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Original article

A counting problem on lattice points in two-, three- and four-dimensional spaces

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ABSTRACT

A counting problem on lattice points in n-dimensional space with rectangular coordinate system was considered. Lattice points are all the points having integer coordinates. The distances of these lattice points to the origin O are denoted from small to large as $r_{n,0} < r_{n,1} < r_{n,2} < \ldots$, where $r_{n,0} = 0$ denotes the origin itself. All the lattice points scatter on a series of concentric spherical surfaces with the center O and the radii $r_{n,k}, k = 0, 1, 2, \ldots$. The number of lattice points on the spherical surface with the radius $r_{n,k}$ is denoted as $N_{n,k}$. Several properties about the sequences $r_{n,k}$ and $N_{n,k}, k = 0, 1, 2, \ldots$, were investigated. The relevant generating function was derived in terms of the elliptic theta functions for convenient calculation of $r_{n,k}$ and $N_{n,k}$. We proved that for the 2-dimensional case, the number of lattice points is 4 on each circles with the radii satisfying $r_{2,s}^2 = 2^h, h = 0, 1, 2, \ldots$; for the 3-dimensional case, the number of lattice points is 6 on each spherical surfaces with the radii satisfying $r_{3,s}^2 = 4^h, h = 0, 1, 2, \ldots$; for the 4-dimensional case, the number of lattice points is 24 on each hyper-spherical surfaces with the radii satisfying $r_{4,s}^2 = 2^h, h = 1, 2, \ldots$.

1. Introduction

In molecular dynamics simulations, the coordination shells around an atom are often considered, such as in pairwise potentials (Kittel, 2005), the Van der Waals interactions (Mittemeijer, 2010), the embedded atom potentials (Daw and Baskes, 1984; Finnis and Sinclair, 1984; Duan and Liu, 2020) and the radial distribution function (Callister, 2001). Mirjalili and Vahdati-Khaki (2008) calculated the melting point of nano-particles by introducing and using the mean coordination number. Peresypkina and Blatov (1999) and Peresypkina and Blatov (2000) considered the molecular coordination numbers in crystal structures of simple substances and organic compounds. Wang et al. (2010) investigated the coordination numbers and geometrical conformation of rare earth metal. In Duan et al. (2020), computational problems of multilayered coordination radii and coordination numbers in cubic crystals were considered, respectively for simple cubic, body-centered cubic and face-centered cubic crystals. These problems were solved by modelling the enumeration of lattice points in 3-dimensional space by means of the Diophantine equations and generating functions.

The calculation problem of coordination numbers of cubic crystals, especially the simple cubic crystals, may be modeled as counting of lattice points in the Cartesian coordinate system. In a 2-dimensional space, the calculation of lattice points within a circle is related to an ancient puzzle, known as the Gauss's circle problem (Hardy and Landau, 1924; Berndt et al., 2018), which is still an open problem (Berndt et al., 2018) the resolution of which involves the application of advanced number theory and special functions (Andrews, 2015; Travaglini, 2015; Grosswald, 1985). Its counterpart in 3-dimensional space has been considered in (Grosswald, 1985; Fraser and Gotlieb, 1962; Arkhipova, 2008; Fomenko, 2014). Further, a new field, the geometry on the integer lattices, was developed in Maehara and Martini (2018). Owing to the complicacy of computation problem on lattices, the lattice theory has been applied to the field of cryptography (Micciancio et al., 2011; Wang et al., 2016).

In this article, we consider a counting problem on lattice points in the n-dimensional space with the Cartesian rectangular coordinate system. Lattice points are all the points with the integer coordinates. The following notations are used:

n: the dimension of space under consideration.

r: the distance to the origin O of the Cartesian rectangular coordinate system.

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$r_{n,k}$: the distances from lattice points to the origin O in n-dimensional rectangular coordinate system, ordered from small to large as $r_{n,0} < r_{n,1} < r_{n,2} < \ldots$, where $r_{n,0} = 0$ means the distance of the origin O to itself. So $r^2_{n,k}$ is just the $(k+1)$th non-negative integer in natural order that may be expressed as sum of n square numbers.

$N_{n,k}$: the number of lattice points on the spherical surface with the radius $r_{n,k}, k = 0, 1, \ldots$.

$L_{n,k}$: the total of lattice points on or inside the spherical surface with the radius $r_{n,k}, k = 0, 1, \ldots$.

$\mathbb{Z}$: the set of all the integers.

In the next section, we discuss the properties of the sequence $r_{n,k}$ and express $N_{n,k}$ as the number of integer solutions of a quadratic indefinite equation. Further, we derive the generating function for the sequences $N_{n,k}$ and $r^2_{n,k}, k = 0, 1, \ldots$, in terms of the elliptic theta functions. So convenient computing methods for $N_{n,k}$ and $r^2_{n,k}$ are obtained. In Section 3, we consider the properties of the sequences $N_{n,k}$ and $L_{n,k}, k = 0, 1, \ldots$, especially focused on the cases of $n = 2, 3$ and 4.

2. Sequences $r_{n,k}$ and $N_{n,k}, k = 0, 1, \ldots$, and the generating function

We consider the lattice points in n-dimensional space with rectangular coordinate system. Suppose the basis vectors of the unit orthogonal basis to be $\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_n$. Then, every lattice point A may uniquely be represented as a vector

$$\boldsymbol{r}_A = \overrightarrow{OA} = \sum_{i=1}^{n} x_i \boldsymbol{e}_i, \tag{1}$$

where $x_i \in \mathbb{Z}$. The square of the distance of the lattice point A to the origin O is

$$r^2 = |\boldsymbol{r}_A|^2 = \sum_{i=1}^{n} x_i^2. \tag{2}$$

The set of all possible values of r^2 is countable, assumed to be $r^2_{n,k}, k = 0, 1, 2, \ldots$, and

$$r_{n,0} < r_{n,1} < r_{n,2} < \ldots.$$

All of the number $r^2_{n,k}, k = 0, 1, 2, \ldots$, are exactly the set of all of the sums of n square numbers. It is obvious that

$$r_{n,0} = 0, \; r_{n,1} = 1, \tag{3}$$

which correspond to the origin O and the nearest $2n$ lattice points from O in n-dimensional space:

$$(\pm 1, 0, \ldots, 0), \; (0, \pm 1, \ldots, 0), \; \ldots, \; (0, \ldots, 0, \pm 1).$$

In 2-dimensional case, $r^2_{2,k}$ cannot equal 3, i.e. the first positive integer which cannot be represented as the quadratic sum of two integers is 3. In 3-dimensional case, $r^2_{3,k}$ cannot equal 7.

Whether a given positive integer can be represented into a quadratic sum of two, three or four integers is a classical and attractive problem. We list the related results in the following three theorems (Andrews, 2015; Travaglini, 2015; Grosswald, 1985; Feng, 2011).

Theorem 1. *A positive integer m can be expressed as the sum of two square numbers if and only if each prime factor of m in the form of $p = 4k + 3$ has an even power, where k is a nonnegative integer.*

Theorem 2. *A positive integer m cannot be expressed as the sum of three square numbers if and only if m can be expressed as the form of $m = 4^l(8k + 7)$, where l and k are nonnegative integers.*

Theorem 3 (*Lagrange's four-square theorem*). *Every positive integer can be expressed as the quadratic sum of four integers.*

If a positive integer m can be expressed as a sum of p square numbers, then m can be expressed as a sum of more than p square numbers either because some terms in the sum are already sum of squares or by trivially adding as many zeros squared as one wants. It can be derived that the sequence $\left\{r^2_{2,k}\right\}$ is a subsequence of $\left\{r^2_{3,k}\right\}$, and the sequence $\left\{r^2_{3,k}\right\}$ is a subsequence of $\left\{r^2_{4,k}\right\}$. From Theorem 3, if $n \geqslant 4$, then the sequence $\left\{r^2_{n,k}\right\}$ is just all the non-negative integers, i.e.

$$r^2_{n,k} = k, \quad k = 0, 1, 2, \ldots, \quad \text{for} \quad n \geqslant 4. \tag{4}$$

We notice that for the higher dimensional cases, $n \geqslant 4$, the sequence $\left\{r^2_{n,k}\right\}$ is very simple. But for the 2-dimensional and 3-dimensional cases, namely $n = 2, 3$, it is difficult to find a general term formula or recurrence relation for the sequence $\left\{r^2_{n,k}\right\}$. By means of the software MATHEMATICA 8.0, the plots of $r^2_{n,k}$ versus k for $k = 0, 1, \ldots, 49$ are shown in Fig. 1, where n is taken as 2, 3 and 4, respectively.

The plots of $r^2_{n,k}$ versus k for $k = 1$ through $k = 20000$ were examined visually for $n = 2$ and 3, and we found that for $n = 3$, the plot is almost a straight line, while for $n = 2$, the plot appears to be slightly concave. By linear fitting, the obtained results are

$$\hat{r}^2_{3,k} = 1.1999k - 2.579, \tag{5}$$

$$\hat{r}^2_{2,k} = 4.1641k - 1596.5. \tag{6}$$

We also examined the fitting effects by adding a nonlinear term in the form of $ak + b + ck^d$, and find that for the case of $n = 3$, the fitting result nearly does not change and $d = 1$ again, while for the case of $n = 2$, the fitting result is $\hat{r}^2_{2,k} = -2.1113k - 119.88 + 4.3433k^{1.0366}$.

For any nonnegative integer k, the number of lattice points, $N_{n,k}$, on the spherical surface $|\boldsymbol{r}_A| = r_{n,k}$, introduced in the last section, is just the number of the n-tuples, $(x_1, x_2, \ldots, x_n) \in \mathbb{Z}^n$, the integer solutions of the quadratic indefinite equation

$$\sum_{i=1}^{n} x_i^2 = r^2_{n,k}. \tag{7}$$

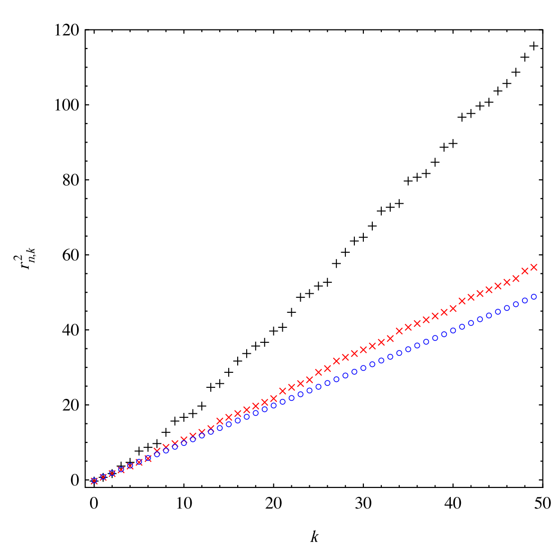

Fig. 1. Plots of $r^2_{n,k}$ versus k for $k = 0, 1, \ldots, 49$ (+: $n = 2$, $\times$: $n = 3$, $\circ$: $n = 4$).

Next, we consider the generating function $G_n(t)$ of the sequence $N_{n,k}, k = 0, 1, 2, \ldots$, starting from the equation

$$\sum_{x_1, x_2, \ldots, x_n = -\infty}^{\infty} t^{x_1^2 + x_2^2 + \ldots + x_n^2} = \left(\sum_{j=-\infty}^{\infty} t^{j^2} \right)^n. \tag{8}$$

Considering Eq. (7), combining the terms with same powers on the left hand side of Eq. (8) forms a power series on t, which is just in the form of $\sum_{k=0}^{\infty} N_{n,k} t^{r_{n,k}^2}$. So we obtain the generating function for the sequences $N_{n,k}$ and $r_{n,k}^2, k = 0, 1, 2, \ldots$, as

$$G_n(t) = \sum_{k=0}^{\infty} N_{n,k} t^{r_{n,k}^2} = \left(1 + 2 \sum_{j=1}^{\infty} t^{j^2} \right)^n = (\theta_3(0, t))^n, \tag{9}$$

where $\theta_3(c, t)$ is the elliptic theta function of the third type, defined as Olver et al. (2010)

$$\theta_3(c, t) = 1 + 2 \sum_{j=1}^{\infty} t^{j^2} \cos(2jc), \ |t| < 1. \tag{10}$$

We can resort to a computer software to expand the power of the elliptic theta function in Eq. (9) into power series to obtain the values of $r_{n,k}^2$ and $N_{n,k}$. We note that the elliptic theta function is built-in in MATHEMATICA 8.0. Let $L_{n,k} = \sum_{i=0}^{k} N_{n,i}$. In Table 1, the first ten values of the sequences $\left\{ r_{n,k}^2 \right\}, \{N_{n,k}\}$ and $\{L_{n,k}\}$ for $n = 2, 3, 4$ are listed.

3. Properties of sequences $N_{n,k}$ and $L_{n,k}, k = 0, 1, 2, \ldots$

In this section, we investigate properties of the sequence $N_{n,k}$ and $L_{n,k}, k = 0, 1, 2, \ldots$, especially for the cases of $n = 2, 3$ and 4.

Theorem 4. *For any positive integers $k \geqslant 1$ and $p \geqslant 2$, there exists a positive integer $s > k$, such that $pr_{n,k} = r_{n,s}$ and $N_{n,k} \leqslant N_{n,s}$.*

Proof. Suppose $(l_1, \ldots, l_n)$ is an integer solution of the indefinite equation $\sum_{i=1}^{n} x_i^2 = r_{n,k}^2$.Then we have $\sum_{i=1}^{n} (pl_i)^2 = (pr_{n,k})^2$. This implies that there exists a positive integer $s > k$, such that $pr_{n,k} = r_{n,s}$ and $(pl_1, \ldots, pl_n)$ is an integer solution of the indefinite equation $\sum_{i=1}^{n} x_i^2 = r_{n,s}^2$. Therefore, the inequality $N_{n,k} \leqslant N_{n,s}$ holds. ■.

Theorem 5. (i) *If $n = 2$ or 3, then for each $r_{n,k}, k \geqslant 1$, there exists a positive integer $s > k$, such that $2r_{n,k} = r_{n,s}$ and $N_{n,k} = N_{n,s}$.*

(ii) For the case of $n = 4$, if $r_{4,k}^2$ is a positive even number, then there exists a positive integer $s > k$, such that $2r_{4,k} = r_{4,s}$ and $N_{4,k} = N_{4,s}$.

Proof. By Theorem 4, we only need to explain the inequality $N_{n,k} \geqslant N_{n,s}$ holds. Suppose $(l_1, \ldots, l_n)$ is an integer solution of the equation $\sum_{i=1}^{n} x_i^2 = r_{n,s}^2$. Then

$$\sum_{i=1}^{n} l_i^2 = 4r_{n,k}^2. \tag{11}$$

In the following we show that all of l_i for $i = 1, \ldots, n$ are even.

(i) If $n = 2$, then l_1 and l_2 in Eq. (11) are both even. In fact, it is obvious that there cannot be exactly one even. Suppose both l_1 and l_2 are odd, then

$$l_1^2 + l_2^2 = (2u + 1)^2 + (2v + 1)^2 = 2\left(2u^2 + 2u + 2v^2 + 2v + 1\right),$$

where u, v are integers. Eq. (11) cannot hold.

If $n = 3$, Eq. (11) implies evidently that l_1, l_2 and l_3 cannot be all odd, nor exactly one odd. Suppose there are exactly two being odd, then we have

$$\begin{aligned} \sum_{i=1}^{3} l_i^2 &= (2u + 1)^2 + (2v + 1)^2 + 4g \\ &= 2\left(2u^2 + 2u + 2v^2 + 2v + 2g + 1\right), \end{aligned} \tag{12}$$

where u, v, g are integers. Eq. (11) cannot hold too.

Hence if $n = 2$ or 3, all l_i in Eq. (11) are even. Thus $(l_1/2, \ldots, l_n/2)$ is an integer solution of the equation $\sum_{i=1}^{n} x_i^2 = r_{n,k}^2$. It follows that $N_{n,k} \geqslant N_{n,s}$.

(ii) If $n = 4$, Eq. (11) implies obviously that among l_1, l_2, l_3 and l_4, there cannot be exactly one or three being odd. If there were exactly two being odd, a counterpart with Eq. (12) would derived. So Eq. (11) cannot hold. If all the four were odd, then

$$\begin{aligned} \sum_{i=1}^{4} l_i^2 &= (2u + 1)^2 + (2v + 1)^2 + (2g + 1)^2 + (2h + 1)^2 \\ &= 4(u(u + 1) + v(v + 1) + g(g + 1) + h(h + 1) + 1), \end{aligned} \tag{13}$$

where u, v, g, h are integers. But by the assumptions for the case $n = 4$, Eq. (11) has the form

$$\sum_{i=1}^{4} l_i^2 = 4 \times 2p, \ p = 1, 2, \ldots. \tag{14}$$

This is contradictory to Eq. (13). Hence if $n = 4$, all l_i in Eq. (11) are even. Thus $(l_1/2, \ldots, l_4/2)$ is an integer solution for the equation $\sum_{i=1}^{4} x_i^2 = r_{n,k}^2$. It follows that $N_{n,k} \geqslant N_{n,s}$. The proof is completed. ■.

Theorem 5 indicates that for the 2-dimensional or 3-dimensional cases, the numbers of lattice points on the spherical surfaces remain the same when the radius doubles; for the 4-dimensional case, if the square of the radius is even, then as the

Table 1
The first ten values of the sequences $\left\{ r_{n,k}^2 \right\}, \{N_{n,k}\}$ and $\{L_{n,k}\}$ for $n = 2, 3, 4$.

k	$r_{2,k}^2$	$N_{2,k}$	$L_{2,k}$	$r_{3,k}^2$	$N_{3,k}$	$L_{3,k}$	$r_{4,k}^2$	$N_{4,k}$	$L_{4,k}$
0	0	1	1	0	1	1	0	1	1
1	1	4	5	1	6	7	1	8	9
2	2	4	9	2	12	19	2	24	33
3	4	4	13	3	8	27	3	32	65
4	5	8	21	4	6	33	4	24	89
5	8	4	25	5	24	57	5	48	137
6	9	4	29	6	24	81	6	96	233
7	10	8	37	8	12	93	7	64	297
8	13	8	45	9	30	123	8	24	321
9	16	4	49	10	24	147	9	104	425

radius doubles, the number of lattice points on the spherical surface remains unchanged. For the 4-dimensional case, if the square of the radius is odd, such invariant property cannot hold by the following theorem.

Theorem 6. *For the case of $n = 4$, if $r^2_{4,k}$ is an odd number and $2r_{4,k} = r_{4,s}$, then the inequality $N_{4,k} < N_{4,s}$ holds.*

Proof. Let $r^2_{4,k} = 2m + 1, m = 0, 1, \ldots$. By definition we know that $N_{4,k}$ is the number of the integer solutions of the equation

$$\sum_{i=1}^{4} x_i^2 = 2m + 1, \tag{15}$$

while $N_{4,s}$ is the number of the integer solutions of the equation

$$\sum_{i=1}^{4} x_i^2 = 4(2m + 1). \tag{16}$$

It is obvious that the double of any solution of Eq. (15) is a solution of Eq. (16). Now we write $4(2m + 1) = 8m + 3 + 1$. By Theorem 2, $8m + 3$ can be expressed as the sum of three square numbers. Thus we find a solution of Eq. (16) with at least one odd component 1. This solution of Eq. (16) cannot be a double of any integer solution of Eq. (15). The inequality $N_{4,k} < N_{4,s}$ is proved. ■.

In Fig. 2, plots of $N_{n,k}$ versus k for $k = 1$ through 260 are shown for $n = 2$, 3 and 4, respectively. From Theorem 5, for the 2-dimensional or 3-dimensional cases, for any $s \geqslant 1$, there are infinitely many terms in the sequence $\{N_{n,k}\}$ taking the same value with $N_{n,s}$. This properties are reflected in Figs. 2a and 2b.

By using Eq. (4), the results in Theorems 5 (ii) and 6 mean

$$N_{4,k} = N_{4,4k}, \text{ if } k \text{ is even}, \tag{17}$$

$$N_{4,k} < N_{4,4k}, \text{ if } k \text{ is odd}. \tag{18}$$

Theorem 7. *(i) For the 2-dimensional case, every $N_{2,k}$ for $k \geqslant 1$ is a multiple of 4. For every $h, h = 0, 1, 2, \ldots$, there exists a positive integer s, such that*

$$r^2_{2,s} = 2^h, \quad N_{2,s} = 4, \tag{19}$$

which is the least value of $N_{2,k}$ for $k \geqslant 1$.

(ii) For the 3-dimensional case, every $N_{3,k}$ for $k \geqslant 1$ has the form $6\delta + 12p + 8q$, where $\delta = 0$ or 1, $p, q \geqslant 0, \delta, p, q$ are not all zeros. For every $h, h = 0, 1, 2, \ldots$, there exists a positive integer s, such that

$$r^2_{3,s} = 4^h, \quad N_{3,s} = 6, \tag{20}$$

which is the least value of $N_{3,k}$ for $k \geqslant 1$.

(iii) For the 4-dimensional case, every $N_{4,k}$ for $k \geqslant 2$ has the form $8\delta + 24p + 32q + 16w$, where $\delta = 0$ or 1, $p, q, w \geqslant 0, p, q, w$ are not all zeros, and if $w = 1$, then $\delta = 1$. For every $h, h = 1, 2, \ldots$, the following equalities hold

$$N_{4,2^h} = 24, \ h = 1, 2, \ldots, \tag{21}$$

which is the least value of $N_{4,k}$ for $k \geqslant 2$.

Proof. (i) For the 2-dimensional case, by symmetry, every $N_{2,k}$ for $k \geqslant 1$ is a multiple of 4. From $r^2_{2,1} = 1, N_{2,1} = 4$ and Theorem 5 (i), for any $l \geqslant 0$, there exists a positive integer s_1, such that

$$r^2_{2,s_1} = 4^l = 2^{2l}, \ N_{2,s_1} = 4.$$

Since $r^2_{2,2} = 2 = (\pm 1)^2 + (\pm 1)^2$ and $N_{2,2} = 4$, so for any $l \geqslant 0$, there exists a positive integer s_2, such that

$$r^2_{2,s_2} = 4^l \times 2 = 2^{2l+1}, \ N_{2,s_2} = 4.$$

Thus for every $h, h = 0, 1, 2, \ldots$, there exists a positive integer s, such that

$$r^2_{2,s} = 2^h, \quad N_{2,s} = 4,$$

which is the least value of $N_{2,k}$ for $k \geqslant 1$.

(ii) For the 3-dimensional case, we can classify the $N_{3,k}$ lattice points for $k \geqslant 1$ into those on axes with only one nonzero coordinate, those on planes with exactly two nonzero coordinates, and those inside octants with three nonzero coordinates. There are six first kind points, if any, a multiple of 12 of the second kind points, and a multiple of 8 of the third kind points. Therefore, every $N_{3,k}$ for $k \geqslant 1$ has the form $6\delta + 12p + 8q$, where $\delta = 0$ or 1, $p, q \geqslant 0, \delta, p, q$ are not all zeros.

From $r^2_{3,1} = 1, N_{3,1} = 6$ and Theorem 5 (i), for every $h, h = 0, 1, 2, \ldots$, there exists a positive integer s, such that

$$r^2_{3,s} = 4^h r^2_{3,1} = 4^h, \quad N_{3,s} = 6,$$

which is the least value of $N_{3,k}$ for $k \geqslant 1$.

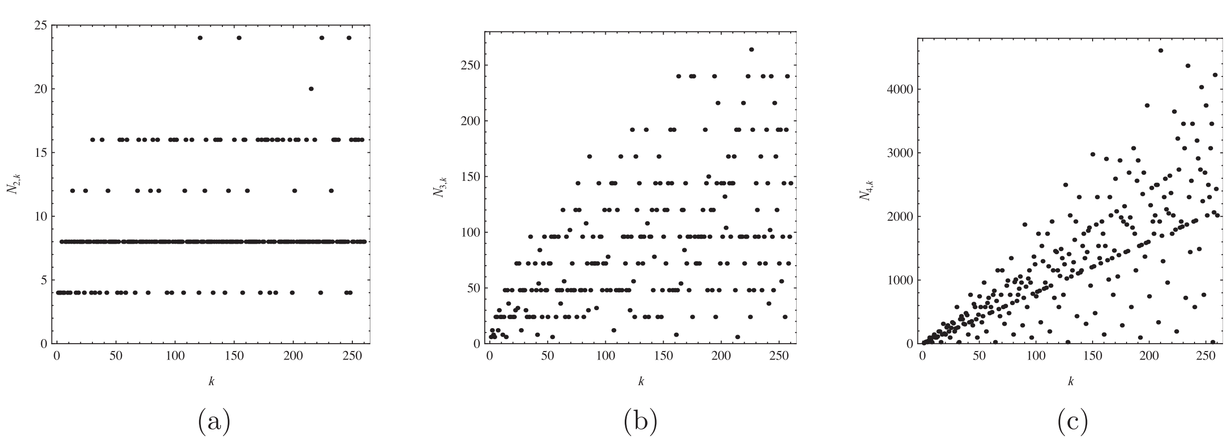

Fig. 2. Plots of $N_{n,k}$ versus k for $k = 1$ through 260 ((a) $n = 2$, (b) $n = 3$, (c) $n = 4$).

(iii) For the 4-dimensional case, we classify the $N_{4,k}$ lattice points for $k \geqslant 2$ into four classes: those with only one nonzero coordinate, there being 8 points, if any; those with exactly two nonzero coordinates, the number of points being a multiple of 24; those with exactly three nonzero coordinates, the number being a multiple of 32; and those with four nonzero coordinates, the number being a multiple of 16. So every $N_{4,k}$ for $k \geqslant 2$ has the form $8\delta + 24p + 32q + 16w$, where $\delta = 0$ or 1, $p, q, w \geqslant 0$.

Next, we show that even if $\delta = 1, p, q, w$ are not all zeros. If $N_{4,k}$ for $k \geqslant 2$ has the expression $8 + 24p + 32q + 16w$, then $r_{4,k}^2$ is a square number, i.e. the partitions of four square numbers of $r_{4,k}^2$ include the case of only one nonzero part. In this case, $r_{4,k}^2$ can be expressed as the sum of at least two nonzero square numbers. In fact, if $r_{4,k}^2 = (2m)^2$, then it has the expression $r_{4,k}^2 = m^2 + m^2 + m^2 + m^2$. If $r_{4,k}^2 = (2m+1)^2$, then $r_{4,k}^2 = (2m)^2 + 4m + 1$. By Theorem 2, $4m+1$ can be expressed as the sum of three square numbers since there is the expression $4m+1 = 8u+1$ or $4m+1 = 8u+5$ corresponding to even m or odd m, respectively. Therefore, p, q, w are not all zeros by the last paragraph.

Further, we show that if $w = 1$, then $\delta = 1$. $w = 1$ means there is only one lattice point with four positive coordinates. The four coordinates of such lattice point must be identical as $(m, m, m, m), m > 0$. Otherwise, more lattice points with four positive coordinates were found by exchanging different coordinates. Thus we have $r_{4,k}^2 = m^2 + m^2 + m^2 + m^2 = (2m)^2$, a square number. Therefore, we have $\delta = 1$.

Finally, due to $N_{4,2} = 24$ and Eq. (17), we have $N_{4,4^l \cdot 2} = N_{4,2^{2l+1}} = 24,\ l \geqslant 0$. Similarly, due to $N_{4,4} = 24$ and Eq. (17), we have $N_{4,4^l \cdot 4} = N_{4,2^{2l+2}} = 24,\ l \geqslant 0$. In conclusion, for every $h, h = 1, 2, \ldots,$ the equalities $N_{4,2^h} = 24,\ h = 1, 2, \ldots,$ hold, and which is the least value of $N_{4,k}$ for $k \geqslant 2$ from the above analysis. ■.

Because one lattice point occupies one n-dimensional unit cube and the n-dimensional sphere with the radius r has the volume $V_n(r) = \frac{\pi^{n/2} r^n}{\Gamma\left(\frac{n}{2}+1\right)}$,where $\Gamma(\cdot)$ is the gamma function, so we have the asymptotic behavior for the sequence $L_{n,k}$ as

$$L_{n,k} \sim V_n(r_{n,k}) = \frac{\pi^{n/2} r_{n,k}^n}{\Gamma\left(\frac{n}{2}+1\right)},\ k \to \infty. \tag{22}$$

This means

$$\lim_{k\to\infty} \frac{L_{n,k}}{V_n(r_{n,k})} = 1. \tag{23}$$

We checked the results for $n = 2, 3$ and 4, and the data are plotted in Fig. 3.

Unlike the sequence $L_{n,k}, k = 0, 1, 2, \ldots,$in Eqs. (22) and (23), the sequence $N_{n,k}, k = 0, 1, 2, \ldots,$does not have an asymptotic behavior for our considered cases $n = 2, 3$and 4. Instead, we may consider the sequence of mean values

$$\overline{N}_{n,k} = \frac{L_{n,k}}{k+1},\ k = 0, 1, 2, \ldots. \tag{24}$$

From Eq. (22), it has the asymptotic behavior

$$\overline{N}_{n,k} \sim \frac{\pi^{n/2} r_{n,k}^n}{(k+1)\Gamma\left(\frac{n}{2}+1\right)},\ k \to \infty. \tag{25}$$

For the case of $n = 4$, a simple result may be derived considering Eq. (4) as $\overline{N}_{4,k} \sim \frac{\pi^2 k}{2},\ k \to \infty$.For the cases of $n = 2$ and $n = 3$, we only have $\overline{N}_{2,k} \sim \frac{\pi r_{2,k}^2}{k}$and $\overline{N}_{3,k} \sim \frac{4\pi r_{3,k}^3}{3k}$ as $k \to \infty$, since we do not know the asymptotic behaviors of the sequences $\{r_{2,k}\}$ and $\{r_{3,k}\}$.

4. Conclusions

Lattice points in n-dimensional space scatter on a series of concentric spherical surfaces with the center O and the radii $r_{n,k}$, where $0 = r_{n,0} < r_{n,1} < r_{n,2} < \ldots$. All of the number $r_{n,k}^2, k = 0, 1, 2, \ldots,$ are exactly the set of all of the sums of n square numbers. If $n \geqslant 4$, the sequence $\left\{r_{n,k}^2\right\}$ is just the sequence of all the nonnegative integers, i.e. $r_{n,k}^2 = k,\ k = 0, 1, 2, \ldots$.The number of lattice points, $N_{n,k}$, on the spherical surface with the radius $r_{n,k}$ equals the number of integer solutions of the quadratic indefinite equation $\sum_{i=1}^n x_i^2 = r_{n,k}^2$. The generating function is derived as $G_n(t) = \sum_{k=0}^\infty N_{n,k} t^{r_{n,k}^2} = (\theta_3(0,t))^n$ in terms of the elliptic theta functions for convenient calculation of $r_{n,k}$ and $N_{n,k}$.

We proved that for the 2-dimensional or 3-dimensional cases, the numbers of lattice points on the spherical surfaces, $N_{n,k}$, remain the same when the radius doubles; for the 4-dimensional case, if the square of the radius is even, then as the radius doubles, the number of lattice points on the spherical surface remains unchanged, while if the square of the radius is odd, such invariant property does not hold.

For the 2-dimensional case, for every $h, h = 0, 1, 2, \ldots,$ there exists a positive integer s, such that $r_{2,s}^2 = 2^h$ and $N_{2,s} = 4$.For the 3-dimensional case, for every $h, h = 0, 1, 2, \ldots,$ there exists a positive integer s, such that $r_{3,s}^2 = 4^h$ and $N_{3,s} = 6$. For the 4-dimensional case, for every $h, h = 1, 2, \ldots,$ the equalities $N_{4,2^h} = 24$ hold and 24 is the least value of $N_{4,k}$ for $k \geqslant 2$. Finally, the asymptotic behaviors of the sequences $L_{n,k}$ and $\overline{N}_{n,k}$ are given.

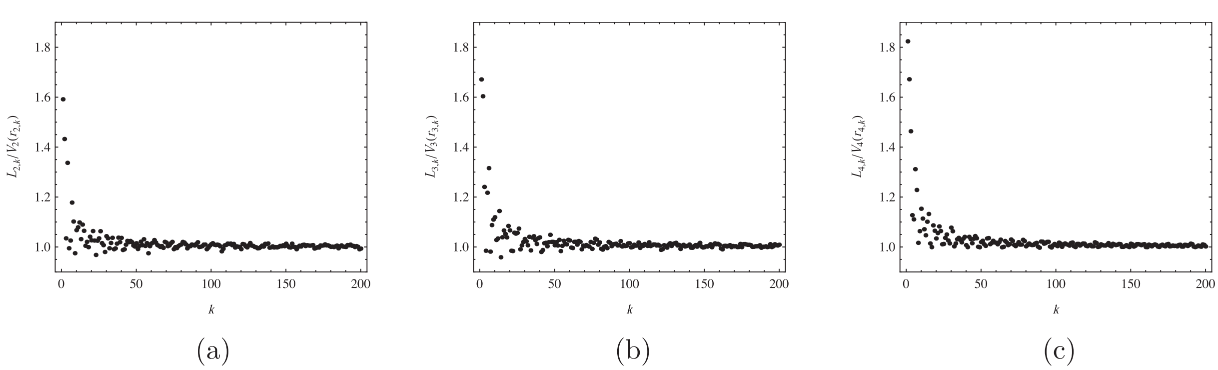

Fig. 3. Plots of $L_{n,k}/V_n(r_{n,k})$ versus k for $k = 1$ through 200 ((a) $n = 2$, (b) $n = 3$, (c) $n = 4$).

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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References

Andrews, G.E., 2015. Number Theory. Dover Publications, New York.
Arkhipova, L.G., 2008. Number of lattice points in a sphere. Moscow Univ. Math. Bull. 63 (5), 214–215.
Berndt, B.C., Kim, S., Zaharescu, A., 2018. The circle problem of Gauss and the divisor problem of Dirichlet - still unsolved. Am. Math. Mon. 125 (2), 99–114.
Callister Jr., W.D., 2001. Foundations of Materials Science and Engineering. John Wiley & Sons Inc, New York.
Daw, M.S., Baskes, M.I., 1984. Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. Phys. Rev. B 29, 6443–6453.
Duan, L., Liu, Y., 2020. Relationships between elastic constants and EAM/FS potential functions for cubic crystals. Acta Metall. Sin. 56 (1), 112–118.
Duan, L., Liu, Y., Duan, J., 2020. Calculation of radii and atom numbers of different coordination shells in cubic crystals. Mater. Today Commun. 22, 100768.
Feng, K.Q., 2011. Quadratic Sum. Harbin Institute of Technology, Harbin.
Finnis, M.W., Sinclair, J.E., 1984. A simple empirical N-body potential for transition metals. Philos. Mag. A 50, 45–55.
Fomenko, O.M., 2014. Lattice points in the circle and sphere. J. Math. Sci. 200 (5), 632–645.
Fraser, W., Gotlieb, C.C., 1962. A calculation of the number of lattice points in the circle and sphere. Math. Comp. 16, 282–290.
Grosswald, E., 1985. Representations of Integers as Sums of Squares. Springer, New York, NY.
Hardy, G.H., Landau, E., 1924. The lattice points of a circle. Proc. Royal Soc. London A 105 (731), 244–258.
Kittel, C., 2005. Introduction to Solid State Physics. John Wiley & Sons Inc, Hoboken, NJ.
Maehara, H., Martini, H., 2018. Elementary geometry on the integer lattice. Aequat. Math. 92, 763–800.
Micciancio, D., 2011. The geometry of lattice cryptography. In: Aldini, A., Gorrieri, R. (Eds.), Foundations of Security Analysis and Design VI. Springer, Berlin/Heidelberg, pp. 185–210.
Mirjalili, M., Vahdati-Khaki, J., 2008. Prediction of nanoparticles' size-dependent melting temperature using mean coordination number concept. J. Phys. Chem. Solids 69, 2116–2123.
Mittemeijer, E.J., 2010. Fundamentals of Materials Science. Springer-Verlag, Berlin.
Olver, F.W.J., Lozier, D.W., Boisvert, R.F., Clark, C.W., 2010. NIST Handbook of Mathematical Functions. Cambridge University Press, New York.
Peresypkina, E.V., Blatov, V.A., 1999. Molecular coordination numbers and crystal structure of simple substances. J. Mol. Struc.-Theochem 489, 225–236.
Peresypkina, E.V., Blatov, V.A., 2000. Molecular coordination numbers in crystal structures of organic compounds. Acta Cryst. B 56, 501–511.
Travaglini, G., 2015. Number Theory, Fourier Analysis and Geometric Discrepancy. Cambridge University Press, London.
Wang, J., Hu, P., Liu, B., Jin, X., Kong, Y., Gao, J., Wang, D., Wang, B., Xu, R., Zhang, X., 2010. Investigation on coordination number and geometrical conformation of rare earth complexes with catenulate aminopolycarboxylic acid ligands. J. Coord. Chem. 63 (13), 2193–2222.
Wang, X., Xu, G., Wang, M., Meng, X., 2016. Mathematical foundations of public key cryptography. CRC Press, Boca Raton, FL.