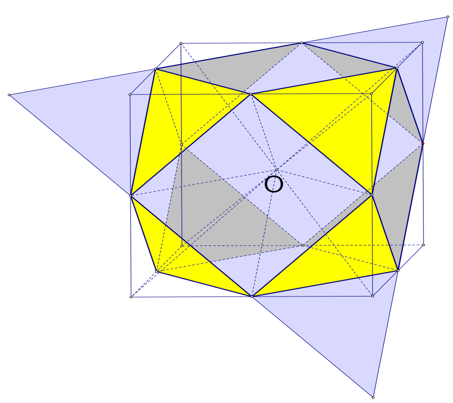

Figure 6: Eight tetrahedra and essentially one cube

If one takes all the possible values for m and n such that $m^2 - mn + n^2 = 1$, there are six regular tetrahedra generated this way, from a plane (colored blue in Figure 6), three on one side and the other three on the other side, but if one looks at the Figure 6, one might observe that in fact there are eight regular tetrahedra all generating essentially the same cube (up to translations of integer coordinates). So, our code needs to take into acount this property and we will only use one of the choices for the values for m and n. Summarizing, there are in general four planes containing the center of a given cube in $\mathbb{Z}^3$, corresponding to normals given by the directions of the four big diagonals in the cube which may generate the cube as before, some may have a value of $k > 1$. For this reason, one needs to check for repetitions when writing the code. For this purpose, our approach is to generate an exhaustive list, $\mathcal{L}$, of cubes in $\mathbb{N}_0^3$ ($\mathbb{N}_0 = \mathbb{N} \cup \{0\}$) which are irreducible (cannot be scaled to a smaller cube in $\mathbb{Z}^3$). One other property of each cube in $\mathcal{L}$ is that it cannot be translated in the negative direction along any of the axes of coordinates and remain in $\mathbb{N}_0^3$. Unfortunately, the cubes in $\mathcal{L}$ are not uniquely defined this way, because of the possible symmetries involved here. These 48 symmetries form a group which can be identified with the symmetry group of a regular octahedron (see [14]).

3. The Minimal List and Other Considerations

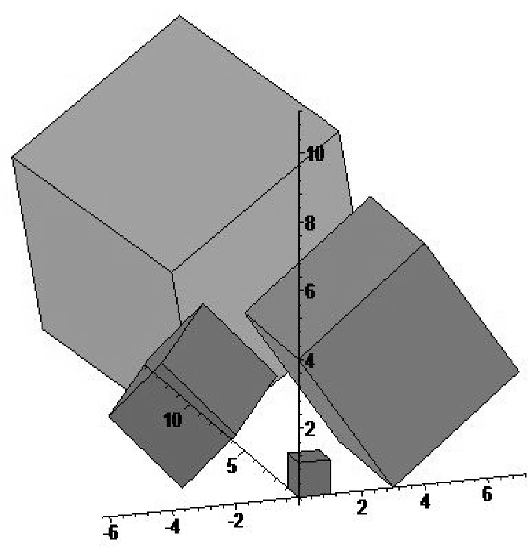

Figure 7: First cubes in $\mathcal{L}$

A dozen cubes (listed in non-decreasing order of their side-lengths) in the list $\mathcal{L}$ that we found using our code, are included in the table below. The first column represents the side-lengths, the second column gives the dimension of the smallest cube $C_m := [0, m]^3$ containing the cube in column three.

n	m	A cube	k-values	invariants
1	1	$[0,0,0], [0,0,1], [0,1,0], [0,1,1],$ $[1,0,0], [1,0,1], [1,1,0], [1,1,1]$	1	[1, 1, 0, 0]
3	5	$[0,3,2], [1,1,4], [2,2,0], [2,5,3],$ $[3,0,2], [3,3,5], [4,4,1], [5,2,3]$	1,3	[4, 4, 0, 0]
5	7	$[0,0,4], [0,5,4], [3,0,0], [3,5,0],$ $[4,0,7], [4,5,7], [7,0,3], [7,5,3]$	1	[12, 18, 4, 0]
7	11	$[0,6,8], [2,9,2], [3,0,6], [5,3,0],$ $[6,8,11], [8,11,5], [9,2,9], [11,5,3]$	1,7	[8, 8, 0, 0]
9	15	$[0,5,5], [4,4,13], [4,13,4], [7,1,1],$ $[8,12,12], [11,0,9], [11,9,0], [15,8,8]$	1,3	[24,108, 48, 16]
11	19	$[0,11,13], [2,2,7], [6,17,6], [8,8,0],$ $[9,9,19], [11,0,13], [15,15,12], [17,6,6]$	1	[24, 108, 48, 16]
13	19	$[0,12,15], [3,16,3], [4,0,12], [7,4,0],$ $[12,15,19], [15,19,7], [16,3,16], [19,7,4]$	1, 13	[8, 8, 0, 0]
13	17	$[0,0,12], [0,13,12], [5,0,0], [5,13,0],$ $[12,0,17], [12,13,17], [17,0,5], [17,13,5]$	1	[12, 30,8, 0]
15	25	$[0,5,10], [2,19,15], [10,0,20], [11,7,0],$ $[12,14,25], [13,21,5], [21,2,10], [23,16,15]$	1, 3	[48, 360, 176, 64]
17	29	$[0,20,9], [1,8,21], [12,12,0], [12,29,17],$ $[13,0,12], [13,17,29], [24,21,8], [25,9,20]$	1	[24, 60, 16, 0]
17	23	$[0,0,15], [0,17,15], [8,0,0], [8,17,0],$ $[15,0,23], [15,17,23], [23,0,8], [23,17,8]$	1	[12, 42, 12, 0]
19	31	$[0,16,10], [6,6,25], [10,31,16], [15,10,0],$ $[16,21,31], [21,0,15], [25,25,6], [31,15,21]$	1, 19	[8, 8, 0, 0]

Table 1

In the fourth column we list the values of k which can be used in the construction described in Section 2 to generate the cube in column three. The list of invariants in the last column are as follows. First, we have the number of cubes in the orbit obtained by applying the group of 48 transformations, determined by the orthogonal matrices (3 by 3) with coefficients 0 and ± 1, to the cube in column three. Let us denote this number by α_0. We observe that α_0 is a divisor of 48 as expected (Lagrange's Theorem). We expect that in general such a cube will have no special symmetry and so, more often than otherwise we will get $\alpha_0 = 48$. The second number in the invariants list is the number of cubes in the *generalized* orbit, obtained by the previous orbit together with all its integer translations along the axes of coordinates that remain in C_m, a number that we are going to denote by α. The third number in the list, β, is the cardinality of the intersection between this former orbit and its translation along $(0, 0, 1)$. Finally, the last number, γ, is defined by the cardinality of the generalized orbit with its translation along $(0, -1, 1)$. It turns out that these last three numbers are enough to determine the number of cubes that one can fit by translating the given cube in all possible ways within a bigger cube of size $k \geq m$. This fact has been essentially proved in Theorem 2.2 ([10]). The formula that gives this number is

$$(k-m+1)^3\alpha - 3(k-m)(k-m+1)^2\beta + 3(k-m+1)(k-m)^2\gamma. \qquad (14)$$

One other observation that we make, about Table 1, is that this set of invariants is not complete, since we see that the same numbers appear for various irreducible cubes. The most surprising are those cubes in rows six and seven. A good problem here is to determine the exact number of such cubes, which go into a certain side-length n, in terms of n. We see that the first n for which we have two such cubes is $n = 13$. Let us also observe that in column four we see a 1 for each cube. As we mentioned earlier, this is not always the case.

Also, each cube in Table 1 with side-lengths n, gives rise to an orthogonal matrix with rational coefficients having denominators in $\frac{1}{n}\mathbb{Z}$ (obtained by taking the normalized vectors along the sides of the cube that form an orthogonal basis). In [14] we computed a few of them:

$$T_3 := \frac{1}{3}\begin{bmatrix} 1 & -2 & 2 \\ 2 & -1 & -2 \\ -2 & -2 & -1 \end{bmatrix}, T_5 := \frac{1}{5}\begin{bmatrix} 4 & 0 & 3 \\ 3 & 0 & -4 \\ 0 & -5 & 0 \end{bmatrix}, T_7 := \frac{1}{7}\begin{bmatrix} -2 & -3 & 6 \\ 3 & -6 & -2 \\ -6 & -2 & -3 \end{bmatrix},$$

$$T_9 := \frac{1}{9}\begin{bmatrix} -7 & -4 & 4 \\ 4 & 1 & 8 \\ -4 & 8 & 1 \end{bmatrix}, T_{11} := \frac{1}{11}\begin{bmatrix} 2 & -9 & -6 \\ 9 & -2 & 6 \\ -6 & -6 & 7 \end{bmatrix},$$

$$T_{13} := \frac{1}{13}\begin{bmatrix} -4 & -12 & -3 \\ 12 & -3 & -4 \\ 3 & -4 & 12 \end{bmatrix}, \hat{T}_{13} := \frac{1}{13}\begin{bmatrix} 0 & -13 & 0 \\ 12 & 0 & 5 \\ -5 & 0 & 12 \end{bmatrix}.$$

The next matrix can be obtained by multiplying T_3 with T_5. We notice a multiplicative structure on this set of matrices. For the next two sizes (prime numbers) we have essentially two orthogonal matrices in each case.

$$T_{17} := \frac{1}{17}\begin{bmatrix} 12 & -8 & -9 \\ 12 & 9 & 8 \\ 1 & -12 & 12 \end{bmatrix}, \hat{T_{17}} := \frac{1}{17}\begin{bmatrix} 15 & 0 & 8 \\ 8 & 0 & -15 \\ 0 & -17 & 0 \end{bmatrix},$$

$$T_{19} := \frac{1}{19}\begin{bmatrix} 6 & -18 & 1 \\ 17 & 6 & 6 \\ -6 & -1 & 18 \end{bmatrix}, \hat{T}_{19} := \frac{1}{19}\begin{bmatrix} 15 & -6 & -10 \\ 10 & 15 & 6 \\ 6 & -10 & 15 \end{bmatrix}.$$

From T_5, $\hat{T}_{13}$, and $\hat{T}_{17}$ it is clear that there is a natural imbedding of the primitive Pythagorean Triples into this sequence of orthogonal matrices (well known in the literature). One essential property of the list $\mathcal{L}$ is that each cube in the list generates under translations and rotations cubes in C_k and two different cubes cannot generate the same cube. We accomplish this by making sure that the four planes given by diagonals are different for two different cubes in the list. So, in order to count all the cubes in C_k, we first compute the list of irreducible cubes in $\mathcal{L}$, up to the side length k, and then for each one we use the formula (14) to find out how many are generated by each cube in the $\mathcal{L}$ that are in C_k. This operation is not enough though since there are cubes in C_k which are reducible. So, in the end we multiply each cube in the list $\mathcal{L}$ by an integer factor in such a way the resulting cube still fits in C_k. Then, we recalculate the invariants on this cube and use the same formula (14) to find the contribution of the reducible cubes. In the end, we add up all these numbers and that gives, $NC(k)$, the number of cubes in C_k .

The first 100 values of $NC(n)$ are:

$1, 9, 36, 100, 229, 473, 910, 1648, 2795, 4469,$	$n = 1 \dots 10$
$6818, 10032, 14315, 19907, 27190, 36502, 48233, 62803, 80736, 102550,$	$n = 11 \dots 20$
$128847, 160271, 197516, 241314, 292737,$	$n = 21 \dots 25$
$352591, 421764, 501204, 592257, 696281,$	$n = 26 \dots 30$
$814450, 948112, 1098607, 1267367, 1456292,$	$n = 31 \dots 35$
$1666998, 1901633, 2162179, 2450440, 2768346,$	$n = 36 \dots 40$
$3117935, 3501389, 3923178, 4384792, 4889323,$	$n = 41 \dots 45$
$5439155, 6037660, 6687358, 7391669, 8154671,$	$n = 46 \dots 50$
$8979750, 9870158, 10830095, 11862711, 12972046,$	$n = 51 \dots 56$
$14161848, 15436931, 16801993, 18263634, 19825948,$	$n = 57 \dots 60$
$21493019, 23269647, 25160816, 27171482, 29308957,$	$n = 61 \dots 65$
$31577319, 33986616, 36540004, 39244371, 42106267,$	$n = 66 \dots 70$
$45131996, 48327502, 51700279, 55258019, 59011634,$	$n = 71 \dots 75$
$62965766, 67132037, 71515527, 76127374, 80973598,$	$n = 76 \dots 80$
$86062187, 91401297, 96999986, 102866282, 109014085,$	$n = 81 \dots 85$
$115457359, 122206348, 129266410, 136648555, 144364071,$	$n = 86 \dots 90$
$152426724, 160843660, 169626467, 178787563, 188347314,$	$n = 91 \dots 95$
$198309846, 208694461, 219509943, 230767760, 242483634.$	$n = 96 \dots 100$

In [15], an earlier version of this paper, we included the code of our algorithm written for Mathematica, together with the necessary explanations for each step. For further studies we are going to look into the problem of counting the number of regular octahedra in C_k (see [12]) and of course one may ask similar questions about other polyhedra with integer vertices, semi-regular or with various other properties. Our techniques easily adapt to other similar situations. This opens a wide range of investigations which seem appropriate for undergraduate research projects.

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