Rod-packing arrangements of invariant tori in solenoidal vector fields with cubic symmetries

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Abstract
The arrangements of invariant tori that resemble rod packings with cubic symmetries are considered in three-dimensional solenoidal vector fields. To find them systematically, vector fields whose components are represented in the form of multiple Fourier series with finite terms are classified using magnetic groups. The maximal magnetic group compatible with each arrangement is specified on the assumption that the cores of the nested invariant tori are straight and located on the lines corresponding to the central axes of the rods packed. Desired rod-packing arrangements are demonstrated by selecting vector fields whose magnetic groups are the maximal ones and by drawing their integral curves that twine around invariant tori. In the demonstration of chiral arrangements, Beltrami flows (or force-free fields in plasma physics), which have the strongest chirality of all solenoidal vector fields satisfying the same vector Helmholtz equation, are used. As by-products, several chain-like arrangements of closed invariant tori were found. One of the chains consists of knotted invariant tori. In all vector fields (chiral or achiral) selected for the demonstration, the volume percentages of ordered regions formed by invariant tori in a unit cell were roughly measured with the aid of a supervised machine learning technique.

Keywords Rod packing · Cubic symmetry · Invariant torus · Solenoidal vector field · Beltrami flow · Magnetic group

Mathematics subject classification 37C10 · 37J15 · 82D25
Introduction

The problem of sphere packings has a long history since Kepler [1] mentioned it in 1611 after becoming aware of the work of T. Harriot (see [2] for the history and the proof of the so-called Kepler conjecture on dense sphere packings). By contrast, the problem of rod (or cylinder) packings is much newer. The pioneering work of O’Keeffe and Andersson [3] in inorganic chemistry was published in 1977. Recently, rod packings have attracted the interest of chemists in the design of materials such as metal–organic frameworks or covalent organic frameworks [4, 5]. The rod-packing problem was generalised by assuming that rods are not necessarily straight but may be zigzagged, curved or tangled [5, 6].
Fig. 3  The $\Omega$ rod packing. Left: $^+\Omega$ rod packing. Right: $^-\Omega$ rod packing

Fig. 4  The $\Pi^*$ rod packing (in eight unit cells)

Fig. 5  The $\Sigma^*$ rod packing

Fig. 6  The $\Gamma$ rod packing
Various rod packings exist even when only considering those with cubic symmetries [7]. However, if we restrict ourselves to invariant cubic rod packings, then the number of packings is six (or nine if a pair of enantiomorphs is counted as two). Here, an invariant cubic rod packing means a packing in which the axes of rods coincide with the rotation or screw rotation axes (with or without inversion centres) specified in a cubic space group. The six (or nine) packings were named $\Pi$, $\Sigma$, $\Omega$, $+\Pi$, $-\Pi$, $+\Sigma$, $-\Sigma$, $+\Omega$, $-\Omega$, $\Pi^*$, $\Sigma^*$ and $\Gamma$ in [8] (see also [5, Fig. 16]), and their rods are arranged as shown in Figs. 1, 2, 3, 4, 5, and 6. Here, the signs $\pm$ distinguish enantiomorphs, and the sign $*$ indicates the union of the enantiomorphs.

O’Keeffe [9] referred to the $\Pi$ and $\Pi^*$ packings as $\beta$-Mn and $\beta$-W packings, respectively, because they are convenient for describing the crystal structures of $\beta$-manganese and $\beta$-tungsten. For the same reason, the $\Sigma$, $\Sigma^*$ and $\Gamma$ packings (except $\Omega$) were referred to as the SrSi$_2$, $\gamma$-Si and garnet packings, respectively. The $\Pi$ and $\Pi^*$ packings also arise in blue phases I and II, respectively, of cholesteric liquid crystals. They were theoretically proposed in the 1980s [10, 11] and experimentally observed approximately 30 years later [12]. The rods in the blue phases are called double-twist cylinders. Each double-twist cylinder consists of a nested set of coaxial cylindrical surfaces around which liquid crystalline molecules wrap helically (see e.g. [13, 14]).

Intriguingly, a figure similar to that in Fig. 1 was presented in a fluid mechanics paper [15], which investigated the structure of integral curves (or streamlines) of the Arnold–Beltrami–Childress (ABC) flow

$$U(x, y, z) = A \begin{pmatrix} \sin z \\ \cos z \\ 0 \end{pmatrix} + B \begin{pmatrix} 0 \\ \sin x \\ \cos x \end{pmatrix} + C \begin{pmatrix} \cos y \\ 0 \\ \sin y \end{pmatrix}$$

with arbitrary real constants $A$, $B$ and $C$. The figure [15, Fig. 4] sketched the arrangement of tubes, consisting of nested tubelike surfaces helically wound around by integral curves of $U$ with $ABC \neq 0$. In studies of dynamical systems, such a tubelike surface is referred to as an invariant torus [16, 17]. When $|A| = |B| = |C| \neq 0$, the ABC flow $U$ acquires cubic symmetry. Figure 7a shows a family of its invariant tori, which were called principal vortices in [15]. Apart from their undulations, they are arranged similarly to the rods in the $-\Pi$ packing in Fig. 1. Each invariant torus in Fig. 7a is depicted by numerically calculating the integral of $U$:

$$r(t) = \begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix} = r_0 + \int_0^t U(r(s)) ds,$$

which is the solution to the dynamical system

$$\frac{dr}{dt} = U(r), \quad r(0) = r_0.$$
and plotting the curve of \( r(t) \) modulo the unit cell \([\pi/2, 5\pi/2]^3\). The flow \( \mathbf{U} \) with \( |A| = |B| = |C| \neq 0 \) also has invariant tori of another family, which were called secondary vortices in [15]. Two of these are shown in Fig. 7b, in which an eight times larger cell is used to clearly show that the two tori form a double helix\(^1\) along a rod in the \( ^+\Sigma \) packing. Hereafter, for brevity, we refer to the arrangement of invariant tori along the rods in the \( ^+\Pi \) packing, etc. as the \( ^+\Pi \) arrangement, etc.

In general, invariant tori in three dimensions arise in the integration of solenoidal (i.e. volume-preserving) vector fields. Indeed, \( \mathbf{U} \) satisfies \( \text{div} \mathbf{U} = 0 \). If an initial point is chosen outside the invariant tori (and moreover, it is neither a zero of the vector field nor located on a heteroclinic trajectory connecting two zeros), then the integral curve chaotically wanders without belonging to any invariant torus, as shown for \( \mathbf{U} \) in Fig. 8.\(^2\) In other words, space is divided into an ordered part with invariant tori and a chaotic part with chaotic integral curves. The former and the latter are sometimes called “islands” and a “sea”, respectively, by their appearances on the Poincaré section (e.g. [18, p. 427]). For example, \( \mathbf{U} \) with \( ABC = 0 \) is analytically integrable (see [15]), and there exists no “sea”. By contrast, in \( \mathbf{U} \) with \( |A| = |B| = |C| \neq 0 \), the volume percentages of the above mentioned \( ^-\Pi \)- and \( ^+\Sigma \)-arranged ordered regions and the chaotic region per unit cell are estimated to be 87.5%, 5.6% and 6.9%, respectively, using the method explained in Sect. 2. In every vector field investigated in this study, a nonzero percentage of a unit cell is chaotic. We should note that chaos in solenoidal vector fields is different from chaos in

\[^1\] This is not a triple helix although located along a 3\(_1\) screw axis.

\[^2\] Figure 8 is to show that the integral curve is chaotic and does not lie on any surface. The numerical drawing of a chaotic integral curve outside the invariant tori is error-prone, and the larger \( t \) becomes, the less accurate the drawn curve.
non-solenoidal vector fields such as Lorenz’s volume-contracting flow, which is well known for its chaos attractor.

In the late 1980s, a research group in the Soviet Union, e.g. [19, 20], investigated nearly two-dimensional solenoidal vector fields that have crystal or quasicrystal structures. Because each of these vector fields is not integrable but nearly integrable, its chaotic integral curves are confined in a thin region, which was called a stochastic web. The cross section of this thin region shows a periodic or quasiperiodic pattern. By contrast, in a fully three-dimensional solenoidal vector field without integrability, like ours, the chaotic region is not usually thin and its complement, the ordered region with invariant tori, is easier to study.

Noticing the resemblance between the Π arrangements of invariant tori in U and of double-twist cylinders in blue phase I, we [21] derived three solenoidal fluid flows associated with cubic space groups that had been used in studies of blue phases. The flows were shown to have Γ-, ω- and π*-arranged invariant tori [21, Figs. 4, 8 and 11], although the connection with the rod packings was not mentioned. In addition, the first flow has +Σ*-arranged invariant tori, as well [21, Fig. 7a]. We [22] extended our study to solenoidal fluid flows with hexagonal symmetries and reported that there exist various arrangements of invariant tori, two of which resemble the Λ and Δ rod packings (see [5, Fig. 16] for these hexagonal packings).

One of the aims of this study is to investigate the type of solenoidal vector field (not restricted to fluid flow) having invariant tori whose arrangement resembles each of the six (or nine) cubic rod packings. For simplicity, we focus on the cases in which the cores of nested invariant tori are straight and located on the same lines as the central axes of the rods. Following the procedure used in [22], we apply magnetic groups to vector fields\(^3\) \(v_{klm} = (u, v, w)\) such that each of \(u, v\) and \(w\) is written in the form of multiple Fourier series with at most 48 (= 3! \cdot 8) terms:

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\(^3\) In this paper, the \(x, y\) and \(z\) components of a vector field are written in text style \((\cdot, \cdot, \cdot)\) as well as in a column vector.
Here, \( a_{pqri} (i = 1, 2, \ldots, 8) \) are constants, \( k, l \) and \( m \) are non-negative integers such that \((k, l, m) \neq (0, 0, 0)\) and \((k/n, l/n, m/n) \notin \mathbb{Z}^3\) for any integer \( n \geq 2 \), and \( P(k, l, m) \) is the set of all permutations of \((k, l, m)\). We will restrict the coefficients \( a_{pqri} \) by specifying the magnetic group of \( \mathbf{V}_{klm} \), and clarify which magnetic group is compatible with each rod-packing arrangement of invariant tori with straight cores.

The other aim of this study is to demonstrate the desired arrangements of invariant tori. Unlike rods in the rod packings, two interlaced sets of nested invariant tori cannot touch because of the uniqueness of the integral curve to a given initial point, and their gap is filled with chaotic integral curves (in the “sea” of chaos). Moreover, even if the cores of invariant tori are straight, the shapes and sizes of the cross sections of off-core invariant tori are nonconstant. Therefore, the volume percentage of invariant tori in each rod-packing arrangement is different from (generally, lower than) the percentage of rods packed. We will show how different they are in each vector field used as an example.

When \( \mathbf{V}_{klm} \) is solenoidal, we write it as \( \mathbf{V}_{klm,S} \). Because every \( \mathbf{V}_{klm} \) has the \( x, y \) and \( z \) components in the form (1) and satisfies the vector Helmholtz equation

\[
- \nabla^2 \mathbf{V}_{klm} = \kappa^2 \mathbf{V}_{klm}
\]

with

\[
\kappa = \sqrt{k^2 + l^2 + m^2},
\]

the solenoidal field \( \mathbf{V}_{klm,S} \) is also a solution to (2). Consequently, the vector field \( \mathbf{v} \) defined as \( \mathbf{v} = \mathbf{V}_{klm,S} \exp(\imath \kappa c_0 t) \) with a constant \( c_0 > 0 \) satisfies the vector wave equation

\[
\frac{1}{c_0^2} \frac{\partial^2 \mathbf{v}}{\partial t^2} = \nabla^2 \mathbf{v}
\]

as well as the equation \( \text{div} \mathbf{v} = 0 \). This means that \( \mathbf{v} \) can be realised in an electric or a magnetic field by superposing monochromatic electromagnetic waves. Therefore, the study of the arrangements of invariant tori has the potential to be useful in materials science. For example, if we can orientate rod-like molecules along the electric or magnetic force lines and somehow maintain their orientation, then the construction of crystals with artificial double-twist cylinders will be possible.
As vector fields with chirality, we define $\mathbf{V}_{klm,LB}$ and $\mathbf{V}_{klm,RB}$ by restricting the constants $a_{pqri}$ of $\mathbf{V}_{klm}$ in (1) so that

$$\text{rot } \mathbf{V}_{klm,LB} = \kappa \mathbf{V}_{klm,LB} \quad \text{and} \quad \text{rot } \mathbf{V}_{klm,RB} = -\kappa \mathbf{V}_{klm,RB},$$

(4)

respectively, are satisfied. These are special cases of $\mathbf{V}_{klm,S}$ (indeed, $\text{div } \mathbf{V}_{klm,LB} = \kappa^{-1} \text{div rot } \mathbf{V}_{klm,LB} = 0$ etc.). The ABC flow $\mathbf{U}$ is an example of $\mathbf{V}_{001,LB}$. The labels LB and RB represent the left- and right-handed Beltrami flows, respectively. In general, a solenoidal vector field $\mathbf{B}$ that parallels nontrivial rot $\mathbf{B}$ is called a Beltrami flow (or a force-free field in plasma physics). At the point where the ratio of rot $\mathbf{B}$ to $\mathbf{B}$ is positive (resp. negative), $\mathbf{B}$ locally twists like a left-handed (resp. right-handed) helix. Indeed, the simplest Beltrami flows $\mathbf{u}_{LB} = (\sin \kappa_0 z, \cos \kappa_0 z, 0)$ ($= \kappa_0^{-1} \text{rot } \mathbf{u}_{LB}$) and $\mathbf{u}_{RB} = (\cos \kappa_0 z, \sin \kappa_0 z, 0)$ ($= -\kappa_0^{-1} \text{rot } \mathbf{u}_{RB}$) with a positive constant $\kappa_0$ twist left- and right-handed helically, respectively, at all points. See [23] for details on the local geometry of Beltrami flows.

Because every $\mathbf{V}_{klm,S}$ is a solution to (2), it also satisfies

$$\text{rot rot } \mathbf{V}_{klm,S} = \kappa^2 \mathbf{V}_{klm,S}.$$

Using this fact, we can verify that an arbitrary non-Beltrami field $\mathbf{V}_{klm,S}$ is represented by the sum of

$$\frac{1}{2} (1 + \kappa^{-1} \text{rot}) \mathbf{V}_{klm,S} \quad \text{and} \quad \frac{1}{2} (1 - \kappa^{-1} \text{rot}) \mathbf{V}_{klm,S},$$

and these two fields are left- and right-handed Beltrami flows, respectively (as shown by calculating their curls). See [24], in which the same fact was mentioned in terms of the Fourier series. The decomposition of $\mathbf{V}_{klm,S}$ into $\mathbf{V}_{klm,LB}$ and $\mathbf{V}_{klm,RB}$ is analogous to the decomposition of linearly or elliptically polarised light into left- and right-handed circularly polarised light. For this reason, we can regard $\mathbf{V}_{klm,LB}$ and $\mathbf{V}_{klm,RB}$ to have the strongest left- and right-handed chirality, respectively, of all $\mathbf{V}_{klm,S}$. A remarkable difference between $\mathbf{V}_{klm,LB}$ and $\mathbf{V}_{klm,RB}$ appears in their integral curves, which wind around invariant tori (if existing) helically right- and left-handed, respectively, with the handedness opposite to that mentioned above (see Fig. 9). As in our previous papers [21, 22], we will mainly use $\mathbf{V}_{klm,RB}$, rather than $\mathbf{V}_{klm,LB}$, for chiral arrangements of invariant tori. For achiral arrangements, we will use $\mathbf{V}_{klm,S}$, which are represented with both $\mathbf{V}_{klm,LB}$ and $\mathbf{V}_{klm,RB}$ (as it were, analogously to racemic bodies in chemistry). In the achiral arrangements, the type of invariant torus in Fig. 9 and its mirror image coexist.

To integrate vector fields and draw their integral curves as in Fig. 7 or Fig. 8, we used the command “NDSolve” in the software Mathematica. To estimate the volume percentages of ordered or chaotic regions, we applied the machine learning command “Classify” (with the option “Method” designated as “LogisticRegression”) to a huge quantity of figures showing integral curves whose initial points are equally distributed in a unit cell. After that, we counted the figures of curves in each region by the command “Count”, considering their ratio to all figures to approximate the volume percentage of the region. In Sect. 2, details of how to find the rod-packing arrangements of invariant tori are explained after
introducing magnetic groups. In Sect. 3, the Π and Σ arrangements are considered using some magnetic groups of the I4132 family. In Sect. 4, the Σ* arrangement is found in a vector field whose magnetic group belongs to the Ia3d family, which is the superfamily of the I4132 family. In Sect. 5, a magnetic group of the Ia3 family is used for the Π̂ arrangement. In addition to this achiral Π̂ arrangement, a chiral Π̂ arrangement is found using a magnetic group of the I4132 family in Sect. 5, as well. The I4132 family is also applied to the Γ arrangement in Sect. 6. The Ω arrangement is treated with a magnetic group of the I432 family in Sect. 7. Lastly, in Sect. 8, the results of this study are summarised and discussed.

2 Preliminaries

2.1 Magnetic groups

As demonstrated in [22], magnetic groups are convenient to derive vector fields whose sets of integral curves have desired symmetries. In the three-dimensional case, there are 230, 230 and 1191 magnetic groups of the first, second and third types, respectively [25]. Each of the third-type magnetic groups consists of isometry transformations \{S | σ\} and \{T | τ\}' (with S, T ∈ O(3) and σ, τ ∈ \mathbb{R}^3) that map r to Sr + σ and Tr + τ, and work as symmetry and antisymmetry operations, respectively, of an axial vector field W:

\[
W(\{S | σ\} r) = (\det S)SW(r), \quad W(\{T | τ\}' r) = -(\det T)TW(r). \tag{5}
\]

By contrast, each first-type magnetic group consists of symmetry operations \{S | σ\} only, and is denoted by the same international symbol with a space group. Attention is required when a first- or third-type magnetic group is applied to a polar vector field. Because the symmetry and antisymmetry operations of a polar vector field are defined by (5) with the factors det S and det T removed, every element \{S | σ\} with det S = −1 (resp. \{T | τ\}' with det T = −1) of the magnetic group works as an antisymmetry (resp. a symmetry) operation of the polar vector field. In this study, all vectors are assumed to be axial so that we can use first- or third-type magnetic groups without such attention. If W is equated with −W, like a director field in liquid crystals, then its magnetic group is a second-type group, which is the direct product of a space group by the two-order group \{1, 1'\} with the operation 1' (W → −W), and contains both \{S | σ\} and \{S | σ\}'. For an element \{S | σ\} or \{T | τ\}' of a magnetic group (of any type), the point \{S | σ\} r or \{T | τ\}' r is called an equivalent point to r (in the magnetic group).

Each of the total 1651 magnetic groups was numbered in the form a.b.c by Litvin [26]. Here, a (= 1, 2, …, 230) is the international number of the associated space group, b (= 1, 2, 3, …) classifies the magnetic groups with the same a, and c (= 1, 2, …, 1651) is a serial number. The first- and second-type magnetic groups have b = 1 and 2, respectively, whereas the third-type groups have b ≥ 3. We denote V_{klm} with (1) whose magnetic group number is a.b.c by V_{klm}^{(a,b)} (without using c). In the same way, V_{klm, S}, V_{klm, LB} and V_{klm, RB} are written as V_{klm, S}^{(a,b)}, V_{klm, LB}^{(a,b)} and V_{klm, RB}^{(a,b)}.
respectively. The ABC flow $U$ with $|A| = |B| = |C| \neq 0$ is an example of $V^{(214.4)}_{001,1,LB}$ because its magnetic group $I_{p}A_{1},32$ is numbered as 214.4.1570 in [26].

### 2.2 Process

The rod-packing arrangements of invariant tori are found according to the following process:

1. Let $G$ be the following space group (or a cubic subgroup$^4$ of it when returned from step 7): $I_{4_{1}},32$ (No. 214) for $\Pi$ and $\Sigma$; $I_{432}$ (No. 211) for $\Omega$; $Pm\bar{3}n$ (No. 223) or $Ia\bar{3}d$ (No. 230) for $\Pi^{*}$; $Ia\bar{3}d$ for $\Sigma^{*}$ and $\Gamma$.
2. Select a magnetic group numbered in [26] as $a.b.c$, where $a$ is the international number of $G$ and $b \neq 2$. Denote the magnetic group by $G$.
3. Restrict $a_{pqri}$ in (1) so that $V_{klm} = (u, v, w)$ becomes $V_{klm}^{(a,b)}$, using equivalent points to $(x, y, z)$, especially those yielded by the “generators selected” of $G$ in [26]. Because the coordinates of the equivalent points were listed modulo 1 in [26], convert them into those modulo $2\pi$.
4. Restrict $a_{pqri}$ further so that $V_{klm}^{(a,b)}$ becomes $V_{klm,S}^{(a,b)}$ (if $G$ is an achiral space group) or $V_{klm,RB}^{(a,b)}$ (if $G$ is chiral).
5. Define $W$ by $V_{klm,S}^{(a,b)}$ or $V_{klm,RB}^{(a,b)}$, obtained in step 4, or a linear combination of vector fields with the same $(a,b)$ and the same label (S or RB) but different $\kappa$ of (3), such as $V_{klm,S}^{(a,b)} + \lambda' V_{k'p'm',S}^{(a,b)} + \cdots + \lambda'' V_{k''p''m'',S}^{(a,b)}$ with constants $\lambda', \lambda''$ etc. In the last case, a linear combination whose $\sqrt{k^2 + l^2 + m^2}$, $\sqrt{k'^2 + l'^2 + m'^2}$ etc. have rational ratio is preferable from a physical viewpoint (e.g. in electromagnetic waves mentioned in Sect. 1).

$^4$ Cubic subgroups (except those of $I_{432}$) are listed in [9, Table 1].
6. Specify all constants contained in $\mathbf{W}$. If the cores of invariant tori are required to be straight, give appropriate values to the constants so that the orthogonal component of $\mathbf{W}$ is zero on the line corresponding to the central axis of a rod in the rod packing.

7. Find an initial point $\mathbf{r}_0$ such that the integral curve of $\mathbf{W}$, i.e. the solution curve $\mathbf{r}(t)$ of

$$\frac{d\mathbf{r}}{dt} = \mathbf{W}(\mathbf{r})$$

with $\mathbf{r}(0) = \mathbf{r}_0$, winds around an invariant torus when numerically drawn modulo a unit cell until an appropriately given upper bound $t = t_{\text{max}}$. If a desired invariant torus cannot be found, return to step 6 and resppecify the constants, or start again from step 2 with another $\mathcal{G}$. If no desired invariant torus is found for any $\mathcal{G}$ of the same $a$, return to step 1.

8. Draw all the other invariant tori by taking equivalent points to $\mathbf{r}_0$ as new initial points in step 7.

We should note that, if (5) is satisfied, then (6) with $\mathbf{r}$ replaced by $\{\mathbf{S} | \sigma\} \mathbf{r}$ and by $\{\mathbf{T} | \tau\}' \mathbf{r}$ yield

$$\frac{d\mathbf{r}}{dt} = (\det \mathbf{S}) \mathbf{W}(\mathbf{r}) \quad \text{and} \quad \frac{d\mathbf{r}}{dt} = -(\det \mathbf{T}) \mathbf{W}(\mathbf{r}),$$

respectively. Because $|\det \mathbf{S}| = |\det \mathbf{T}| = 1$, and the integral curve $\mathbf{r}(t)$ ($-\infty < t < \infty$) of $\mathbf{W}$ is the same as of $-\mathbf{W}$ (if the same $\mathbf{r}(0)$ is given), both $\{\mathbf{S} | \sigma\}$ and $\{\mathbf{T} | \tau\}'$ preserve the set of all integral curves of $\mathbf{W}$. Moreover, $\{\mathbf{T} | \tau\}$ also preserves the set. Therefore, the space group of the set is $\mathcal{G}$, which is obtained by changing all antisymmetry operations to symmetry operations (as $\{\mathbf{T} | \tau\}'$ to $\{\mathbf{T} | \tau\}$) in $\mathcal{G}$. This is why the above process works.

Assume that the cores of invariant tori are straight and one of them coincides with the line $\mathbf{r} = \mathbf{p} + s\mathbf{q}$, where $\mathbf{p} \in \mathbb{R}^3$ is a fixed position vector, $s \in \mathbb{R}$ is a parameter and $\mathbf{q}$ is the direction vector defined as

$$\mathbf{q} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \text{for the } \Pi \text{ or } \Pi^* \text{ arrangement;}$$

$$\mathbf{q} = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} \quad \text{for the } \Sigma, \Omega, \Sigma^* \text{ or } \Gamma \text{ arrangement.}$$

Then, we notice that

$$\mathbf{W} \neq \mathbf{0} \text{ and } \mathbf{q} \parallel \mathbf{W} \text{ everywhere on the line } \mathbf{r} = \mathbf{p} + s\mathbf{q}$$

(7)
(see Fig. 9). In other words, if \( \mathbf{V}^{(a,b)}_{klm} \) obtained in step 3 satisfies

\[
\mathbf{q} \cdot \mathbf{V}^{(a,b)}_{klm} (\mathbf{p} + s_\ast \mathbf{q}) = 0 \quad \text{with a constant } s_\ast \text{ for all possible } (k, l, m) \tag{8}
\]

or

\[
\int_{0}^{2\pi} \mathbf{q} \cdot \mathbf{V}^{(a,b)}_{klm} (\mathbf{p} + s \mathbf{q}) \, ds = 0 \quad \text{for all possible } (k, l, m), \tag{9}
\]

then every \( \mathbf{W} \) in step 6 that satisfies \(|\mathbf{q} \times \mathbf{W}(\mathbf{p} + s \mathbf{q})| = 0 \) for all \( s \) also satisfies \( \mathbf{q} \cdot \mathbf{W}(\mathbf{p} + s \mathbf{q}) = 0 \) for some \( s \), meaning (7) is impossible; thus, the line \( \mathbf{r} = \mathbf{p} + s \mathbf{q} \) cannot become a core of invariant tori. Using (8) or (9) as a sufficient condition for the nonexistence of invariant tori with straight cores, we can judge whether the selection of \( \widetilde{\mathbf{G}} \) in step 2 is inappropriate or not. Also, using the negation of (8) or (9) as a necessary condition for the existence of the desired invariant tori, we can judge whether \( \widetilde{\mathbf{G}} \) is worth investigating.

In this study, body-centred cubic space groups are used as \( \mathbf{G} \). In such a body-centred cubic case, the volume percentage of an ordered region with invariant tori or of a chaotic region is roughly measured by the following simple method:

i. Make \( 4N^3 \) figures of integral curves starting from the equally distributed initial points \( \mathbf{r}_0 = (n_x - \epsilon_x, n_y - \epsilon_y, n_z - \epsilon_z)\pi/N \). Here, \( n_x \) and \( n_y \) are integers from 1 to 2\( N \), whereas \( n_z \) is an integer from 1 to \( N \). The small constants \( \epsilon_x, \epsilon_y \) and \( \epsilon_z \) are for deviating \( \mathbf{r}_0 \) from the symmetry axes or planes on which zeros or heteroclinic trajectories are located. We set \( N = 20 \), \( \epsilon_x = 0.1 \), \( \epsilon_y = 0.2 \) and \( \epsilon_z = 0.3 \), i.e.

\[
\mathbf{r}_0 = \left( \frac{n_x - 0.1}{20} \pi, \frac{n_y - 0.2}{20} \pi, \frac{n_z - 0.3}{20} \pi \right). \tag{10}
\]

ii. Count the figures with integral curves winding around invariant tori of the same family or the figures with chaotic integral curves. If the number is \( M \), then \( M/(4N^3) \) is an approximate value of the volume fraction of the ordered or chaotic region. Because \( 4N^3 \) is a huge number when \( N = 20 \), we classified all the \( 4N^3 \) figures into several categories according to (dis)orderedness or the shapes of invariant tori by a supervised machine learning technique (and personally corrected misclassifications) before counting.

The reason for taking \( 4N^3 \) initial points, not \((2N)^3\), in step i is that the unit cube \([0, 2\pi]^3\) has twice the volume of a primitive unit parallelepiped when \( \mathbf{G} \) is body-centred cubic.
3 The $\Pi$ and $\Sigma$ arrangements

3.1 General forms of $V_{klm}^{(214,b)}$ and $V_{klm, RB}^{(214,b)}$

When $I4_132$ is taken as the space group $G$ in the process in Sect. 2.2, the magnetic group $\tilde{G}$ in step 2 is one of the $I4_132$ family: $I4_132$ (No. 214.1.1567), $I4_132'$ (No. 214.3.1569), $I_{p4}4_3$2 (No. 214.4.1570) and $I_{p4}4_32'$ (No. 214.5.1571). In the appropriate setting of the origin and the $x$, $y$ and $z$ axes, the conditions for $V_{klm} = (u, v, w)$ to be $V_{klm}^{(214,b)} (b = 1, 3, 4, 5)$ in step 3 are

$$V_{klm}(-x + \pi, -y, z + \pi) = (-u(x, y, z), -v(x, y, z), w(x, y, z)), \quad (11)$$

$$V_{klm}^b(y + \pi/2, x + 3\pi/2, -z + 3\pi/2)$$

$$\begin{cases} 
(v(x, y, z), u(x, y, z), -w(x, y, z)) & \text{for } b = 1 \text{ or } 4, \\
(-v(x, y, z), -u(x, y, z), w(x, y, z)) & \text{for } b = 3 \text{ or } 5,
\end{cases} \quad (12)$$

$$V_{klm}(x + \pi, y + \pi, z + \pi) = \begin{cases} 
V_{klm}^b(x, y, z) & \text{for } b = 1 \text{ or } 3, \\
-V_{klm}^b(x, y, z) & \text{for } b = 4 \text{ or } 5.
\end{cases} \quad (13)$$

Here, $-x + \pi, -y, z + \pi$ and $(y + \pi/2, x + 3\pi/2, -z + 3\pi/2)$ are the equivalent points to $(x, y, z)$ yielded by Nos. 2 and 13 of the “generators selected” of each magnetic group in [26], whereas $(x + \pi, y + \pi, z + \pi)$ is yielded by $i(1/2, 1/2, 1/2)$ or $i'(1/2, 1/2, 1/2)$ of the generators. Due to the forms of $v$ and $w$ in (1), the equivalent points yielded by Nos. 3 and 5 of the generators are not necessary. We should note that, if all of $k$, $l$ and $m$ are odd, then cubic $V_{klm}$ has the face-centred structure: $V_{klm}(x + \pi, y + \pi, z) = V_{klm}(x, y, z)$, and its magnetic group is not of the $I4_132$ family. Moreover, because (1) has the same form even if $k$, $l$ and $m$ are permuted, $k$ and $m$ can be assumed to be even and odd, respectively, without generality loss. On this assumption, we introduce the following four cases:

$$[k \equiv 0 \text{ and } l \equiv m(\equiv 1 \text{ or } 3) \text{ mod } 4] \text{ or } [k \equiv 2, l \equiv 1 \text{ and } m \equiv 3 \text{ mod } 4], \quad (14)$$

$$[k \equiv 0, l \equiv 1 \text{ and } m \equiv 3 \text{ mod } 4] \text{ or } [k \equiv 2 \text{ and } l \equiv m(\equiv 1 \text{ or } 3) \text{ mod } 4], \quad (15)$$

$$[k \equiv l(\equiv 0 \text{ or } 2) \text{ and } m \equiv 1 \text{ mod } 4] \text{ or } [k \equiv 0, l \equiv 2 \text{ and } m \equiv 3 \text{ mod } 4], \quad (16)$$

$$[k \equiv 0, l \equiv 2 \text{ and } m \equiv 1 \text{ mod } 4] \text{ or } [k \equiv l(\equiv 0 \text{ or } 2) \text{ and } m \equiv 3 \text{ mod } 4]. \quad (17)$$

Additionally, $l \leq m$ if $l \equiv m$ (mod 4) and $k \leq l$ if $k \equiv l$ (mod 4) are assumed. The general forms of the $x$ components $u$ of $V_{klm}^{(214,b)} (b = 1, 3, 4, 5)$ are tabulated in Table 1. In the table, the following are referred to:
\[ u = c_1 (\cos kx \cos ly \sin mz \mp \cos kx \cos my \sin lz) \]
\[ + c_2 (\sin kx \sin ly \cos mz \pm \sin kx \sin my \cos lz) \]
\[ + c_3 (\cos lx \cos my \cos kz \mp \sin lx \cos ky \sin mz) \]
\[ + c_4 (\sin lx \sin ky \sin kx \pm \cos lx \sin ky \cos mz) \]
\[ + c_5 (\cos mx \sin ky \cos lz \pm \sin mx \sin ly \sin kx) \]
\[ + c_6 (\sin mx \cos ky \sin lz \mp \cos mx \cos ly \cos kx). \]

(18)

\[ u = c_7 (\cos kx \cos ly \cos mz \mp \cos kx \sin my \sin lz) \]
\[ + c_8 (\sin kx \sin ly \sin mz \mp \sin kx \cos my \sin lz) \]
\[ + c_9 (\cos lx \sin my \cos kz \mp \cos lx \sin ky \cos mz) \]
\[ + c_{10} (\sin lx \cos my \sin kx \pm \sin lx \sin ky \sin mz) \]
\[ + c_{11} (\cos mx \cos ky \sin lz \pm \sin mx \sin ly \cos kz) \]
\[ + c_{12} (\sin mx \sin ky \cos lz \pm \cos mx \cos ly \sin kz). \]

(19)

Here, the constants \( c_i \) (\( i = 1, 2, \ldots, 12 \)) are generally nonzero, although some can vanish unless \( u \) becomes what will appear in Sect. 4.1. The conditions for \( \mathbf{V}^{(214,b)}_{klm} \) to become \( \mathbf{V}^{(214,b)}_{klm,RB} \) in step 4 of the process are also listed in Table 1 by referring to

\[ c_1 = (l^2 + m^2)\alpha, \quad c_2 = (l^2 + m^2)\beta, \quad c_3 = -mk\alpha + kl\beta, \]
\[ c_4 = k\alpha + mk\beta, \quad c_5 = -mk\alpha - l\kappa\beta, \quad c_6 = -lk\alpha - mk\beta, \]
\[ c_7 = (l^2 + m^2)\alpha, \quad c_8 = (l^2 + m^2)\beta, \quad c_9 = mk\alpha + kl\beta, \]
\[ c_{10} = k\alpha - mk\beta, \quad c_{11} = -lk\alpha + mk\beta, \quad c_{12} = mk\alpha + lk\beta. \]

(20)

(21)

Table 1: General forms of the \( x \) components of \( \mathbf{V}^{(214,b)}_{klm} \) and \( \mathbf{V}^{(214,b)}_{klm,RB} \) when the origin and the coordinate axes are appropriately set

| Vector field | Magnetic group | Case | General form of the \( x \) component | Conditions to become \( \mathbf{V}^{(214,b)}_{klm,RB} \) |
|--------------|---------------|------|--------------------------------------|---------------------------------|
| \( \mathbf{V}^{(214,1)}_{klm} \) | \( I_{4,32} \) | (14) and \( klm \neq 011 \) | (18) (upper signs) | (20) |
| \( \mathbf{V}^{(214,3)}_{klm} \) | \( I_{4',32'} \) | (15) | (18) (lower signs) | (20) |
| \( \mathbf{V}^{(214,4)}_{klm} \) | \( I_{4,4',32} \) | (16) | (19) (upper signs) | (21) and \( klm \neq 001 \) |
| \( \mathbf{V}^{(214,5)}_{klm} \) | \( I_{4',4',32'} \) | (17) | (19) (lower signs) | (21) |

The \( y \) and \( z \) components are obtained from (1)

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where \( \alpha \) and \( \beta \) are generally nonzero constants, and \( \kappa \) is from (3). In the case of (14) with \((k, l, m) = (0, 1, 1)\), excluded in Table 1, the \( x \) component (18) with the upper signs is not of \( \mathbf{V}^{(214.1)}_{klm} \) but of \( \mathbf{V}^{(230.1)}_{klm} \), which is a gradient field associated with the “gyroid” as pointed out in [21, Sect. 4.1]. In addition, (21) with \((k, l, m) = (0, 0, 1)\) is also excluded in Table 1 because \( \mathbf{V}^{(214.4)}_{klm, RB} \) becomes trivial.

We can easily show that, if \( k = 0 \) or \( k = l \) or \( l = m \), then each of \( \mathbf{V}^{(214,b)}_{klm, RB} \) \((b = 1, 3, 4, 5)\) is determined uniquely up to constant multiples. We can also show that

\[
\mathbf{V}^{(214.1)}_{klm, RB}(-x, -y, -z) = \mathbf{V}^{(214.1)}_{klm, LB}(x, y, z), \tag{22}
\]

\[
\mathbf{V}^{(214.3)}_{klm, RB}(-x, -y, -z) = \mathbf{V}^{(214.3)}_{klm, LB}(x, y, z), \tag{23}
\]

\[
\mathbf{V}^{(214.4)}_{klm, RB}(-x, -y, -z) = \mathbf{V}^{(214.5)}_{klm, LB}(x, y, z), \tag{24}
\]

\[
\mathbf{V}^{(214.5)}_{klm, RB}(-x, -y, -z) = \mathbf{V}^{(214.4)}_{klm, LB}(x, y, z), \tag{25}
\]

where \((k, l, m) \neq (0, 1, 1)\) in (22) and \((k, l, m) \neq (0, 0, 1)\) in (24).

### 3.2 The \( \Pi \) Arrangement

In the \(+\Pi\) (resp. \(-\Pi\)) rod packing, the central axes of rods coincide with the \( 4_1 \) (resp. \( 4_3 \)) screw axes in \( I4_132 \). Because one of these screw axes is represented as \((\pi/2, 0, z)\) (resp. \((3\pi/2, 0, z)\)) with any \( z \) in our coordinates (see [8, 9]), we set \( p = (\pi/2, 0, 0) \) (resp. \((3\pi/2, 0, 0)\)) and \( q = (0, 0, 1) \) in (8) or (9). The \( x \) component (18) with (14) or (15) yields

\[
w(\pi/2, 0, z) = u(z, \pi/2, 0) = c_2 \sin k z \left( \sin \frac{l \pi}{2} \pm \sin \frac{m \pi}{2} \right),
\]

\[
w(3\pi/2, 0, z) = u(z, 3\pi/2, 0) = c_2 \sin k z \left( \sin \frac{3l \pi}{2} \pm \sin \frac{3m \pi}{2} \right).
\]

They vanish at \( z = 0 \) (or for all \( z \) if \( k = 0 \)) and (8) holds for \( \mathbf{V}^{(214.1)}_{klm} \) and \( \mathbf{V}^{(214.3)}_{klm} \) (see Table 1). Therefore, the magnetic groups \( I4_132 \) and \( I4_1'32' \) are excluded from candidates for appropriate \( G \). By contrast, (19) with (16) or (17) yields

\[
w(\pi/2, 0, z) = u(z, \pi/2, 0) = c_7 \cos k z \left( \cos \frac{l \pi}{2} \mp \sin \frac{m \pi}{2} \right) + c_9 \cos l z \left( \sin \frac{m \pi}{2} \mp \cos \frac{k \pi}{2} \right).
\]

The term with \( c_7 \) is a nonzero constant and (9) does not hold when (16) (resp. (17)) with \( k = 0 \) holds and the lower (resp. upper) sign in the term is taken. In the same way, \( w(3\pi/2, 0, z) \) obtained from (19) has a term that does not vanish when (17) (resp. (16)) with \( k = 0 \) holds and the lower (resp. upper) sign is taken. Therefore,
taking Table 1 into account, we expect that linear combinations $W$ containing $V_{0l,m,\text{RB}}^{(214,5)}$ and $V_{0l,m,\text{RB}}^{(214,4)}$ have invariant tori with straight cores $+\Pi$- and $-\Pi$-arranged, respectively. Moreover, the vector fields used in a linear combination should have the same $m$. Indeed, in the $^+\Pi$ arrangement, (19) yields

$$u(\pi/2, 0, z) = \left(c_7 \cos \frac{k\pi}{2} + c_9 \cos \frac{l\pi}{2}\right) \cos mz,$$

which should be cancelled by $u(\pi/2, 0, z)$ of the other field(s) in the linear combination.

From Table 1, we obtain

\begin{itemize}
\item[(a)] Fig. 10 Invariant tori in $V_{0l,m,\text{RB}}^{(214,5)} + \frac{1}{2} V_{0l,m,\text{RB}}^{(214,5)}$ with (26) and (27). a The $^+\Pi$ arrangement. One of the initial points is (10) with $(n_x, n_y, n_z) = (12, 3, 5)$. b Chain-like arrangement of ring-shaped invariant tori. Every four rings form a (4, 4)-torus link. One of the initial points is (10) with $(n_x, n_y, n_z) = (14, 40, 20)$. c A knotted invariant torus linking to another. The knot is of type $8_{19}$ (“true-lovers’ knot”). One of the initial points is (10) with $(n_x, n_y, n_z) = (38, 1, 5)$
\end{itemize}
\[
\mathbf{V}_{001,\text{RB}}^{(214.5)} = \begin{pmatrix}
\cos z + \sin y \\
\cos x + \sin z \\
\cos y + \sin x
\end{pmatrix}
\]

(26)

when \( \alpha = 1/2 \) in (21). Because the ABC flow \( \mathbf{U} \) with \( A = B = C = 1 \), which is written as \( \mathbf{V}_{001,\text{RB}}^{(214.5)}(-x + \pi/2, -y + \pi/2, -z + \pi/2) \) or \( \mathbf{V}_{001,\text{LB}}^{(214.4)}(x - \pi/2, y - \pi/2, z - \pi/2) \) (see (25)), has undulating \((-\Pi)\)-arranged invariant tori as in Fig. 7a, an enantiomorph (26) has undulating \((\Pi)\)-arranged invariant tori. To straighten their cores, we take a linear combination \( \mathbf{W} = \mathbf{V}_{001,\text{RB}}^{(214.5)} + \lambda \mathbf{V}_{221,\text{RB}}^{(214.5)} \) in step 5 of the process in Sect. 2.2. Here, the \( \frac{1}{3} \)-wavelength field \( \mathbf{V}_{221,\text{RB}}^{(214.5)} \) is obtained from Table 1 as

\[
\mathbf{V}_{221,\text{RB}}^{(214.5)} = \begin{pmatrix}
\cos z + \sin y \\
\cos x + \sin z \\
\cos y + \sin x
\end{pmatrix},
\]

\[
\mathbf{W}(\pi/2, 0, z) = \begin{pmatrix}
(1 - 2\lambda) \cos z \\
(1 - 2\lambda) \sin z
\end{pmatrix}
\]

by setting \( 4\alpha + 2\beta = 1 \) in (21). The constant \( \lambda \) is given so that (7) holds on the \( 4_1 \) screw axes. Because the linear combination \( \mathbf{W} \) leads to

on the \( 4_1 \) screw axis \( (\pi/2, 0, z) \), we expect \((\Pi)\)-arranged invariant tori with straight cores when \( \lambda = 1/2 \). In fact, desired invariant tori are observed, as depicted in Fig. 10a. The volume percentage of the ordered region with invariant tori of this family is estimated at 7.7\%, which is much lower than the volume percentage of rods in the \((\Pi)\) or \((-\Pi)\) packing \((3\pi/32 = 29.45 \ldots \% , \text{see [7, 9]}\)).

Interestingly, a larger part of a unit cell, estimated at 21.9\%, is occupied by ring-shaped invariant tori linked like a chain in \( \mathbf{V}_{001,\text{RB}}^{(214.5)} + \frac{1}{4} \mathbf{V}_{221,\text{RB}}^{(214.5)} \). Each of the rings links with nine other rings, as shown in Fig. 10b. Moreover, every four rings linking with one another form a \((4, 4)\)-torus link, whose enantiomorph was pictured in [27, Fig. 2]. It is notable that the vector field \( \mathbf{V}_{001,\text{RB}}^{(214.5)} + \frac{1}{3} \mathbf{V}_{221,\text{RB}}^{(214.5)} \) has another chain of closed invariant tori each of which forms “true-lovers knot”, i.e. a knot of type \( 8^1 \) (see [28, Fig. 1.5]). Two of the linked knots are depicted in Fig. 10c. The chain of the knots occupies approximately 11.1\% of a unit cell.

We next show that the \((-\Pi)\) arrangement of invariant tori with straight cores is realised (not only with \( \mathbf{V}_{001,\text{RB}}^{(214.5)}(-\mathbf{r}) = \mathbf{V}_{001,\text{LB}}^{(214.4)}(\mathbf{r}) \) but also) with \( \mathbf{V}_{001,\text{LB}}^{(214.4)} \), as hypothesised at the beginning of this subsection. For this, we use \( \mathbf{V}_{021,\text{RB}}^{(214.4)} \) and \( \mathbf{V}_{041,\text{RB}}^{(214.4)} \), although the ratio of their wavelengths is not rational. They are obtained from Table 1 as

\[
\mathbf{V}_{021,\text{RB}}^{(214.4)} = \begin{pmatrix}
\cos z + \sin y \\
\cos x + \sin z \\
\cos y + \sin x
\end{pmatrix},
\]

\[
\mathbf{V}_{041,\text{RB}}^{(214.4)} = \begin{pmatrix}
\cos z + \sin y \\
\cos x + \sin z \\
\cos y + \sin x
\end{pmatrix},
\]

\[
u(x, y, z) = \begin{pmatrix}
\cos z + \sin y \\
\cos x + \sin z \\
\cos y + \sin x
\end{pmatrix} + \sqrt{5}(\cos 2y \cos z + \sin y \cos 2z) + 2\cos 2(x \sin y + \cos z) \]

\[
(28)
\]
\[
\mathbf{V}^{(214.4)}_{041, RB} = \begin{pmatrix}
 u(x, y, z) \\
 u(y, z, x) \\
 u(z, x, y)
\end{pmatrix},
\]

\[
u(x, y, z) = \sqrt{17}(\cos 4y \cos z - \sin y \cos 4z) + \cos 4x(\sin y - \cos z) - 4(\cos x \sin 4z + \sin x \sin 4y)
\]

with constant multiples appropriately set. From now on, vector fields unique up to constant multiples will be introduced with appropriate values given to the constants, which are independent of the shapes of invariant tori. Each of (28) and (29) has undulating invariant tori along the \(4_3\) screw axes. When

\[
\lambda = -\frac{\sqrt{5} - 1}{\sqrt{17} - 1} = -0.3957 \ldots,
\]

the linear combination \(\mathbf{W} = \mathbf{V}^{(214.4)}_{021, RB} + \lambda \mathbf{V}^{(214.4)}_{041, RB}\) is proven to satisfy (7) on the \(4_3\) screw axes (e.g. \((3\pi/2, 0, z)\) with any \(z\)) and expected to have \(-\Pi\)-arranged invariant tori with straight cores. Indeed, these tori are observed as shown in Fig. 11. The volume percentage of the ordered region formed by them is estimated at 5.3\%. As explained by Fig. 9 in Sect. 1, integral curves in a right-handed Beltrami flow wind around invariant tori left-handed helically. This left-handedly helical winding is confirmed in Fig. 11 as well as in Fig. 10a (cf. Fig. 7a).

### 3.3 The \(\Sigma\) arrangement

In the \(+\Sigma\) (resp. \(-\Sigma\)) rod packing, the central axes of rods coincide with the \(3_1\) (resp. \(3_2\)) screw axes in \(I4_132\), one of which is represented as \((2\pi/3 + s, 4\pi/3 + s, s)\) (resp. \((4\pi/3 + s, 2\pi/3 + s, s)\)) with any \(s\) in our coordinates (see [8, 9]). Let us show that \(I4_1'32' (a, b = 214.3)\) is the only magnetic group of the \(I4_132\) family that is compatible with \(+\Sigma\)- or \(-\Sigma\)-arranged invariant tori with straight cores. The composition of (11) and (12) yields

\[
\mathbf{V}^{(214,b)}_{klm}(-y + \pi/2, -x + \pi/2, -z + \pi/2) = \begin{cases}
 -v(x, y, z), & -u(x, y, z), \ w(x, y, z) \\
 u(x, y, z), & w(x, y, z)
\end{cases}
\]

for \(b = 1\) or \(4\),

\[
(y(x, y, z), \ u(x, y, z), \ w(x, y, z))
\]

for \(b = 3\) or \(5\).

Here, \((-y + \pi/2, -x + \pi/2, -z + \pi/2)\) corresponds to the equivalent point to \((x, y, z)\) numbered as 14 in each magnetic group of the \(I4_132\) family [26]. The scalar product of (31) by \(\mathbf{q} = (1, 1, 1)\) leads to

\[
\mathbf{q} \cdot \mathbf{V}^{(214,b)}_{klm}(-y + \pi/2, -x + \pi/2, -z + \pi/2) = \begin{cases}
 -\mathbf{q} \cdot \mathbf{V}^{(214,b)}_{klm}(x, y, z) & \text{for } b = 1 \text{ or } 4, \\
 \mathbf{q} \cdot \mathbf{V}^{(214,b)}_{klm}(x, y, z) & \text{for } b = 3 \text{ or } 5.
\end{cases}
\]

Substituting \((11\pi/12, 19\pi/12, \pi/4)\) or \((19\pi/12, 11\pi/12, \pi/4)\) for \((x, y, z)\) and using the \(2\pi\) periodicity of \(\mathbf{V}^{(214,b)}_{klm}\) in \(x\) or \(y\), we deduce that
The use of the following invariant tori in \( V_{021,\text{RB}}^{(214,4)} + \lambda V_{041,\text{RB}}^{(214,4)} \) with (28), (29) and (30). One of the initial points is (10) with \((n_x, n_y, n_z) = (29, 2, 1)\)

\[
\begin{align*}
q \cdot V_{klm}^{(214,b)}(11\pi/12, 19\pi/12, \pi/4) &= 0 \\
q \cdot V_{klm}^{(214,b)}(19\pi/12, 11\pi/12, \pi/4) &= 0
\end{align*}
\]

for \( b = 1 \) or 4.

The two points \((11\pi/12, 19\pi/12, \pi/4)\) and \((19\pi/12, 11\pi/12, \pi/4)\) are located on the \(3_1\) screw axis \((2\pi/3 + s, 4\pi/3 + s, s)\) and the \(3_2\) screw axis \((4\pi/3 + s, 2\pi/3 + s, s)\), respectively. Therefore, the case \( b = 1 \) or 4 is discarded, for (8) holds on the two axes and neither axis can be a core of invariant tori. Furthermore, the case \( b = 5 \) is also discarded, for (13) shows that (9) holds for \( V_{klm}^{(214,5)} \) on the axis \((2\pi/3 + s, 4\pi/3 + s, s)\) or \((4\pi/3 + s, 2\pi/3 + s, s)\). Then, only the case \( b = 3 \) remains.

From Table 1, we obtain

\[
V_{011,\text{RB}}^{(214,3)} = \begin{pmatrix}
\sqrt{2} \cos y \sin z - \cos x \cos y - \sin x \sin z \\
\sqrt{2} \cos z \sin x - \cos y \cos z - \sin y \sin x \\
\sqrt{2} \cos x \sin y - \cos z \cos x - \sin z \sin y
\end{pmatrix}.
\]

This has thick undulating invariant tori along the \(3_1\) screw axes, as shown in [21, Fig. 7a]. To cancel its orthogonal component on the \(3_1\) or \(3_2\) screw axes, we make use of the following \(\frac{1}{5}\)-wavelength field:

\[
V_{453,\text{RB}}^{(214,3)} = \begin{pmatrix}
u(x, y, z) \\
u(y, z, x) \\
u(z, x, y)
\end{pmatrix},
\]

\[
u(x, y, z) = 34\alpha(\cos 4x \cos 5y \sin 3z - \cos 4x \cos 3y \sin 5z)
+ 34\beta(\sin 4x \sin 5y \cos 3z + \sin 4x \sin 3y \cos 5z)
+ (-15\sqrt{2}\alpha + 20\beta) (\cos 5x \cos 3y \cos 4z - \sin 5x \cos 4y \sin 3z)
+ (20\alpha + 15\sqrt{2}\beta)(\sin 5x \sin 3y \sin 4z + \cos 5x \sin 4y \cos 3z)
+ (-12\alpha + 25\sqrt{2}\beta)(\cos 3x \sin 4y \cos 5z + \sin 3x \sin 5y \sin 4z)
+ (-25\sqrt{2}\alpha - 12\beta)(\sin 3x \cos 4y \sin 5z - \cos 3x \cos 5y \cos 4z).
\]
Note that \( V_{klm, RB}^{(214, b)} \) is not unique even up to constant multiples when \( k, l \) and \( m \) are nonzero and different from one another. The constants \( \alpha \) and \( \beta \) for which the sum of (32) and (33) has zero orthogonal component on the \( 3_1 \) screw axes are obtained by algebraic computation with Mathematica as

\[
\alpha = \frac{15\sqrt{2} (61 + 10\sqrt{6})}{2 \cdot 17 \cdot 3121} = 0.01709 \ldots , \tag{34}
\]

\[
\beta = -\frac{8428 + 3991\sqrt{6}}{2 \cdot 17 \cdot 3121} = -0.1715 \ldots .
\]

Even if these hold, \(+\Sigma\)-arranged invariant tori with straight cores are not observed. This is because \( W = V_{011, RB}^{(214, 3)} + V_{453, RB}^{(214, 3)} \) with (34) has zeros on the \( 3_1 \) screw axes and (7) is not satisfied. Then, we additionally use \( V_{011, RB}^{(214, 3)} (3x, 3y, 3z) \) as a field of period \( 2\pi \) in \( x, y \) and \( z \). Because it satisfies not only the latter of (4) with \( \kappa = \sqrt{3^2 + 3^2} \) but also (11)–(13) for \( b = 3 \), we write it as \( V_{033, RB}^{(214, 3)} (x, y, z) \), i.e.

\[
V_{033, RB}^{(214, 3)} (2\pi/3 + s, 4\pi/3 + s, s) = \left( \frac{1}{\sqrt{2}} \sin 6s - 1 \right) \left( \begin{array}{c} 1 \\ 1 \\ 1 \end{array} \right) \parallel \left( \begin{array}{c} 2\pi/3 + s \\ 4\pi/3 + s \\ s \end{array} \right).
\]

Therefore, \( \lambda \) can be selected without changing (34) so that (7) holds for \( W = V_{011, RB}^{(214, 3)} + V_{453, RB}^{(214, 3)} + \lambda V_{033, RB}^{(214, 3)} \) and \(+\Sigma\)-arranged invariant tori with straight cores are found. In fact, such tori exist as shown in Fig. 12a, where \( \lambda = -9 \). The volume percentage of the ordered region formed by them is estimated at 1.4\%. This is lower than the percentage of rods in the \(+\Sigma\) or \(-\Sigma\) packing \( (\sqrt{3} \pi/72 = 7.55 \ldots \% \), see [7, 9]).

The vector field \( V_{011, RB}^{(214, 3)} + V_{453, RB}^{(214, 3)} + \lambda V_{033, RB}^{(214, 3)} \) can be made to have \(-\Sigma\)-arranged invariant tori with straight cores by redefining \( \alpha \) and \( \beta \) as

\[
\alpha = \frac{15\sqrt{2} (61 - 10\sqrt{6})}{2 \cdot 17 \cdot 3121} = 0.007297 \ldots , \tag{36}
\]

\[
\beta = -\frac{8428 + 3991\sqrt{6}}{2 \cdot 17 \cdot 3121} = 0.01270 \ldots .
\]

For these \( \alpha \) and \( \beta \), the orthogonal component of the vector field vanishes on the \( 3_2 \) screw axes independently of \( \lambda \). When we set \( \lambda = 3 \), thin \(-\Sigma\)-arranged invariant tori, which occupy approximately 0.7\% of a unit cell, are observed as in Fig. 12b. In
addition, three satellite sets of undulating invariant tori that run parallel to each $3_2$ screw axis are also observed and their volume percentage is estimated at 0.6%.

4 The $\Sigma^*$ arrangement

4.1 General forms of $V_{klm}^{(230,b)}$ and $V_{klm,5}^{(230,b)}$

When $Ia\bar{3}d$ is taken as the space group $G$ in the process in Sect. 2.2, the magnetic group $\bar{G}$ is one of $Ia\bar{3}d$ (No. 230.1.1647), $Ia'\bar{3}'d$ (No. 230.3.1649), $Ia\bar{3}d'$ (No. 230.4.1650) and $Ia'\bar{3}'d'$ (No. 230.5.1651). When the origin and the coordinate axes are appropriately set, the condition for $V_{klm} = (u, v, w)$ to be $V_{klm}^{(230,b)} (b = 1, 3, 4, 5)$ is to satisfy (11) and the following three equations:

$$V_{klm}(y + \pi/2, x + 3\pi/2, -z + 3\pi/2) = \begin{cases} (v(x, y, z), u(x, y, z), -w(x, y, z)) & \text{for } b = 1 \text{ or } 5, \\ (-v(x, y, z), -u(x, y, z), w(x, y, z)) & \text{for } b = 3 \text{ or } 4, \end{cases}$$

(37)

$$V_{klm}(-x, -y, -z) = \begin{cases} V_{klm}(x, y, z) & \text{for } b = 1 \text{ or } 4, \\ -V_{klm}(x, y, z) & \text{for } b = 3 \text{ or } 5, \end{cases}$$

(38)

$$V_{klm}(x + \pi, y + \pi, z + \pi) = V_{klm}(x, y, z).$$

(39)

The four equations (11) and (37)–(39) correspond to Nos. 2, 13, 25 and t(1/2, 1/2, 1/2), respectively, of the “generators selected” of each magnetic group in [26]. For the same reason as in Sect. 3.1, we assume that $k$ and $m$ are even and
odd, respectively. Moreover, (39) implies that \( k + l + m \) is even; thus, we restrict ourselves to the cases (14) and (15). Comparing (37) and (39) with (12) and (13), we notice that \( \mathbf{V}_{klm}^{(230.1)} \) and \( \mathbf{V}_{klm}^{(230.5)} \) are obtained by imposing (38) on \( \mathbf{V}_{klm}^{(214.1)} \), whereas \( \mathbf{V}_{klm}^{(230.3)} \) and \( \mathbf{V}_{klm}^{(230.4)} \) are obtained from \( \mathbf{V}_{klm}^{(214.3)} \). The general forms of the \( x \) components of \( \mathbf{V}_{klm}^{(230,b)} (b = 1, 3, 4, 5) \) are tabulated in Table 2, together with the conditions for \( \mathbf{V}_{klm}^{(230,b)} \) to become solenoidal. In the table, the following are referred to:

\[
\begin{align*}
\mathbf{u} &= c_2 (\sin kx \sin ly \cos mz \pm \sin kx \sin my \cos lz) \\
&\quad + c_3 (\cos lx \cos my \cos kx \mp \sin lx \cos ky \sin mz) \\
&\quad + c_6 (\sin mx \cos ky \sin lz \mp \cos mx \cos ly \cos kx), \\
\mathbf{u} &= c_1 (\cos kx \cos ly \sin mz \mp \cos kx \cos my \sin lz) \\
&\quad + c_4 (\sin lx \sin my \sin kx \mp \cos lx \sin ky \cos mz) \\
&\quad + c_5 (\cos mx \sin ky \cos lz \mp \sin mx \sin ly \sin kx),
\end{align*}
\]

\[
kc_2 - lc_3 + mc_6 = 0, \\
kc_1 - lc_4 + mc_5 = 0.
\]

There are two places where the case \( (k, l, m) = (0, 1, 1) \) is excluded in Table 2, for the vector fields become trivial.

Comparing (40)–(43) with (18) and (20) and taking (22) and (23) into account, we can verify the following “racemic” representations up to constant multiples:

\[
\begin{align*}
\mathbf{V}_{klm,S}^{(230.1)} &= \mathbf{V}_{klm,\text{RB}}^{(214.1)} + \mathbf{V}_{klm,\text{LB}^*}^{(214.1)}, \\
\mathbf{V}_{klm,S}^{(230.3)} &= \mathbf{V}_{klm,\text{RB}}^{(214.3)} - \mathbf{V}_{klm,\text{LB}^*}^{(214.3)}, \\
\mathbf{V}_{klm,S}^{(230.4)} &= \mathbf{V}_{klm,\text{RB}}^{(214.3)} + \mathbf{V}_{klm,\text{LB}^*}^{(214.3)}, \\
\mathbf{V}_{klm,S}^{(230.5)} &= \mathbf{V}_{klm,\text{RB}}^{(214.1)} - \mathbf{V}_{klm,\text{LB}^*}^{(214.1)},
\end{align*}
\]

where \( (k, l, m) \neq (0, 1, 1) \) in (44) and (47).

### 4.2 The \( \Sigma^* \) arrangement

In the \( \Sigma^* \) rod packing, the central axes of rods coincide with the \( 3_1 \) or \( 3_2 \) screw axes in \( Ia\overline{3}d \). One of these screw axes is represented as \( (2\pi/3 + s, 4\pi/3 + s, s) \) or \( (4\pi/3 + s, 2\pi/3 + s, s) \) with any \( s \) in our coordinates (see [8, 9]). In the same way as in Sect. 3.3, we see that \( \Sigma^* \)-arranged invariant tori with straight cores are impossible when the magnetic group \( Ia\overline{3}d \) or \( Ia'\overline{3}'d' \) is selected as \( \widetilde{G} \) in the process. Therefore, we can restrict ourselves to investigating \( \mathbf{V}_{klm,S}^{(230.3)} \) or \( \mathbf{V}_{klm,S}^{(230.4)} \) (see (45) and (46)).
From (23) and (46) with (32) and (33) or from Table 2, we obtain

\[
\mathbf{v}^{(230.4)}_{klm} = \begin{pmatrix} 
\cos x \cos y + \sin x \sin z \\
\cos y \cos z + \sin y \sin x \\
\cos z \cos x + \sin z \sin y 
\end{pmatrix}
\]  

(48)

and

\[
\mathbf{v}^{(230.4)}_{453, S} = \begin{pmatrix} 
u(x, y, z) \\
u(y, z, x) \\
u(z, x, y) 
\end{pmatrix},
\]

\[
u(x, y, z) = 5\bar{\alpha} \sin 4x (\sin 5y \cos 3z + \sin 3y \cos 5z) + (4\bar{\alpha} + 3\bar{\beta})(\cos 5x \cos 3y \cos 4z - \sin 5x \cos 4y \sin 3z) + 5\bar{\beta}(\sin 3x \cos 4y \sin 5z - \cos 3x \cos 5y \cos 4z)
\]  

(49)

The \(y\) and \(z\) components are obtained from (1)

Fig. 13 The \(\Sigma^*\) arrangement of invariant tori in \(\mathbf{v}^{(230.4)}_{011, S} + \mathbf{v}^{(230.4)}_{453, S} - 9 \mathbf{v}^{(230.4)}_{033, S}\) with (48)–(51). One of the initial points is (10) with \((n_x, n_y, n_z) = (16, 27, 1)\)
with constants $\tilde{\alpha}$ and $\tilde{\beta}$. Moreover, for the same reason as for $V_{033, RB}^{(214, 3)}$ in Sect. 3.3, we introduce

$$V_{033, S}^{(230, 4)} = \begin{pmatrix} \cos 3x \cos 3y + \sin 3x \sin 3z \\ \cos 3y \cos 3z + \sin 3y \sin 3x \\ \cos 3z \cos 3x + \sin 3z \sin 3y \end{pmatrix},$$  \hfill (50)

which is not obtained from Table 2. The orthogonal component of the linear combination $V_{011, S}^{(230, 4)} + V_{453, S}^{(230, 4)} + \lambda V_{033, S}^{(230, 4)}$ on the $3_1$ or $3_2$ screw axes is shown with Mathematica to vanish independently of $\lambda$ when

$$\tilde{\alpha} = -\frac{13}{20}, \quad \tilde{\beta} = \frac{9}{20}.$$  \hfill (51)

Adjusting the value of $\lambda$, we can find $\Sigma^*$-arranged invariant tori with straight cores as shown in Fig. 13, where $\lambda = -9$. The invariant tori along the $3_1$ and $3_2$ screw axes are wound around by integral curves right- and left-handed helically, respectively. The volume percentage of the ordered region formed by them is estimated at 4.3%, which is much lower than the volume percentage of rods in the $\Sigma^*$ rod packing ($\sqrt{3} \pi / 36 = 15.11 \ldots \%$, see [7, 9]).

The existence or nonexistence of $\Sigma^*$-arranged invariant tori with straight cores in a linear combination of $V_{klm, S}^{(230, 3)}$ continues to be a problem.

5 The $\Pi^*$ arrangement

The 14 cubic space groups that are compatible with the $\beta$-W (i.e. $\Pi^*$) rod packing were listed in [9, Table 1]. They were classified into three categories. The first consists of $Ia\bar{3}d$ and its three achiral subgroups: $I\bar{4}3d$, $Ia\bar{3}$, $Pa\bar{3}$ (Nos. 220, 206, 205). The second consists of $I4_132$ and its four chiral subgroups: $P4_132$, $P4_321$, $I2_13$, $P2_13$ (Nos. 213, 212, 199, 198). The third consists of $Pm\bar{3}n$ and its four achiral or chiral subgroups: $P\bar{4}3n$, $P4_232$, $Pm\bar{3}$, $P23$ (Nos. 218, 208, 200, 195).

If $G$ is a space group of the third category, then the central axis of a rod in the $G$-symmetric $\Pi^*$ packing coincides with the line $(0, 1/2, z)$ or $(1/2, 0, z)$ when using the coordinates in [9]. In this case, $\tilde{G}$ in step 2 of the process in Sect. 2.2 is one of 14 first- or third-type magnetic groups. In the part “Positions” in the pages about each $\tilde{G}$ in [26], we observe that the coordinate $(0, 1/2, 1/2)$ (resp. $(1/2, 0, 1/2)$) is accompanied by the vector $[0, 0, 0]$ or $[u, 0, 0]$ (resp. $[0, u, 0]$). This means that every continuous vector field whose magnetic group is $\tilde{G}$ becomes the vector, namely zero or perpendicular to the line $(0, 1/2, z)$ (resp. $(1/2, 0, 1/2)$) at $(0, 1/2, 1/2)$ (resp. $(1/2, 0, 1/2)$). Therefore, (8) holds and neither $(0, 1/2, z)$ nor $(1/2, 0, z)$ can be a core of nested invariant tori. For this reason, we exclude all the space groups of the third category from our consideration. We note that not all are discarded if curved cores of invariant tori are allowed. Indeed, in [21, Fig. 11], we previously showed the $\Pi^*$ arrangement of double helical invariant tori in $V_{113, RB}^{(208, 4)}$, whose magnetic group is $Pf\bar{4}22$ (No. 208.4.1549) of the $P4_232$ family.
Table 3: General forms of the $x$ components of $\mathbf{V}_{klm}^{(206,b)}$ and $\mathbf{V}_{klm,S}^{(206,b)}$ when the origin and the coordinate axes are appropriately set

| Vector field $\mathbf{V}_{klm}^{(206,b)}$ | Magnetic group | Case (with $k$ even, $m$ odd) | General form of the $x$ component | Conditions to become $\mathbf{V}_{klm,S}^{(206,b)}$ |
|--------------------------------------|----------------|--------------------------------|----------------------------------|----------------------------------|
| $\mathbf{V}_{klm}^{(206.1)}$ | $I\alpha 3$ | $l$ odd | (52) | (55) and $klm \neq 011$ |
| $\mathbf{V}_{klm}^{(206.3)}$ | $I\alpha 3'$ | $l$ odd and $klm \neq 011$ | (53) | (56) or $k = 0$ |
| $\mathbf{V}_{klm}^{(206.4)}$ | $I\mu a 3'$ | $l$ even | (54) | (57) |

The $y$ and $z$ components are obtained from (1).

We discuss the case in which $G$ is a space group of the first (achiral) category in Sect. 5.2 after studying $\mathbf{V}_{klm,S}^{(206,b)}$ in Sect. 5.1. The case in which $G$ belongs to the second (chiral) category is treated in Sect. 5.3.

5.1 General forms of $\mathbf{V}_{klm}^{(206,b)}$ and $\mathbf{V}_{klm,S}^{(206,b)}$

To prepare for the discussion in Sect. 5.2, we study $\mathbf{V}_{klm,S}^{(206,b)}$, whose magnetic groups belong to the $I\alpha \bar{3}$ family: $I\alpha \bar{3}$ (No. 206.1.1538), $I\alpha \bar{3}'$ (No. 206.3.1540) and $I\mu a \bar{3}'$ (No. 206.4.1541). When the origin and the $x$, $y$ and $z$ axes are appropriately set, the conditions for $\mathbf{V}_{klm} = (u, v, w)$ to be $\mathbf{V}_{klm}^{(206,b)}$ ($b = 1, 3, 4$) are (11), (13) with $b = 5$ removed, and

$$\mathbf{V}_{klm}(-x, -y, -z) = \begin{cases} \mathbf{V}_{klm}(x, y, z) & \text{for } b = 1, \\ -\mathbf{V}_{klm}(x, y, z) & \text{for } b = 3 \text{ or } 4. \end{cases}$$

These conditions are yielded by the “generators selected” of each magnetic group in [26]. As in the previous sections, we assume that $k$ is even and $m$ is odd. The general forms of the $x$ components $u$ of $\mathbf{V}_{klm}^{(206,b)}$ are tabulated in Table 3, in which the following are referred to:

$$u = C_1 \sin kx \sin ly \cos mz + C_2 \sin kx \sin my \cos lx \cos my \cos kz + C_4 \sin lx \cos ky \sin mz + C_5 \sin mx \cos ky \sin lz + C_6 \cos mx \cos ly \cos kz, \quad (52)$$
$$u = C_7 \cos kx \cos ly \sin mz + C_8 \cos kx \cos my \sin lz + C_9 \sin lx \sin my \sin kz + C_{10} \cos lx \sin ky \cos mz + C_{11} \cos mx \sin ky \cos lz + C_{12} \sin mx \sin ly \sin kz, \quad (53)$$
$$u = C_{13} \sin kx \sin ly \sin mz + C_{14} \cos kx \sin my \cos lz + C_{15} \cos lx \sin my \cos kz + C_{16} \sin lx \sin ky \sin mz + C_{17} \cos mx \cos ky \sin lz + C_{18} \cos mx \cos ly \sin kz. \quad (54)$$

Here, $C_i \ (i = 1, 2, \ldots, 12)$ are constants for which $u$ does not become (40) or (41) in Sect. 4.1, whereas $C_i \ (i = 13, 14, \ldots, 18)$ are constants for which $u$ is not trivial. In the case $(k, l, m) = (0, 1, 1)$ excluded in $\mathbf{V}_{klm}^{(206,3)}$ in Table 3, the $x$ component (53) is of
The conditions for \( V_{011}^{(230.3)} \) (see Table 2). The conditions for \( V_{klm}^{(206,b)} \) to become \( V_{klm_S}^{(206,b)} \) are also listed in Table 3, in which the following are referred to:

\[
kC_1 - lC_3 + mC_5 = 0, \quad kC_2 + lC_4 - mC_6 = 0, \tag{55}
\]

\[
kC_7 - lC_9 + mC_{11} = 0, \quad kC_8 + lC_{10} - mC_{12} = 0, \tag{56}
\]

\[
kC_{13} - lC_{15} - mC_{17} = 0, \quad kC_{14} - lC_{16} + mC_{18} = 0. \tag{57}
\]

In the case \((k, l, m) = (0, 1, 1)\) excluded from \( V_{klm_S}^{(206.1)} \) in Table 3, the \( x \) component \((52)\) with \((55)\) is the \( x \) component of \( V_{011.5}^{(44)−(47)} \).

Let \( k, l \) and \( m \) satisfy one of \((14)−(17)\). Then, comparing \((52)−(57)\) with \((18)−(21)\) and taking \((22)−(25)\) into account, we can obtain the following “racemic” representations valid up to constant multiples:

\[
V_{klm_S}^{(206.1)} = \mu[V_{klm_{RB}}^{(214.1)} + V_{klm_{LB}}^{(214.1)}] + \nu[V_{klm_{RB}}^{(214.3)} + V_{klm_{LB}}^{(214.3)}],
\]

\((k, l, m) \neq (0, 1, 1), \tag{58}\)

\[
V_{klm_S}^{(206.3)} = \mu[V_{klm_{RB}}^{(214.1)} - V_{klm_{LB}}^{(214.1)}] + \nu[V_{klm_{RB}}^{(214.3)} - V_{klm_{LB}}^{(214.3)}],
\]

\((k, l, m) \neq (0, 1, 1), \tag{59}\)

\[
V_{klm_S}^{(206.4)} = \begin{cases} \mu[V_{klm_{RB}}^{(214.4)} - V_{klm_{LB}}^{(214.5)}] + \nu[V_{klm_{RB}}^{(214.5)} - V_{klm_{LB}}^{(214.4)}] & \text{if } (k, l, m) \neq (0, 0, 1), \\ \begin{pmatrix} [214.5]_{01.\text{RB}} - [214.4]_{01.\text{LB}} \end{pmatrix} & \text{if } (k, l, m) = (0, 0, 1). \end{cases} \tag{60}\)

Here, \( \mu \) and \( \nu \) are constants such that \( \mu \nu \neq 0 \) in \((58)\) and \((59)\), whereas \( (\mu, \nu) \neq (0, 0) \) in \((60)\). Clearly, \((58)\) and \((59)\) can be rewritten in terms of \( V_{klm_S}^{(230.5)} \) \((b = 1, 3, 4, 5)\) due to \((44)−(47)\).

### 5.2 Achiral \( \Pi' \) arrangement

As mentioned at the beginning of Sect. 5, we start the process taking \( Ia\overline{3}d \) as \( G \). According to the columns “\( \beta\)-W (\( \times2 \))” in [9, Table 1], the central axis of a rod in the \( Ia\overline{3}d \)-symmetric \( \Pi' \) packing coincides with the line \((0, \pi/2, z)\) or \((\pi/2, 0, z)\) in our coordinates. In this case, the eight unit cells in Fig. 4 becomes one unit cell, as indicated by “\( \times2 \)” in [9, Table 1].

Let us prove that the line \((0, \pi/2, z)\) in \( V_{klm_S}^{(230.1)} \) cannot become a core of invariant tori. We can verify that each \( V_{klm_S}^{(230.1)} \) in Table 2 satisfies

\[
V_{klm}^{(230.3)}(x, -y + \pi, z + \pi) = \begin{cases} (-u(x, y, z), v(x, y, z), -w(x, y, z)) & \text{for } b = 1 \text{ or } 4, \\ (u(x, y, z), -v(x, y, z), w(x, y, z)) & \text{for } b = 3 \text{ or } 5. \end{cases} \tag{61}\]
where \((x, -y + \pi, z + \pi)\) is yielded from \((x, y, z)\) by the symmetry or antisymmetry operation No. 27 (the \(c\) glide on the plane \(y = \pi/2\)) in each magnetic group in [26]. If \((x, y, z) = (\rho \cos \phi, \pi/2 + \rho \sin \phi, s)\) with \(\rho = \rho(s)\) and \(\phi = \phi(s)\) represents a helical curve whose axis is \((0, \pi/2, z)\), then \((x, -y + \pi, z + \pi) = (\rho \cos \phi, \pi/2 - \rho \sin \phi, s + \pi)\) represents another helical curve with the opposite handedness. Therefore, when the existence of an invariant torus around the line \((0, \pi/2, z)\) is supposed in \(V_{klm,S}^{(230,b)}\), there would exist an enantiomorphic invariant torus around the same line. Thus, the line \((0, \pi/2, z)\) cannot become a core of invariant tori. This impossibility can be also deduced from the following equalities:

\[
V_{klm}^{(230,b)}(-y + \pi/2, x + \pi/2, -z + 3\pi/2) = \begin{cases} 
(v(x, y, z), -u(x, y, z), w(x, y, z)) & \text{for } b = 1 \text{ or } 3, \\
(-v(x, y, z), u(x, y, z), -w(x, y, z)) & \text{for } b = 4 \text{ or } 5.
\end{cases}
\]

Here, \((-y + \pi/2, x + \pi/2, -z + 3\pi/2)\) is yielded from \((x, y, z)\) by the \(4\) rotation around \((0, \pi/2, z)\), i.e., by the operation No. 39 and the body-centring \((x, y, z) \mapsto (x + \pi, y + \pi, z + \pi)\) in each magnetic group in [26].

In addition, the line \((\pi/2, 0, z)\) in \(V_{klm,S}^{(230,b)}\) cannot become a core of invariant tori, either. Indeed, at the point \((\pi/2, 0, 0)\) on the line, \(w(\pi/2, 0, 0) (= u(0, \pi/2, 0))\) is equal to zero in (40) and (41), namely (8) holds. Thus, the \(\Pi^*\) arrangement of straight invariant tori cannot be expected when \(Ia\overline{3}d\) is chosen as \(G\). The maximal non-isomorphic subgroups of \(Ia\overline{3}d\) are \(I43d, I4_132\) and \(Ia\overline{3}d\). The first one is discarded in the same way as \(Ia\overline{3}d\). The second one will be taken as \(G\) in Sect. 5.3.

When the third one, \(Ia\overline{5}\), is taken as \(G\), none of the resulting fields \(V_{klm,S}^{(206,b)}\) (see Table 3) has a core of invariant tori on the line \((0, \pi/2, z)\). This is because (61) remains valid even if \(V_{klm,S}^{(230,b)}\) is replaced with \(V_{klm,S}^{(206,b)}\) (with \(b = 5\) removed). Furthermore, \(w(\pi/2, 0, 0) (= u(0, \pi/2, 0))\) vanishes in (52) and (53); thus, (8) holds and neither \(V_{klm,S}^{(206,d)}\) nor \(V_{klm,S}^{(206,3)}\) has a core of invariant tori on the line \((\pi/2, 0, z)\). For these reasons, using \(V_{klm,S}^{(206,4)}\), we search for the \(\Pi^*\) arrangement in which a core of invariant tori is located on \((\pi/2, 0, z)\), a \(2\) screw axis.

The simplest field of all \(V_{klm,S}^{r(206,4)}\) in Table 3 is

\[
V_{001,S}^{(206,4)} = \begin{pmatrix} \sin y \\ \sin z \\ \sin x \end{pmatrix}.
\]

It has no remarkable invariant torus except very thin crooked tori. Indeed, Galloway and Proctor [29] reported that almost all integral curves are chaotic in numerically solving

\[
\frac{d}{dt} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \sin z \\ \sin x \\ \sin y \end{pmatrix},
\]

in which interchanging \(y\) and \(z\) on the left and right sides yields
As far as we know, the best example of the \( \Pi^* \) arrangement of invariant tori with straight cores is observed in \( u_1 \odot u_2 \), \( S_{01} \). Here, \( S_{01} \) is obtained from Table 3. Because of the necessary condition (7) for the line \( (u_1 \odot 2, 0, z) \) to be a core of invariant tori reads that is,

\[
\begin{aligned}
\frac{d}{dt} \begin{pmatrix} x \\ y \\ z \end{pmatrix} &= \begin{pmatrix} \sin y \\ \sin z \\ \sin x \end{pmatrix} \\
&= V_{001,S}^{(206.4)} + V_{021,S}^{(206.4)}.
\end{aligned}
\]

Figure 14 shows \( \Pi^* \)-arranged invariant tori in the sum of (62), (63) with (64). One of the initial points is \( (10) \) with \( (n_x, n_y, n_z) = (10, 1, 1) \)

\[
\begin{pmatrix} x \\ y \\ z \end{pmatrix} = V_{001,S}^{(206.4)} + V_{021,S}^{(206.4)}.
\]

is obtained from Table 3. Because of

\[
W(\pi/2, 0, z) = V_{001,S}^{(206.4)}(\pi/2, 0, z) + V_{021,S}^{(206.4)}(\pi/2, 0, z) = \begin{pmatrix} 0 \\ (1 - C_{14} + C_{15}) \sin z \\ 1 + C_{14} + C_{15} \cos 2z \end{pmatrix},
\]

the necessary condition (7) for the line \( (\pi/2, 0, z) \) to be a core of invariant tori reads

\[
1 - C_{14} + C_{15} = 0 \quad \text{and} \quad |1 + C_{14}| > |C_{15}|,
\]

that is,

\[
C_{14} - C_{15} = 1 \quad \text{and} \quad C_{14} > 0.
\]

Figure 14 shows \( \Pi^* \)-arranged invariant tori in the sum of (62) and (63) with

\[
C_{14} = \frac{9}{11}, \quad C_{15} = -\frac{2}{11}.
\]

Although obscure in the figure, the invariant torus along the line \( (\pi/2, 0, z) \) (resp. \( (3\pi/2, 0, z) \)) is left-handed helically (resp. right-handed helically) wound around by integral curves. The volume percentage of the \( \Pi^* \)-arranged ordered region is
estimated at 5.8%. This is not to be compared with the volume percentage of rods in the $\Pi^*$ rod packing ($3/\sqrt{16} = 58.90 \ldots \%$, see [7, 9]).

5.3 Chiral $\Pi^*$ arrangement

When rods are ordinary cylinders, the $\Pi^*$ rod packing is achiral and does not have an enantiomorph. However, it can be chiral when all rods have the same chirality. According to [9, Table 1], the central axes of rods in the $\Pi^*$ packing with the symmetry of $I_{4_1}32$ coincide with twofold rotation axes, one of which is located on the line $(0, \pi/2, z)$ in our coordinates. In this case, the eight unit cells in Fig. 4 are considered as one unit cell whose front side is the $y$–z plane. Because (8) on the line $(0, \pi/2, z)$ follows from $w(0, \pi/2, z) = w(z, 0, \pi/2) = 0$ for (19) in the case (16) or (17), the line $(0, \pi/2, z)$ cannot be a core of invariant tori when $I_{4_1}32$ or $I_{4_1}'32'$ is selected as $\tilde{G}$ (see Table 1). Furthermore, the magnetic group $I_{4_1}32$ is not appropriate for $\tilde{G}$, either, because $V_{kln}^{(214.1)}(0, \pi/2, \pi/4) = 0$ can be proven (see the coordinates $(0, 1/4, 1/8)$ accompanied by the vector $(0, 0, 0)$ in $I_{4_1}32$ in [26]). Then, in Table 1, only $I_{4_1}'32'$ remains as a candidate for $\tilde{G}$. Indeed, as shown in Fig. 15a, straight invariant tori are $\Pi^*$-arranged in

$$
V_{013, RB}^{(214.3)} = \begin{pmatrix}
  u(x, y, z) \\
  u(y, z, x) \\
  u(z, x, y)
\end{pmatrix},
$$

$$
u(x, y, z) = r(\cos y \sin 3z - \cos 3y \sin z)
- 3r(\cos x \cos 3y - \sin x \sin 3z)
- \sin 3x \sin z + \cos 3x \cos y
$$

Fig. 15 Invariant tori in $V_{013, RB}^{(214.3)}$ of (65). a The chiral $\Pi^*$ arrangement. One of the initial points is (10) with $(n_x, n_y, n_z) = (20, 29, 5)$. b Chain-like arrangement of invariant tori. Every two tori form a (12, 2)-torus link. One of the torus links is obtained from (10) with $(n_x, n_y, n_z) = (35, 24, 17)$ and (38, 20, 16).
although very thin. The volume percentage of the \( \Pi^* \)-arranged ordered region is estimated at only 1.0%.

The Beltrami flow \( \mathbf{V}_{013,\text{RB}}^{(214,3)} \) also has chain-like invariant tori, as shown in Fig. 15b. Each of the invariant tori, which is unknotted (although looking as if knotted in the figure), interweaves with another and forms a \((12, 2)\)-torus link. In addition, this pair of invariant tori links with three other pairs. The volume percentage of the chain is estimated at 0.3%.

6 The \( \Gamma \) arrangement

In the \( \Gamma \) rod arrangement, the central axes of rods coincide with the \( \bar{3} \) rotation axes in \( Ia\bar{3}d \). One of these axes is represented as \((s, s, s)\) with any \( s \) (see [8, 9]). Because \( \bar{3} \) rotation axes cannot be cores of invariant tori, we take the maximal chiral subgroup \( I4_132 \) as \( G \) in the process in Sect. 2.2. In this case, the line \((s, s, s)\) becomes a threefold rotation axis. Because (1) means that \( u(s, s, s) = v(s, s, s) = w(s, s, s) \), namely \( \mathbf{V}_{klm}^{(s, s, s)} \) is parallel to the line \((s, s, s)\), the cores of \( \Gamma \)-arranged invariant tori are always straight.

We can show that the only magnetic group of the \( I4_132 \) family that is appropriate for \( G \) in the process is \( I4_132' \) (see Table 1). Indeed, (13) for \( b = 4 \) or 5 implies that (9) holds on the line \((s, s, s)\), and \( I_{p41,32} \) and \( I_{p41',32'} \) are excluded. In addition, (18) at \((x, y, z) = (\pi/4, \pi/4, \pi/4)\) is written as

\[
u(\pi/4, \pi/4, \pi/4) = \left( \begin{array}{c} c_3 \mp c_6 \cos \frac{(l \pm m)\pi}{4} \mp c_1 \sin \frac{(l \mp m)\pi}{4} \cr c_5 \pm c_4 \cos \frac{(l \pm m)\pi}{4} + c_2 \sin \frac{(l \pm m)\pi}{4} \end{array} \right) \cos \frac{k\pi}{4} \sin \frac{k\pi}{4},
\]

which is proven to vanish if \( u \) is of \( \mathbf{V}_{klm}^{(214,1)} \) in Table 1. Thus, (8) holds with \( \mathbf{V}_{klm}^{(214,1)} \) on the line \((s, s, s)\). As a result, the magnetic group \( I4_132 \) is excluded and only \( I4_132' \) remains.

In fact, \( \mathbf{V}_{011,\text{LB}}^{(214,3)} \) of (32) has \( \Gamma \)-arranged invariant tori, as demonstrated in [21, Fig. 4]. Interestingly, when the chirality of (32) is weakened by adding \( \mathbf{V}_{011,\text{LB}}^{(214,3)} \) (see (23)) as

\[
\mathbf{V}_{011,\text{RB}}^{(214,3)} + \lambda \mathbf{V}_{011,\text{LB}}^{(214,3)}
\]

with \( 0 < \lambda \leq 0.8 \) (e.g. \( \lambda = 0.75 \)), the \( \Gamma \)-arranged ordered region is thickened as shown in Fig. 16a (cf. [21, Fig. 4]). The volume percentage of this region for \( \lambda = 0.75 \) is estimated at 32.3%. By contrast, the percentage of rods in the \( \Gamma \) rod packing is \( \sqrt{3} \pi/8 = 68.01 \ldots \% \) [7, 9]. The vector field (66) with \( \lambda = 0.75 \) is also
observed to have chain-like invariant tori (see Fig. 16b), which occupy approximately 1.1\% of a unit cell. Each ring of the chain links with three other rings and the chain structure resembles the polycatenane \textit{lcv-\textit{y}} in [5, Fig. 41]. Here, “lcv” is the abbreviation for lattice complex V (see [30, Sect. 2.4]), and “\textit{y}” was used to represent polycatenanes in [5].

When $\lambda$ approaches 1, each $\Gamma$-arranged invariant torus splits and becomes a bundle of invariant tori. Furthermore, when $\lambda$ reaches 1, the field (66) becomes $\mathbf{V}(230.4)$ (see (48)), and a bundle of six invariant tori are located along each $\overline{3}$ rotation axis.

7 The $\Omega$ arrangement

7.1 General forms of $\mathbf{V}^{(211.b)}_{klm}$ and $\mathbf{V}^{(211.b)}_{klm,\text{RB}}$

When $I432$ is taken as $G$ in the process in Sect. 2.2, candidates for the magnetic group $\overline{G}$ are $I432$ (No. 211.1.1556), $I4',32'$ (No. 211.3.1558), $I_d432$ (No. 211.4.1559) and

Table 4 General forms of the $x$ components of $\mathbf{V}^{(211.b)}_{klm}$ and $\mathbf{V}^{(211.b)}_{klm,\text{RB}}$ when the origin and the coordinate axes are appropriately set

| Vector field | Magnetic group | Case (with $k$ even, $m$ odd and) | General form of the $x$ component | Conditions to become $\mathbf{V}^{(211.b)}_{klm,\text{RB}}$ |
|--------------|----------------|-----------------------------------|-----------------------------------|-----------------------------------|
| $\mathbf{V}^{(211.1)}_{klm}$ | $I432$ | $l$ odd and $klm \neq 011$ | (69) (upper signs) | (70) |
| $\mathbf{V}^{(211.3)}_{klm}$ | $I4',32'$ | $l$ odd | (69) (lower signs) | (70) |
| $\mathbf{V}^{(211.4)}_{klm}$ | $I_d432$ | $l$ even and $klm \neq 001$ | (69) (upper signs) | (70) |
| $\mathbf{V}^{(211.5)}_{klm}$ | $I_d4',32'$ | $l$ even and $klm \neq 001$ | (69) (lower signs) | (70) |

The $y$ and $z$ components are obtained from (1).
I_4^{13} (No. 211.5.1560). When the origin and the x, y and z axes are appropriately set, the conditions for \( \mathbf{V}_{klm} = (u, v, w) \) to be \( \mathbf{V}_{klm}^{(211b)} (b = 1, 3, 4, 5) \) are

\[
\mathbf{V}_{klm}(-x, -y, z) = (-u(x, y, z), -v(x, y, z), w(x, y, z)),
\]

(67)

\[
\mathbf{V}_{klm}(y, x, -z) = \begin{cases} 
(v(x, y, z), u(x, y, z), -w(x, y, z)) & \text{for } b = 1 \text{ or } 4, \\
(-v(x, y, z), -u(x, y, z), w(x, y, z)) & \text{for } b = 3 \text{ or } 5,
\end{cases}
\]

(68)

and (13). These conditions are yielded by the “generators selected” of each magnetic group in [26]. For the same reason as in Sect. 3.1, we can assume that \( k \) is even and \( m \) is odd without generality loss. The general forms of the \( x \) components \( u \) of \( \mathbf{V}_{klm}^{(211b)} \) are tabulated in Table 4, in which the following is referred to:

\[
u = c_1 (\cos kx \sin ly \sin mz \mp \cos kx \sin my \sin lz)
+ c_2 (\sin kx \cos ly \cos mz \pm \sin kx \cos my \cos lz)
+ c_3 (\cos lx \sin my \sin kx \mp \cos lx \sin ky \sin mz)
+ c_4 (\sin lx \cos my \cos kx \pm \sin lx \cos ky \cos mz)
+ c_5 (\cos mx \sin ky \sin lz \mp \cos mx \sin ly \sin kx)
+ c_6 (\sin mx \cos ky \cos lz \pm \sin mx \cos ly \cos kx).
\]

Here, \( c_1, c_2, \ldots, c_6 \) are generally nonzero constants. When they can be written as

\[
c_1 = (l^2 + m^2)\alpha, \quad c_2 = (l^2 + m^2)\beta, \quad c_3 = -kl\alpha + mk\beta,

(70)

\[
c_4 = -mk\alpha - kl\beta, \quad c_5 = -mk\alpha - lk\beta, \quad c_6 = lk\alpha - mk\beta
\]

with nonzero constants \( \alpha \) and \( \beta \) and with \( \kappa \) from (3), the fields \( \mathbf{V}_{klm}^{(211b)} \) become \( \mathbf{V}_{klm, RB}^{(211b)} \). In Table 4, the cases \((k, l, m) = (0, 1, 1)\) for \( I432 \) and \((k, l, m) = (0, 0, 1)\) for \( I_4^{13} \) have been excluded because (69) with upper signs are of the magnetic groups \( Im'3'm' \) (No. 229.5.1642) and \( I_4m'3'm' \) (No. 229.9.1646), respectively. The case \((k, l, m) = (0, 0, 1)\) for \( I_4^{13} \) has been also excluded because \( u \) vanishes in (69) with lower signs. If \( kl = 0 \) or \( k = l = m \), then each of \( \mathbf{V}_{klm, RB}^{(211b)} (b = 1, 3, 4, 5) \) is determined uniquely up to constant multiples.

### 7.2 The \( \Omega \) arrangement

In the \( ^+\Omega \) (resp. \( ^-\Omega \)) rod packing, the central axes of rods coincide with the \( 3_1 \) (resp. \( 3_2 \)) screw axes in \( I432 \). One of these axes is represented as \((2\pi/3 + s, 4\pi/3 + s, s)\) (resp. \((4\pi/3 + s, 2\pi/3 + s, s)\)) with any \( s \) in our coordinates (see [8]). In the same way as in Sect. 3.3, we now show that \( I4^{13} \) is the only magnetic group of the \( I432 \) family that is compatible with \( ^+\Omega \)- or \( ^-\Omega \)-arranged invariant tori with straight cores. The composition of (67) and (68) yields

\[
\mathbf{V}_{klm}^{(211b)}(-y, -x, -z) = \begin{cases} 
(-v(x, y, z), -u(x, y, z), -w(x, y, z)) & \text{for } b = 1 \text{ or } 4, \\
(v(x, y, z), u(x, y, z), w(x, y, z)) & \text{for } b = 3 \text{ or } 5.
\end{cases}
\]

Its scalar product by \( \mathbf{q} = (1, 1, 1) \) leads to
\[ \mathbf{q} \cdot \mathbf{V}_{klm}^{(211.1)}(-y, -x, -z) = \begin{cases} -\mathbf{q} \cdot \mathbf{V}_{klm}^{(211.1)}(x, y, z) & \text{for } b = 1 \text{ or } 4, \\ \mathbf{q} \cdot \mathbf{V}_{klm}^{(211.1)}(x, y, z) & \text{for } b = 3 \text{ or } 5. \end{cases} \]

Substituting \((2\pi/3, 4\pi/3, 0)\) or \((4\pi/3, 2\pi/3, 0)\) for \((x, y, z)\) and using the \(2\pi\) periodicity of \(\mathbf{V}_{klm}^{(211.1)}\) in \(x\) or \(y\), we deduce that

\[ \mathbf{q} \cdot \mathbf{V}_{klm}^{(211.1)}(2\pi/3, 4\pi/3, 0) = \mathbf{q} \cdot \mathbf{V}_{klm}^{(211.1)}(4\pi/3, 2\pi/3, 0) = 0 \quad \text{for } b = 1 \text{ or } 4. \]

Clearly, the two points \((2\pi/3, 4\pi/3, 0)\) and \((4\pi/3, 2\pi/3, 0)\) are located on the \(3_1\) screw axis \((2\pi/3 + s, 4\pi/3 + s, s)\) and the \(3_2\) screw axis \((4\pi/3 + s, 2\pi/3 + s, s)\), respectively. Therefore, (8) holds on the axes and neither axis can be a core of invariant tori in the case \(b = 1 \text{ or } 4\). Furthermore, the case \(b = 5\) is also discarded. Indeed, \(\mathbf{V}_{klm}^{(211.5)}\) has the antisymmetry under the body-centring \(\mathbf{V}_{klm}^{(211.5)}(x + \pi, y + \pi, z + \pi) = -\mathbf{V}_{klm}^{(211.5)}(x, y, z)\), which means that (9) holds on the axis \((2\pi/3 + s, 4\pi/3 + s, s)\) or \((4\pi/3 + s, 2\pi/3 + s, s)\). As a result, only the case \(b = 3\) remains.

In [21, Fig. 8], we showed the \(-\Omega\) arrangement of invariant tori with curved cores in

\[ \mathbf{V}_{011, RB}^{(211.3)} = \begin{pmatrix} \sqrt{2} \sin y \sin z + \sin x (\cos z - \cos y) \\ \sqrt{2} \sin z \sin x + \sin y (\cos x - \cos z) \\ \sqrt{2} \sin x \sin y + \sin z (\cos y - \cos x) \end{pmatrix}. \tag{71} \]

The cores of the invariant tori are straightened by adding a \(1/5\)-wavelength field \(\mathbf{V}_{453, RB}^{(211.3)}\) to (71). In this subsection, however, we investigate the linear combination

\[ \mathbf{W} = \mathbf{V}_{011, RB}^{(211.3)} + \lambda_1 \mathbf{V}_{211, RB}^{(211.3)} + \lambda_2 \mathbf{V}_{013, RB}^{(211.3)} \]

because it has much thicker \(-\Omega\)-arranged invariant tori, and also has \(+\Omega\)-arranged invariant tori for a different pair of \(\lambda_1\) and \(\lambda_2\). Here,

\[ \mathbf{V}_{211, RB}^{(211.3)} = \begin{pmatrix} u(x, y, z) \\ u(y, z, x) \\ u(z, x, y) \end{pmatrix}, \quad u(x, y, z) = 2 \cos 2x \sin y \sin z - 2 \cos x (\sin y \sin 2z + \sin 2y \sin z) - \sqrt{6} \sin x (\cos y \cos 2z - \cos 2y \cos z), \tag{72} \]

\[ \mathbf{V}_{013, RB}^{(211.3)} = \begin{pmatrix} u(x, y, z) \\ u(y, z, x) \\ u(z, x, y) \end{pmatrix}, \quad u(x, y, z) = \sqrt{10} (\sin y \sin 3z + \sin 3y \sin z) - 3 \sin x (\cos 3y - \cos 3z) + \sin 3x (\cos z - \cos y). \tag{73} \]

The linear combination is shown with \textit{Mathematica} to satisfy (7) on the \(3_1\) screw axes when
Fig. 17 Invariant tori in $V^{(211,3)}_{(211,3)} + \lambda_1 V^{(211,3)}_{(011,3)} + \lambda_2 V^{(211,3)}_{(013,3)}$ with (71)–(73). a The $+\Omega$ arrangement when $\lambda_1$ and $\lambda_2$ are from (74). One of the initial points is (10) with $(n_x, n_y, n_z) = (17, 29, 1)$. b The $-\Omega$ arrangement when $\lambda_1$ and $\lambda_2$ are from (75). One of the initial points is (10) with $(n_x, n_y, n_z) = (35, 18, 1)$. c The I-WP-like arrangement when $\lambda_1$ and $\lambda_2$ are from (74). It is covered with a single integral curve that starts from (10) with $(n_x, n_y, n_z) = (19, 20, 14)$ and are plotted modulo $2\pi$

\[
\begin{align*}
\lambda_1 &= -\frac{\sqrt{3} + \sqrt{2}}{6} = -0.5243 \ldots, \\
\lambda_2 &= \frac{\sqrt{3} + \sqrt{2}}{6} \cdot \frac{3\sqrt{2} - 4}{2(\sqrt{10} - \sqrt{3})} = 0.0444 \ldots 
\end{align*}
\]

and on the $3_2$ screw axes when
\[ \lambda_1 = \frac{\sqrt{3} - \sqrt{2}}{6} = 0.0529 \ldots \]
\[ \lambda_2 = \frac{\sqrt{3} - \sqrt{2}}{6} \cdot \frac{3\sqrt{2} + 4}{2(\sqrt{10} + \sqrt{3})} = 0.0446 \ldots \] (75)

Figure 17a and b depict the \(+\Omega\) and \(\ominus\) arrangements of invariant tori with straight cores in the linear combinations with (74) and (75), respectively. The volume percentages of the \(+\Omega\)- and \(\ominus\)-arranged ordered regions are estimated at 12.0% and 29.3%, respectively. By contrast, the percentage of rods in the \(+\Omega\) or \(\ominus\) rod packing is \(\sqrt{3} \pi / 18 = 30.22 \ldots \%\) [7].

In addition to the \(+\Omega\)- and \(\ominus\)-arranged invariant tori, other invariant tori, whose genus is not equal to 1, are observed in the linear combination with (74) or (75). As shown in Fig. 17c, they are surfaces resembling Schoen’s I-WP minimal surface, whose genus is 4 in a primitive kaleidoscopic tetrahedron [31] and 7 in a minimal cubic unit cell [32]. Unlike a usual invariant torus of genus 1, each of the I-WP-like invariant tori contains zeros of the vector field on it. The zeros are located at the points where two of \(x\), \(y\) and \(z\) coordinates are \(i_1\pi\) and \(i_2\pi\) with integers \(i_1\) and \(i_2\) such that \(i_1 \equiv i_2 \mod 2\). The volume percentage of the region occupied by the I-WP-like invariant tori has not been measured because some integral curves on them are difficult to distinguish from chaotic integral curves.

### 8 Summary and discussion

The sets of invariant tori whose arrangements resemble the cubic rod packings in Figs. 1–6 have been considered in solenoidal vector fields. In principle, they are obtained by the process in Sect. 2.2. For chiral arrangements, we used Beltrami flows (see (4)), which have the strongest chirality of all solenoidal vector fields satisfying (2). When the invariant tori are assumed to have straight cores, the sufficient condition (8) or (9) for their nonexistence is convenient to study which magnetic group to select in the process for each rod-packing arrangement. This answer is shown in Table 5. It was analytically derived from (8) or (9) with some symmetry or antisymmetry operations of associated magnetic groups or with the vector fields in Tables 1–4. If familiar with black/red-coloured symmetry/antisymmetry diagrams of magnetic groups in [26], we notice that the rotation or screw rotation axes that coincide with the cores of invariant tori are coloured black and orthogonally intersect with red-coloured twofold rotation axes. The word “Maximal” in Table 5 implies that invariant tori may persist even if small perturbation that violates the symmetry or antisymmetry of the magnetic group is added to the vector field. A demonstration of Table 5 was given using solenoidal vector fields whose magnetic groups are listed in the table, as depicted in Figs. 10–17. If the cores of invariant tori are not assumed to be straight but allowed to curve, then another magnetic group may be selectable.

---

5 There are some colour misprints in twofold rotation axes in the diagrams of \(I\rho A_{1,32}\) and \(I\rho A'_{1,32'}\) in [26].
for each arrangement. Even when restricted to vector fields of the magnetic groups in Table 5, a variety of invariant tori with curved cores are observed in addition to those with straight cores. Especially, chain-like arrangements of closed invariant tori (with or without knots) in Figs. 10b, c, 15b and 16b are notable. They correspond to the polycatenane lec-y (see [5, Fig. 41]) or its variants. Furthermore, an ordered region formed by I-WP-like invariant tori, whose genus is not 1, is also observed as in Fig. 17c.

In each vector field used for drawing Figs. 10–17, the volume percentage of the ordered region formed by nested invariant tori was estimated by counting the figures with invariant tori with the aid of supervised machine learning (based on the logistic regression method). There exist two kinds of errors in this measurement. One comes from the number \( 4N^3 \) of initial points (10). The larger it becomes, the more accurate the percentage becomes. The other comes from the error in the numerical solution \( r(t) \) of (6). If the upper bound of integration \( t_{\text{max}} \) is larger than our setting \( t_{\text{max}} = 125 \), then the error becomes larger and the ratio of figures with chaotic curves (resp. with invariant tori) goes up (resp. down). Judging from these factors, the volume percentages are considered to be reliable up to order 1%, although reported up to order 0.1%.

As mentioned in Sect. 1, some vector fields considered in this study can be realised in electromagnetic standing waves, in which invariant tori are wound around by electric or magnetic force lines (see [33, Fig. 1]). The application of these invariant tori to materials science may be an interesting topic.

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