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LETTER TO THE EDITOR

The Schur rotation as a simple approach to the transition between quasiperiodic and periodic phases

M Baake, D Joseph and P Kramer

Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, D-7400 Tübingen, Federal Republic of Germany

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Abstract. The recently observed transition of CrNiSi from the octahedral to a cubic phase [1] has a natural mathematical counterpart in terms of a one-parameter Schur rotation. We present the corresponding tilings and the diffraction patterns of δ-scatterers at vertex positions for a series of rotation angles. These angles show up as a length scaling in the patterns and provide a measurable order parameter. We comment on the rational reductions and give two further examples, one on a connection between octagonal and dodecagonal patterns and one on a transition between icosahedral and primitive or body-centred cubic phases.

Recently, Kuo [1] has reported on an interesting transition of a Ct–Ni–Si alloy from a quasiperiodic phase with octagonal symmetry (a so-called octagonal T-phase) to a periodic phase of β-Mn type through various intermediate phases with fourfold symmetry. It is the aim of this short note to present a mathematical basis for the development of explicit structure models of this transition.

In the experiment cited, the octagonal T-phase was looked at along the axis of eightfold symmetry wherefore the electron diffraction image showed d_8 symmetry. Heating the probe, Kuo observed the transition to a periodic phase where d_8 is replaced by d_4. To outline our ideas, we will restrict ourselves to a description of the 2D plane perpendicular to the eightfold axis, which is justified by the structure of the T-phase. In the quasiperiodic case, the diffraction pattern is rather well described by a structure based on the well known octagonal quasilattice [2, 3]. The minimal embedding into higher-dimensional space requires dimension 4 and the canonical choice is the hypercubic lattice $\mathbb{Z}^4$. The physical space $\mathbb{E}_\parallel$ is determined as one of the two unique invariant subspaces WRT d_8 which is a subgroup of $\Omega(4)$, the point group of the lattice $\mathbb{Z}^4$. Here, $d_8 = \langle\langle g_8, s\rangle\rangle$ with the representation

$$T(g_8) := \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad T(s) := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}. \tag{1}$$

This reducible representation of d_8 splits into two inequivalent irreducible ones,

$$UT(g)U^{-1} = T^{\mathrm{red}}(g) \qquad g \in d_8 \tag{2}$$

$$T^{\mathrm{red}}(g) = \begin{pmatrix} c & -s & 0 & 0 \\ s & c & 0 & 0 \\ 0 & 0 & c' & -s' \\ 0 & 0 & s' & c' \end{pmatrix} \qquad \text{and} \qquad T^{\mathrm{red}}(s) := \mathbb{1} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3}$$

where

$$c := \cos(\delta) \qquad s := \sin(\delta) \qquad c' := \cos(5\delta) \qquad s' = \sin(5\delta) \tag{4}$$

and $\delta := 2\pi/8$. The choice of 5δ as rotation angle in $\mathbb{E}_\perp$ might look unusual but does not change the pattern and its structure and facilitates the reduction to the subgroup d_4 since $5 \equiv 1 (\mathrm{mod}\, 4)$. The reduction matrix U in (2) reads

$$U := \sqrt{\tfrac{1}{2}} \begin{pmatrix} 1 & \sqrt{\frac{1}{2}} & 0 & -\sqrt{\frac{1}{2}} \\ 0 & \sqrt{\frac{1}{2}} & 1 & \sqrt{\frac{1}{2}} \\ 1 & -\sqrt{\frac{1}{2}} & 0 & \sqrt{\frac{1}{2}} \\ 0 & -\sqrt{\frac{1}{2}} & 1 & -\sqrt{\frac{1}{2}} \end{pmatrix} \tag{5}$$

wherefrom one can extract the projection images $\pi_\|(\boldsymbol{e}_i)$, $\pi_\perp(\boldsymbol{e}_i)$ of the lattice basis in $\mathbb{E}_\|$ and $\mathbb{E}_\perp$, respectively.

Now, if we restrict the representation of d_8 to the subgroup $d_4 = \langle\langle \boldsymbol{g}_4, \boldsymbol{s} \rangle\rangle$, $\boldsymbol{g}_4 = \boldsymbol{g}_8^2$, we find

$$T^{\mathrm{red}}(\boldsymbol{g}_4) := \mathbb{1} \otimes \begin{pmatrix} \cos(\frac{1}{2}\pi) & -\sin(\frac{1}{2}\pi) \\ \sin(\frac{1}{2}\pi) & \cos(\frac{1}{2}\pi) \end{pmatrix} \qquad \text{and} \qquad T^{\mathrm{red}}(\boldsymbol{s}) \text{ as above} \tag{6}$$

i.e., the representations in $\mathbb{E}_\|$ and $\mathbb{E}_\perp$ are identical. The consequences of this general situation were pointed out in the similar situation of the tetrahedral group [4]: According to Schur's lemma, the invariant subspaces $\mathbb{E}_\|$ and $\mathbb{E}_\perp$ are no longer unique; we now have a non-trivial phase freedom,

$$[T^{\mathrm{red}}(\boldsymbol{h}), R(\phi)] = 0 \qquad \boldsymbol{h} \in d_4 \qquad \text{with } R(\phi) := \begin{pmatrix} \cos(\phi) & -\sin(\phi) \\ \sin(\phi) & \cos(\phi) \end{pmatrix} \otimes \mathbb{1}. \tag{7}$$

Therefore we have

$$T^{\mathrm{red}}(\boldsymbol{h}) = U_\phi T(\boldsymbol{h}) U_\phi^{-1} \qquad \boldsymbol{h} \in d_4 \tag{8}$$

with

$$U_\phi = R(\phi) \cdot U \qquad U_0 = U. \tag{9}$$

This means that we obtain a whole one-parameter family of tilings with d_4 symmetry by rotating $\mathbb{E}_\|$ according to the Schur rotation $R(\phi)$ with the 'Schur angle' ϕ. For a dense but countable set of angles ϕ one finds periodic tilings; the generic case is the quasiperiodic one.

It is illustrative to write down the reduction matrix explicitly,

$$U_\phi := \sqrt{\tfrac{1}{2}} \begin{pmatrix} \tilde{c} - \tilde{s} & \sqrt{\frac{1}{2}}(\tilde{c} + \tilde{s}) & 0 & -\sqrt{\frac{1}{2}}(\tilde{c} + \tilde{s}) \\ 0 & \sqrt{\frac{1}{2}}(\tilde{c} + \tilde{s}) & \tilde{c} - \tilde{s} & \sqrt{\frac{1}{2}}(\tilde{c} + \tilde{s}) \\ \tilde{c} + \tilde{s} & -\sqrt{\frac{1}{2}}(\tilde{c} - \tilde{s}) & 0 & \sqrt{\frac{1}{2}}(\tilde{c} - \tilde{s}) \\ 0 & -\sqrt{\frac{1}{2}}(\tilde{c} - \tilde{s}) & (\tilde{c} + \tilde{s}) & -\sqrt{\frac{1}{2}}(\tilde{c} - \tilde{s}) \end{pmatrix} \tag{10}$$

$\tilde{c} = \cos(\phi)$, $\tilde{s} = \sin(\phi)$, because one can see that $\pm\boldsymbol{e}_1$ and $\pm\boldsymbol{e}_3$ on the one hand and $\pm\boldsymbol{e}_2$ and $\pm\boldsymbol{e}_4$ on the other hand build, in the projection to $\mathbb{E}_\|$ or to $\mathbb{E}_\perp$, two regular 4-stars with a relative angle of 45° independent of ϕ. Therefore, the influence of ϕ is on the size of the 4-stars only, and one finds the relative scale to be

$$\eta(\phi) = \frac{|\pi_\|(\boldsymbol{e}_1)|}{|\pi_\|(\boldsymbol{e}_2)|} = \frac{|\pi_\perp(\boldsymbol{e}_2)|}{|\pi_\perp(\boldsymbol{e}_1)|} = \frac{|\cos(\phi) - \sin(\phi)|}{|\cos(\phi) + \sin(\phi)|} = |\tan(\phi - \pi/4)|. \tag{11}$$

The quantity η is just one simple possibility to give ϕ a geometric meaning in $\mathbb{E}_\parallel$ alone and contains nothing new in comparison with ϕ. It can be measured from the diffraction image if one has found a consistent indexing of the spots in the (generic) quasiperiodic case, where $\pi_\parallel(e_1), \ldots, \pi_\parallel(e_4)$ are linearly independent over the integers.

The reduction is rational if and only if $\tan\phi = (p - q\sqrt{2})/(p + q\sqrt{2})$ with coprime integers p and q. Then, we find square lattices $\Gamma_\parallel$ and $\Gamma_\perp$ in $\mathbb{E}_\parallel$ and $\mathbb{E}_\perp$, respectively, such that $\Gamma_\parallel \times \Gamma_\perp$ is a sublattice of $\mathbb{Z}^4$. Let us choose $\Gamma_\parallel$ and $\Gamma_\perp$ to be maximal WRT this property. Then, both $\Gamma_\parallel$ and $\Gamma_\perp$ possess the same lattice constant which turns out to be $\sqrt{p^2+2q^2}$ for p odd and $\sqrt{\frac{1}{2}p^2+q^2}$ for p even. Consequently, the index of the translation subgroup compatible with $\mathbb{E}_\parallel \oplus \mathbb{E}_\perp$ is

$$I = [\mathbb{Z}^4 : \Gamma_\parallel \times \Gamma_\perp] = \begin{cases} (p^2+2q^2)^2 & \text{if } p \text{ odd} \\ \frac{1}{4}(p^2+2q^2)^2 & \text{if } p \text{ even.} \end{cases} \tag{12}$$

From this formula one can try to pick out a suitable periodic phase with the right lattice constant relative to the octagonal quasiperiodic phase at $\phi = 0°$, say. Here, the transition to a periodic phase leads to a tiling with the corresponding periodicity.

To illustrate the mechanism, we show in figure 1 a series of 6 patterns obtained by the standard dualization method [5, 6] for Schur angles between $\phi = 0°$ ($\eta = 1$, octagonal case) and $\phi = 45°$ ($\eta = 0$, periodic case with minimal period). The corresponding kinematic diffraction of δ-scatterers at vertex positions is presented in figure 2 (for details on the construction algorithm and the Fourier formulas used here, see [6, 7]). Figure 2(a) ($\phi = 0°$) presents the eightfold symmetry of the octagonal pattern (figure 1(a)). In figure 2(b) ($\phi = 2°$) the exact eightfold symmetry is broken leaving only fourfold symmetry behind, although many similarities to the eightfold case can still be seen. Figure 2(c) ($\phi = 12°$) and figure 2(d) ($\phi = 20°$) show the transition within the fourfold symmetry. In figure 2(e) ($\phi = 30°$) one can see an obvious step towards the periodic phase with the shortest lattice constant (figure 1(f), figure 2(f)). The small spots which surround the higher intensities will move towards the big spots and decrease simultaneously. Finally, this leads to the periodic case of figure 2(f) ($\phi = 45°$).

Although we have not explicitly calculated the transition from the octagonal to the periodic phase by means of Landau theory, it is plausible that the Schur rotation with a single parameter provides a correct tool to do so and the dimensionless quantity η defined in (11) is the natural candidate for an order parameter which is directly accessible in experiment.

At this point, we would like to mention two other interesting applications of Schur rotations. First, the same technique presented above can be used for the root lattice D_4 to connect quasiperiodic phases with eight- and twelvefold symmetry by a continuous transition that preserved fourfold symmetry [8]. This should prove useful for the description of $V_{15}Ni_{10}Si$ which can coexist in both phases with the same stoichiometry [9, 10]. Like in the $\mathbb{Z}^4$ case one can also get infinitely many periodic phases. Second, the transition between the primitive icosahedral phase and a cubic phase mentioned earlier was obtained by a Schur rotation [4, 11] which preserved tetrahedral symmetry.

Let us explain the situation with the icosahedral group in a little more detail, starting from the hypercubic lattice $\mathbb{Z}^6$. Its point group is the group $\Omega(6)$ [12] which contains the icosahedral group Y_h in such a way that the canonical representation of $\Omega(6)$, when reduced to Y_h, splits into two inequivalent 3D irreps of Y_h [4]:

$$T^{\text{red}}(g) = UT(g)U^{-1} \qquad g \in Y_h \tag{13}$$

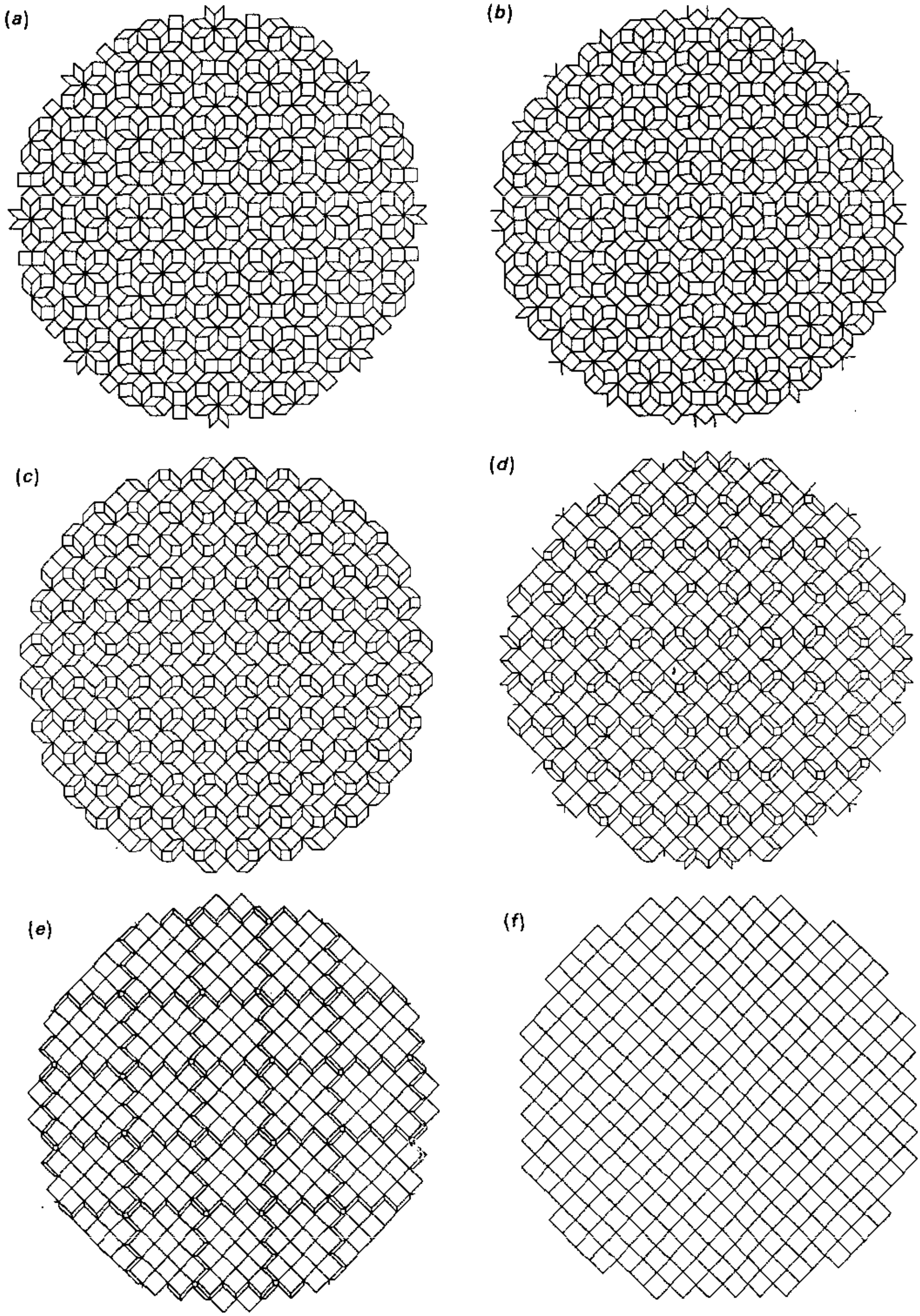

Figure 1. (a) The octagonal quasiperiodic pattern, $\phi = 0°$. (b) A quasiperiodic pattern with fourgold symmetry obtained at $\phi = 2°$, (c) $\phi = 12°$, (d) $\phi = 20°$, (e) $\phi = 30°$, (f) a periodic pattern with fourfold symmetry obtained at $\phi = 45°$.

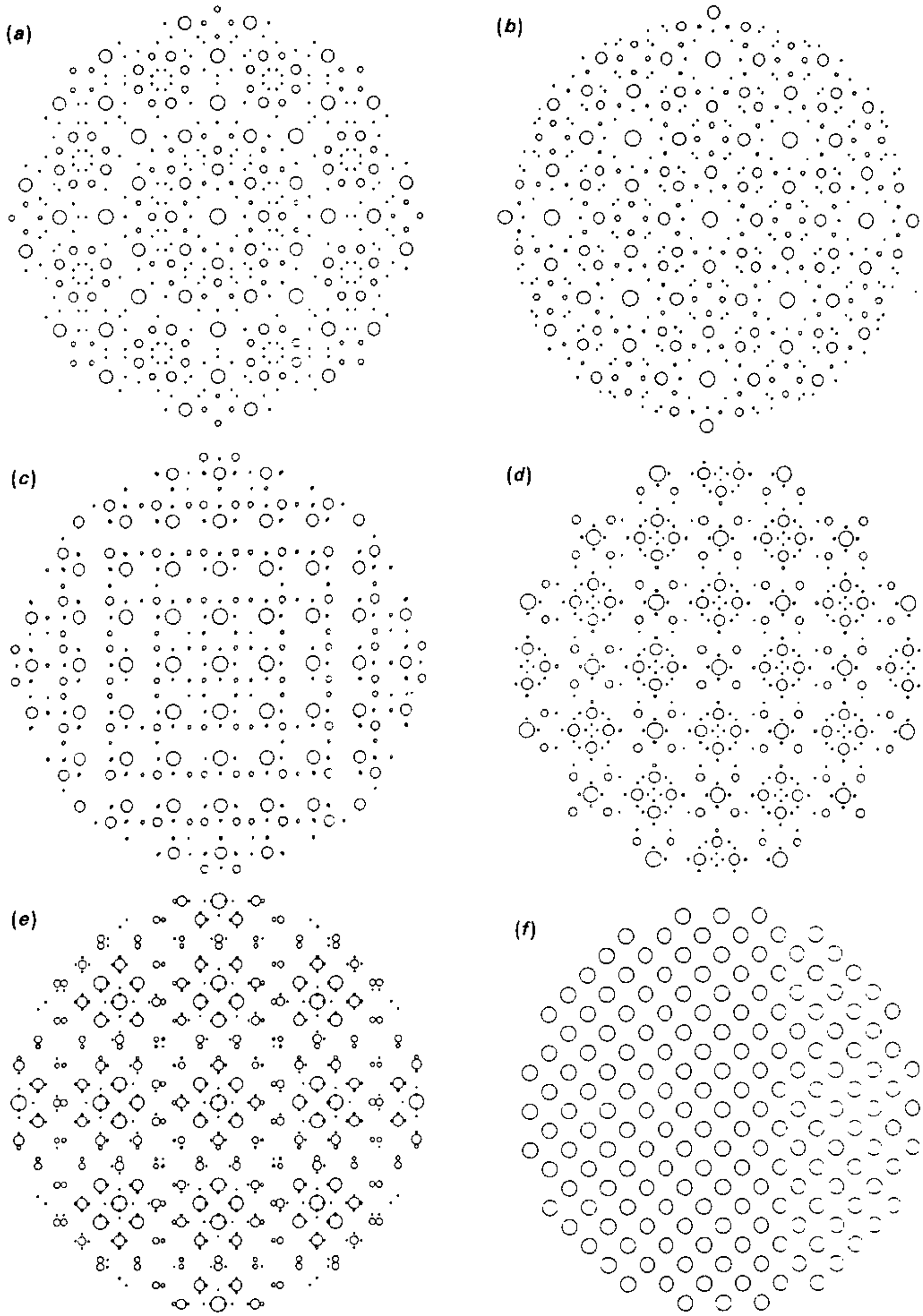

Figure 2. (*a*) The Fourier image of the octagonal quasiperiodic pattern, $\phi = 0°$. (*b*) The Fourier image of the quasiperiodic pattern with fourfold symmetry obtained at $\phi = 2°$, (*c*) $\phi = 12°$, (*d*) $\phi = 20°$, (*e*) $\phi = 30°$, (*f*) the Fourier image of the periodic pattern with fourfold symmetry obtained at $\phi = 45°$.

with

$$U := \sqrt{\tfrac{1}{2}}\begin{pmatrix} 0 & c & s & 0 & c & -s \\ s & 0 & c & -s & 0 & c \\ c & s & 0 & c & -s & 0 \\ 0 & -s & c & 0 & -s & -c \\ c & 0 & -s & -c & 0 & -s \\ -s & c & 0 & -s & -c & 0 \end{pmatrix} \tag{14}$$

and $c = \cos(\alpha)$, $s = \sin(\alpha)$, $\alpha = \frac{1}{2}\tan^{-1}(2)$.

On the other hand, when further restricted to the tetrahedral subgroup, one obtains two identical 3D irreps and thus again the phase freedom for a Schur rotation. Let us take $U = U(\phi)$ as the corresponding reduction matrix where $\phi = \alpha$ gives back (13). Now, for $\tan(\phi) = p/q$, we obtain a rational reduction and we find 3D sublattices $\Gamma_\parallel$ and $\Gamma_\perp$ of $\mathbb{Z}^6$ in $\mathbb{E}_\parallel$ and $\mathbb{E}_\perp$, respectively, with index

$$I = [\mathbb{Z}^6 : \Gamma_\parallel \times \Gamma_\perp] = \begin{cases} 2(p^2+q^2)^3 & \text{if } 0 \not\equiv p \equiv q \bmod 2 \\ 8(p^2+q^2)^3 & \text{if } p \not\equiv q \bmod 2 \end{cases} \tag{15}$$

where we have taken p and q coprime.

The two situations correspond to a body centred cubic lattice ($p \equiv q \bmod 2$) or to a primitive cubic lattice ($p \not\equiv q \bmod 2$) in $\mathbb{E}_\parallel$. All 3D lattices $\Gamma_\parallel$ obtained from rational reduction possess cubic point symmetry which does, however, stem from a $\mathbb{Z}^6$ symmetry only for $\phi = k\pi/4$, $k \in 2\mathbb{Z}+1$. Precisely in the latter cases also the complete structure obtained by the projection method will show the cubic symmetry. In all the other cases, the full cell structure has only tetrahedral point symmetry and the additional, non-tetrahedral point transformations cannot be lifted to a symmetry of $\mathbb{Z}^6$, if we keep the specific embedding of the tetrahedrl group T. This embedding is required in order to get T simultaneously as a subgroup of Y_h and hence to get the link to the quasicrystalline icosahedral phase by Schur rotation.

Let us briefly describe the analogue of (11) where a candidate for an order parameter was given. Here, we have the vectors $e_1+e_2+e_3$ and $e_4+e_5+e_6$ as natural candidates, wherefore we define

$$\eta(\phi) = \frac{|\pi_\parallel(e_1+e_2+e_3)|}{|\pi(e_4+e_5+e_6)|} = \frac{|\cos(\phi)-\sin(\phi)|}{|\cos(\phi)+\sin(\phi)|} = |\tan(\phi - \pi/4)|. \tag{16}$$

These findings are summarized in the following diagram, where—according to the previous remark—the reduction at $\phi = 45°$ is singled out as the rational reduction via the full cubic group $\Omega(3)$ while the cubic symmetry of $\phi = 0°$ is accidental and the reduction leads only to the tetrahedral group T.

$$\begin{tikzcd}
 & \Omega(6) \arrow[dl] \arrow[d] \arrow[dr] & \\
\begin{array}{c} T \\ \phi = 0°,\ \eta = 1 \\ \text{primitive cubic} \end{array} \arrow[dr] & \begin{array}{c} Y_h \\ \phi \simeq 31.7°,\ \eta = \tau^{-3} \\ \text{isocahedral} \end{array} \arrow[d] & \begin{array}{c} \Omega(6) \\ \phi = 45°,\ \eta = 0 \\ \text{bcc} \end{array} \arrow[dl] \\
 & T &
\end{tikzcd} \tag{17}$$

Here, $\tau = \frac{1}{2}(1+\sqrt{5})$ is the golden mean. It is interesting to note that precisely the icosahedral and the bcc phase seem to be related experimentally [13].

Motivated by experimental observations we have outlined the simplest possible scheme of transitions between different phases that maintain the maximal common symmetry. This was achieved by the so-called Schur rotation. Although this is an operation in higher-dimensional space, the rotation angle gives rise to a measurable quantity in physical space $\mathbb{E}_{\|}$. Therefore we think that it could be useful for an explicit structure model as well as for understanding similarities between 'neighbouring' phases.

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