Non-linear generalized elasticity of icosahedral quasicrystals

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Abstract. Quasicrystals can carry, in addition to the classical phonon displacement field, a phason displacement field, which requires a generalized theory of elasticity. In this paper, the third-order strain invariants (including phason strain) of icosahedral quasicrystals are determined. They are connected with 20 independent third-order elastic constants. By means of non-linear elasticity, phason strains with icosahedral irreducible \( \Gamma^4 \)-symmetry can be obtained by phonon stress, which is impossible in linear elasticity.

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1. Introduction

Apart from the ordinary phonon degrees of freedom, quasicrystals (QC) have phason degrees of freedom, referring to relative shifts of the constituent density waves [1, 2]. Therefore, and due to their lack of translational order, quasicrystalline structures are usually constructed as irrational cut of a decorated hyperspace structure by physical space \( E \). The phason degrees of freedom are connected with the displacement field along the orthogonal space \( E^\perp \). The generalized elasticity is described in terms of spatially varying phonon and phason displacement fields [1, 2].

Icosahedral QC have three phonon and three phason degrees of freedom and associated components of a displacement field. Linear elastic theory provides five independent second-order elastic constants, two belonging to pure phonon elasticity, two to pure phason elasticity and one to a coupling between phonons and phasons.

Within linear phonon elasticity, icosahedral QC behave essentially like isotropic media [1]. Faithful icosahedral symmetry exists for physical properties described by tensors of rank \( N \geq 5 \) only [1]. Accordingly, the non-linear elasticity of icosahedral QC is anisotropic [1].

Fundamental research on classical non-linear elasticity has been performed many years ago [3, 4]. The authors of [3, 11, 12, 13] have already determined the four linearly independent, icosahedral elastic tensors of rank six, related to third-order phonon elastic invariants. Contrary to this, in the isotropic case one has only three independent third-order phonon elastic invariants, or elastic constants. Ishii [14] has calculated the pure phason third-order icosahedral invariants. The aim of this paper is to generalize the classical non-linear elasticity and to determine all third-order icosahedral elastic invariants, which occur when phason strains are included. The

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idea leading to this work was to find a possibility to generate phason $\Gamma^4$-strain in icosahedral QC by phonon stress, which is impossible within linear elasticity.

2. Generalized elastic theory of icosahedral QC

According to their icosahedral diffraction pattern, the mass density of icosahedral QC is a sum of density waves indexed by a reciprocal lattice $L$ of icosahedral symmetry: $\rho(x) = \sum_{k \in L} \rho_k \exp[i \mathbf{k} \cdot x] = \sum_{k \in \mathbb{L}} |\rho_k| \exp[i(\mathbf{k} \cdot x + \phi_k)]$. The phases $\phi_k$ of the basis vectors of $\mathbb{L}$ are six degrees of freedom, parametrized by the phonon and phason displacement fields $u$ and $w$ via $\phi_k = \phi_{k,0} - \mathbf{k} \cdot u - \mathbf{k} \cdot w$. Here, $\mathbf{k} \parallel \mathbf{k}$ and $\mathbf{k} \perp$ are the projections of reciprocal six-dimensional hyperlattice vectors onto $E^\parallel$ and $E^\perp$, respectively. The phonon and phason displacement fields $\mathbf{u}$ and $\mathbf{w}$ are the projections of the hyperspace displacement field $\mathbf{u} \oplus \mathbf{w}$ onto $E^\parallel$ and $E^\perp$, respectively.

We denote the position of a point in the undistorted QC $\mathbf{a}$ and the corresponding position in the distorted structure $\mathbf{x}$, where $\mathbf{x} = \mathbf{u} + \mathbf{a}$. In the Lagrangian scheme, all quantities depend on the variable $\mathbf{a} \ [8]$. The phonon strain tensor $\eta^u$ has its components of the classical symmetric form

$$\eta^u_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial a_j} + \frac{\partial u_j}{\partial a_i} \right) + \frac{1}{2} \frac{\partial u_k}{\partial a_i} \frac{\partial u_k}{\partial a_j}$$

or, written in terms of the Jacobian $F_{ij} = \frac{\partial x_i}{\partial a_j}$, $\eta^w_{ij} = \frac{1}{2} (F_{ki} F_{kj} - \delta_{ij})$. This strain tensor is free of rigid rotations. The phason displacement gradient $\frac{\partial w_i}{\partial a_j}$ splits into a $\Gamma^4$ and a $\Gamma^3$ part (see [8]), and both are assumed to increase the elastic energy $\mathbb{E} [\mathbb{E} \ [3]$. Therefore, we have a phason strain tensor $\eta^w$ with

$$\eta^w_{ij} = \frac{\partial w_i}{\partial a_j}.$$  

In the linear limit $|\frac{\partial u}{\partial a}| \ll 1$, the components of $\eta^u$ take their well-known shape $\eta^u_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial a_j} + \frac{\partial u_j}{\partial a_i} \right)$.

The isothermal Helmholtz free energy $F(\eta^u, \eta^w)$ per undistorted volume can be expanded into the Taylor series

$$F = \frac{1}{2} C^{ab}_{ijkl} \eta^a_{ij} \eta^b_{kl} + \frac{1}{6} C^{abc}_{ijklmn} \eta^a_{ij} \eta^b_{kl} \eta^c_{mn} + \ldots = \frac{1}{2} \sum_{ij} C^{ab}_{ij} \eta^a_i \eta^b_j + \frac{1}{6} \sum_{ijklmn} C^{abc}_{ijklmn} \eta^a_i \eta^b_j \eta^c_k + \ldots,$$

with $C^{ab}_{ijkl}$ being second-order and $C^{abc}_{ijklmn}$ third-order cartesian elastic constants due to Brugger [6], which is perhaps the most familiar notation $i, j, k, l, m, n \in \{1, 2, 3\}$, $a, b \in \{u, w\}$. In the right part of (3), the irreducible strain components of Appendix $\mathbb{A}$ are used. Here we have, e.g., $i \in \{1, \ldots, 6\}$ if $a = u$ and $i \in \{1, \ldots, 9\}$ if $a = w$. Because of the index permutation symmetries and the symmetries of the QC, not all of these $C$’s are independent. If the elastic energy is to be written with independent elastic constants $C^{ab}_i$ and $C^{abc}_i$ of second and third order only, one has to use the invariants $I^{ab}_i$ and $I^{abc}_i$ of the generalized elasticity:

$$F = C^{ab}_i I^{ab}_i + C^{abc}_i I^{abc}_i + \ldots.$$  

These invariants (and also the expansions $\mathbb{B}$) must fulfill the condition $I(g \eta^u, g \eta^w) = I(\eta^u, \eta^w)$ for any transformation $g$ of the icosahedral group $Y$ (or $Y_0$). Clearly, symmetries like $I^{uw}_i = I^{uw}_i = \ldots$ and $C^{uw}_i = C^{uw}_i = \ldots$ are assumed to hold. The elastic constants of $\mathbb{B}$ follow from appropriate repeated differentiation with respect to components of $\eta^u$ and $\eta^w$. 

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A generalization of the classical result [10] shows that the generalized Piola-Kirchhoff stresses $t^u$ and $t^w$, which are measured in the undistorted state, have components

$$t^a_{ij} = \frac{\partial F}{\partial \eta^a_{ij}} = C^{ab}_{ijkl} \eta^b_{kl} + \frac{1}{2} C^{abc}_{ijklmn} \eta^b_{kl} \eta^c_{mn} + \ldots = C^{ab}_{k} \frac{\partial I^b_k}{\partial \eta^a_{ij}} + C^{abc}_{k} \frac{\partial I^b_{k}^c}{\partial \eta^a_{ij}} + \ldots \quad (5)$$

The irreducible components of $t^u$ and $t^w$ have the same form as those of $\eta^u$ and $\eta^w$, and it is $t^u_{ij} = \frac{\partial F}{\partial \eta^u_{ij}}$, where the possible pairs of $(a, i)$ are again evident from Appendix A. Cauchy stresses $\sigma^u$ and $\sigma^w$ are measured in the distorted state. They follow immediately from the Piola-Kirchhoff stresses [8]. Because $E^\perp$ remains unchanged even for a finite deformation, the phasonic case must be treated with some care:

$$\sigma^u_{ij} = \Delta^{-1} F_{ik} F_{jk} t^u_{kl}, \quad \sigma^w_{ij} = \Delta^{-1} F_{jk} t^w_{ik}, \quad (6)$$

where $\Delta = \text{det} F$.

Since our intention is to produce certain strains by means of applied stresses, we should rather work with the isothermal Gibbs enthalpy $G(t^u, t^w)$ [14]:

$$G = S^{ab}_{i} I^a_{i} + S^{abc}_{i} I^a_{i}^{bc} + \ldots \quad (7)$$

$S^{ab}_{i}$ and $S^{abc}_{i}$ are independent elastic compliances, and the same invariants as in (4) appear, but this time formulated with components of $t^u$ and $t^w$. One obtains the strain-stress relations

$$\eta^a_{ij} = -\frac{\partial G}{\partial t^a_{ij}} = -S^{ab}_{i} t^b_{kl} - \frac{1}{2} S^{abc}_{i} t^b_{kl} t^c_{mn} + \ldots = -S^{ab}_{k} \frac{\partial I^a_k}{\partial t^a_{ij}} - S^{abc}_{k} \frac{\partial I^a_{k}^c}{\partial t^a_{ij}} + \ldots \quad (8)$$

The irreducible form hereof is obvious.

3. The elastic invariants

First thing of all is to note the transformation behaviour of the strain tensors [3], which follows from the transformation behaviour of vectors in $E^\parallel$ and $E^\perp$:

$$u : \quad \Gamma^3 \otimes \Gamma^3, \quad w : \quad \Gamma^3 \otimes \Gamma^3 = \Gamma^4 \oplus \Gamma^5. \quad (9)$$

Index $s$ means symmetrized. The irreducible components of the strain tensors are given in Appendix A, and the associated transformation matrices are displayed in Table A1. They are deduced from the transformation of the cartesian strain tensors $\eta^u = \eta^u_{ij}$, where $\eta^u_{ij}$ is a basis deformation with component $ij$ being 1 and all others 0: $g \eta^u = \eta^u_{ij}$, $(g \eta^u)_{ij} = (g \eta^u)_{ij}$, $(g \eta^u)_{ij} = D^u_{ik}(g) D^u_{kj}(g) \eta^u_{kl}$, $(g \eta^u)_{ij} = D^u_{ik}(g) D^u_{kj}(g) \eta^u_{kl}$, and $D^u(g), D^w(g)$ are the coordinate transformation matrices of Table A1.

The characters of symmetrized product representations $D = (\tilde{D} \otimes \tilde{D})_s$ and $D = (\tilde{D} \otimes \tilde{D} \otimes \tilde{D})_s$, respectively, of one and the same representation $\tilde{D}$, which the terms occuring in (3) transform after, are

$$\chi^D(g) = \frac{1}{2} \left[ \chi^{\tilde{D}}(g)^2 + \chi^{\tilde{D}}(g^2) \right] \quad \text{and}$$

$$\chi^D(g) = \frac{1}{6} \left[ \chi^{\tilde{D}}(g)^3 + 3 \chi^{\tilde{D}}(g^2) \chi^{\tilde{D}}(g) + 2 \chi^{\tilde{D}}(g^3) \right]. \quad (10)$$
Table 1. Tabulation of symmetrized third-order vector spaces. In the last column, all possible third-order expressions consisting of irreducible strains, referring to orthonormal basis sets, are listed.

| Case   | Dimension dim of symmetrized space | Components with respect to an orthonormal basis set                                                                 |
|--------|-----------------------------------|-------------------------------------------------------------------------------------------------------------------|
| uuu    | 56                                | \((\eta_i^u)^3, \sqrt{3}(\eta_i^u)^2\eta_j^u, \sqrt{2}\eta_i^u\eta_j^u\eta_k^w (i \neq j \neq k \neq i)\) |
| uww    | 189                               | \((\eta_i^u)^2\eta_j^w, \sqrt{2}\eta_i^u\eta_j^u\eta_k^w (i \neq j)\)                                                   |
| uww    | 270                               | \(\eta_i^w(\eta_j^w)^2, \sqrt{2}\eta_i^u\eta_j^w\eta_k^w (j \neq k)\)                                                  |
| www    | 165                               | \((\eta_i^w)^3, \sqrt{3}(\eta_i^w)^2\eta_j^w, \sqrt{2}\eta_i^u\eta_j^w\eta_k^w (i \neq j \neq k \neq i)\) |

Herewith, the following Clebsch-Gordan series for the representations acting in the respective symmetrized product spaces of second-order tensors are straightforward and given below in the order uuu, uww, uww, uww, uww, uww, uww, www [17]:

\[
[(\Gamma^1 \oplus \Gamma^5) \otimes (\Gamma^1 \oplus \Gamma^5)]_s = 2 \Gamma^1 \oplus \Gamma^4 \oplus 3 \Gamma^5, \\
(\Gamma^1 \oplus \Gamma^5) \otimes (\Gamma^4 \oplus \Gamma^5) = \Gamma^1 \oplus 2 \Gamma^3 \oplus 2 \Gamma^3 \oplus 4 \Gamma^4 \oplus 5 \Gamma^5, \\
[(\Gamma^4 \oplus \Gamma^5) \otimes (\Gamma^1 \oplus \Gamma^5)]_s = 2 \Gamma^1 \oplus \Gamma^3 \oplus \Gamma^3 \oplus 3 \Gamma^4 \oplus 5 \Gamma^5, \\
[(\Gamma^1 \oplus \Gamma^5) \otimes (\Gamma^1 \oplus \Gamma^5) \otimes (\Gamma^1 \oplus \Gamma^5)]_s = 4 \Gamma^1 \oplus \Gamma^3 \oplus 4 \Gamma^3 \oplus 4 \Gamma^4 \oplus 6 \Gamma^5, \\
[(\Gamma^1 \oplus \Gamma^5) \otimes (\Gamma^4 \oplus \Gamma^5)]_s = 4 \Gamma^1 \oplus 8 \Gamma^3 \oplus 8 \Gamma^3 \oplus 13 \Gamma^4 \oplus 17 \Gamma^5, \\
(\Gamma^1 \oplus \Gamma^5) \otimes [(\Gamma^4 \oplus \Gamma^5) \otimes (\Gamma^1 \oplus \Gamma^5)]_s = 7 \Gamma^1 \oplus 11 \Gamma^3 \oplus 11 \Gamma^3 \oplus 18 \Gamma^4 \oplus 25 \Gamma^5, \\
[(\Gamma^4 \oplus \Gamma^5) \otimes (\Gamma^1 \oplus \Gamma^5) \otimes (\Gamma^4 \oplus \Gamma^5)]_s = 5 \Gamma^1 \oplus 7 \Gamma^3 \oplus 7 \Gamma^3 \oplus 12 \Gamma^4 \oplus 14 \Gamma^5.
\]

We see that we have the following numbers of invariants: 2 (uu), 1 (uw), 2 (ww), 4 (uuu), 4 (uww), 7 (uww), 5 (www). These numbers have already been calculated in an earlier work [3].

The second-order invariants can readily be written as simple scalar products \(\eta^{u, 1} \cdot \eta^{u, 1}, \eta^{u, 5} \cdot \eta^{u, 5}, \eta^{w, 5} \cdot \eta^{w, 5}, \eta^{w, 4} \cdot \eta^{w, 4}, \eta^{w, 5} \cdot \eta^{w, 5}\) of vectors containing the irreducible strain components (see Appendix A and [19]). Of course, most of the third-order invariants are more complicated.

In Table 1, the symmetrized third-order vector spaces are specified in more detail. Some terms must be weighted with factors to become components for an orthonormal basis set and to transform orthogonal among all others. The third-order elastic invariants are the components for the basis vectors of the identity representation.

Basis vectors for an irreducible group representation \(\alpha\) are obtained by means of the projection operators \(P^\alpha_{ik} = \frac{1}{|G|} \sum_{g \in G} D^\alpha_{ik}^*(g)D(g)\) [20], with \(D(g)\) being the linear operators acting on the full (reducible) vector space (see Table 3). These projectors have the property \(P^\alpha_{ik}e^\beta_{ij} = \delta_{\alpha\beta}\delta_{jk}e^\beta_{ij}\). Here, \(e^\beta_{ij}\) is a basis vector transforming as the index \(j\) of the irreducible representation \(\beta\), and \(1 \leq i \leq n^2_D\), where \(n^2_D\) is the multiplicity of \(\beta\) in \(D\). To split up the full vector space into subspaces spanned by orthogonal irreducible basis vectors, the vectors \(e^\alpha_{i1} \in \text{Im} P^\alpha_{i1}\), \(e^\alpha_{i1} \perp e^\alpha_{j1}\) for \(i \neq j\), must be calculated. The other basis vectors are then \(e^\alpha_{ij} = P^\alpha_{ji}e^\alpha_{i1}\), where \(i \in \{1, \ldots, n^2_D\}\), \(j \in \{2, \ldots, d_{\alpha}\}\). The operators \(D(g)\) are calculated as orthogonal transformation matrices for the components of Table 1.

Herewith, the third-order invariants can be found directly from the full spaces of Table 1. However, we picked the third-order invariants by the following procedure:

\[
\eta_i^u = \sqrt{3}(\eta_i^u)^2, \eta_j^w = \sqrt{2}\eta_i^u\eta_j^w \eta_k^w, \eta_i^w(\eta_j^w)^2, \eta_i^w(\eta_j^w)^2, \eta_i^w\eta_j^w \eta_k^w (i \neq j \neq k \neq i).
\]
Calculate the second-order irreducible components for the irreducible representations $\Gamma^1$, $\Gamma^4$ and $\Gamma^5$ occurring in the first and third series of (11). Then set up all possible invariant scalar products with irreducible components of $\eta^u$ and $\eta^w$ and throw away occurring linearly dependent invariants.

Since the components for different irreducible representations do not mix under transformation, another very elegant method, leading immediately to the ordering with respect to irreducible representations described below, is to expand the triple products of (11) completely, for example $[(\Gamma^4 \oplus \Gamma^5) \otimes (\Gamma^4 \oplus \Gamma^5) \otimes (\Gamma^4 \oplus \Gamma^5)]_s = (\Gamma^4 \otimes \Gamma^4 \otimes \Gamma^4)_s \oplus [(\Gamma^4 \otimes \Gamma^4)_s \otimes (\Gamma^5 \otimes \Gamma^5)]_s \oplus (\Gamma^5 \otimes \Gamma^5 \otimes \Gamma^5)_s$, and search the invariants for each of the arising triple products of irreducible representations separately.

The third-order invariants are listed in Appendix B. They consist of components of as few different irreducible representations as possible (see Table B1). For each of the four cases, they are orthonormal, i.e. $\sum_{k=1}^{dim} v_{i,k} v_{j,k} = \delta_{ij}$, where $dim$ are the respective numbers in the second column of Table I and $v_{i,k}$ is the coefficient of the third-order term $k$ in the invariant $i$. Furthermore, we have tried on the one hand to choose the invariants as short as possible and on the other hand to bring them to a suitable form for comparing with each other and with the invariants of [14] (see Appendix B and Appendix C for details).

4. Discussion

From (11), there are 20 independent third-order elastic invariants, or elastic constants, describing the non-linear elasticity of icosahedral QC. Since there exist four $uvw$-invariants, we have four non-linear phonon-phason couplings. The other third-order invariants are unsuitable if one wants to generate phason strains or stresses. Despite of this, from all the third-order invariants, the four $uvw$ ones will play the most important role because of their influence on the phonon wave propagation. To our knowledge, these third-order phonon elastic constants have not been determined for QC so far.

Generating phason $\Gamma^4$-strains from phonon stresses now is possible through the invariant $I^{uw}$. Due to (8),

$$\eta^u_i = \frac{S^{uw}}{20} \sqrt{30} \left[3 (t_3^w)^2 + 3 (t_2^w)^2 - 2 (t_1^w)^2 - 2 (t_4^w)^2 - 2 (t_5^w)^2 \right],$$

$$\eta^w_2 = -\frac{S^{uw}}{2} \sqrt{3} \left(2 t_3^u t_4^w + \sqrt{2} t_5^w t_6^w \right),$$

$$\eta^w_3 = \frac{S^{uw}}{2} \left(3 t_2^u t_5^w + \sqrt{3} t_3^u t_5^w - \sqrt{6} t_4^u t_6^w \right),$$

$$\eta^w_4 = -\frac{S^{uw}}{2} \left(3 t_2^u t_6^w - \sqrt{3} t_3^u t_6^w + \sqrt{6} t_4^u t_5^w \right).$$

(12)

Here, a perhaps unexpected factor of 3 is present because of the summation rule in (8). From (12), it is obvious that phason $\Gamma^4$-strains arise from shear stresses $t_2^u, \ldots, t_6^u$. $\eta^u_i$ is obtained, for example, by applying the shear stress $t_3^w \equiv t$ and all other $t_j^w = 0$, $\eta^w_2$ by applying $t_3^w \equiv t$, $t_4^w \equiv \sqrt{3}/2 t$, $\eta^w_3$ by applying $t_3^w \equiv t$, $t_5^w \equiv \sqrt{3}/2 t$ and $\eta^w_4$ via $t_3^w \equiv t$, $t_6^w \equiv \sqrt{3}/2 t$. The magnitude of an eventually existing phonon $\Gamma^4$-stress, which is hydrostatic pressure $t_1^w$, has only an indirect effect on the phason $\Gamma^4$ strains, due to the pressure dependence of elastic compliances. Note that the $\Gamma^4$-symmetry is unlikely to exist without simultaneous phason $\Gamma^5$-symmetry, which is generated by
shear stresses even in the linear, but also in the non-linear regime according to higher order compliances (see Table B.1).

Another possibility to obtain phason Γ^4-strains is, for example, the quartic electrostriction [22].

**Appendix A. Icosahedral irreducible strains**

The icosahedral irreducible strain components given below are from [21]. They refer to the same coordinate systems as in [15, 19, 22]. In Table A.1, the icosahedral irreducible transformation matrices are given, which the irreducible strains and stresses transform after. Other coordinate systems in use are compared to our in some detail in [15].

\[
\eta_{u,1}^{w} = \eta_{u}^{w} = \frac{1}{\sqrt{3}}(\eta_{11}^{u} + \eta_{22}^{u} + \eta_{33}^{u}),
\]

\[
\eta_{u,5}^{w} = \left(\begin{array}{c}
\eta_{2}^{w} \\
\eta_{3}^{w} \\
\eta_{4}^{w} \\
\eta_{5}^{w} \\
\eta_{6}^{w}
\end{array}\right) = \left(\begin{array}{c}
\frac{1}{2\sqrt{3}}(-\tau_{11}^{w} + \frac{1}{\sqrt{3}}\eta_{22}^{w} + (\tau + \frac{1}{\sqrt{3}})\eta_{33}^{w}) \\
\frac{1}{2}(\frac{1}{\tau_{11}^{w}} - \tau_{33}^{w}) \\
\frac{1}{\sqrt{2}}(\eta_{21}^{w} + \eta_{31}^{w}) \\
\frac{1}{\sqrt{2}}(\eta_{23}^{w} + \eta_{32}^{w}) \\
\frac{1}{\sqrt{2}}(\eta_{31}^{w} + \eta_{13}^{w})
\end{array}\right),
\]

\[
\eta_{w,4}^{u} = \left(\begin{array}{c}
\eta_{1}^{w} \\
\eta_{2}^{w} \\
\eta_{3}^{w} \\
\eta_{4}^{w} \\
\eta_{5}^{w} \\
\eta_{6}^{w}
\end{array}\right) = \left(\begin{array}{c}
\frac{1}{\sqrt{3}}(\eta_{11}^{w} + \eta_{22}^{w} + \eta_{33}^{w}) \\
\frac{1}{\sqrt{3}}(\eta_{23}^{w} + \eta_{32}^{w}) \\
\frac{1}{\sqrt{3}}(\eta_{12}^{w} + \eta_{21}^{w}) \\
\frac{1}{\sqrt{3}}(\eta_{22}^{w} + \eta_{33}^{w}) \\
\frac{1}{\sqrt{3}}(\eta_{11}^{w} + \eta_{22}^{w}) \\
\frac{1}{\sqrt{3}}(\eta_{11}^{w} + \eta_{22}^{w})
\end{array}\right),
\]

\[
\eta_{w,5}^{u} = \left(\begin{array}{c}
\eta_{5}^{w} \\
\eta_{6}^{w} \\
\eta_{7}^{w} \\
\eta_{8}^{w} \\
\eta_{9}^{w}
\end{array}\right) = \left(\begin{array}{c}
\frac{1}{6}\sqrt{3}(\eta_{11}^{w} - \eta_{22}^{w}) \\
\frac{1}{6}(\eta_{11}^{w} - \eta_{22}^{w}) \\
\frac{1}{6}(\eta_{11}^{w} - \eta_{22}^{w}) \\
\frac{1}{6}(\eta_{11}^{w} - \eta_{22}^{w}) \\
\frac{1}{6}(\eta_{11}^{w} - \eta_{22}^{w})
\end{array}\right).
\]

**Appendix B. Third-order icosahedral invariants**

\[
I_{1}^{uuu} = (\eta_{1}^{u})^{3},
\]

\[
I_{2}^{uuu} = \frac{1}{20}\sqrt{30}\left[ - (\eta_{1}^{u})^{3} + \eta_{2}^{u}(\eta_{5}^{u})^{2} + \eta_{3}^{u}(\eta_{6}^{u})^{2} - 2 \eta_{3}^{u}(\eta_{4}^{u})^{2} + 3 \eta_{3}^{u}(\eta_{5}^{u})^{2} + 4\sqrt{3}\eta_{4}^{u}\eta_{5}^{u}\eta_{6}^{u} + \sqrt{3}\eta_{2}^{u}(\eta_{6}^{u})^{2} - \sqrt{3}\eta_{2}^{u}(\eta_{5}^{u})^{2} \right],
\]

\[
I_{3}^{uuu} = \frac{1}{20}\sqrt{10}\left[ (\eta_{1}^{u})^{3} - 3 \eta_{2}^{u}(\eta_{5}^{u})^{2} + 3 \eta_{3}^{u}(\eta_{6}^{u})^{2} + 3 \eta_{3}^{u}(\eta_{5}^{u})^{2} + 3\sqrt{3}\eta_{3}^{u}(\eta_{5}^{u})^{2} - 3\sqrt{3}\eta_{3}^{u}(\eta_{6}^{u})^{2} \right],
\]

\[
I_{4}^{uuu} = \frac{1}{5}\sqrt{15}\eta_{1}^{u}\left[ (\eta_{2}^{u})^{2} + (\eta_{3}^{u})^{2} + (\eta_{4}^{u})^{2} + (\eta_{5}^{u})^{2} \right],
\]

\[
I_{1}^{uwu} = \frac{1}{60}\sqrt{30}\left[ 2(\eta_{5}^{u})^{2}\eta_{1}^{w} + 2(\eta_{6}^{u})^{2}\eta_{2}^{w} + 2(\eta_{3}^{u})^{2}\eta_{1}^{w} + 3(\eta_{2}^{u})^{2}\eta_{1}^{w} - 3(\eta_{5}^{u})^{2}\eta_{1}^{w} + 2\sqrt{5}\eta_{2}^{u}\eta_{3}^{w}\eta_{4}^{w} + 2\sqrt{5}\eta_{3}^{u}\eta_{4}^{w}\eta_{5}^{w} + 2\sqrt{5}\eta_{3}^{u}\eta_{4}^{w}\eta_{4}^{w} - \sqrt{10}\eta_{2}^{u}\eta_{5}^{w}\eta_{6}^{w} - \sqrt{10}\eta_{3}^{u}\eta_{5}^{w}\eta_{6}^{w} + 2\sqrt{30}\eta_{2}^{u}\eta_{5}^{w}\eta_{6}^{w} + 2\sqrt{30}\eta_{2}^{u}\eta_{5}^{w}\eta_{6}^{w} - \sqrt{30}\eta_{2}^{u}\eta_{5}^{w}\eta_{6}^{w} + \sqrt{30}\eta_{2}^{u}\eta_{5}^{w}\eta_{6}^{w} \right],
\]
Table A1. Tabulation of the transformation matrices for the icosahedral irreducible representations. They are given for two appropriate generating elements of $Y$, i.e. a fivefold rotation $C_5$ and a threefold $C_3$. $\tau = \frac{1}{\phi}$. For $Y_h$, the inversion $i$ must be included. $i$ doesn’t change the strains \[ (B.2) \]

$$
\begin{array}{cccc}
\hline
\Gamma & g = C_5 & g = C_3 \\
\hline
\Gamma^4 \equiv 1 & 1 & 1 \\
\Gamma^3 \equiv 3 & \left( \begin{array}{ccc}
\tau & \tau - 1 & -1 \\
\tau - 1 & 1 & \tau \\
1 & -\tau & \tau - 1 \\
\end{array} \right) & \left( \begin{array}{ccc}
0 & 0 & 1 \\
1 & 0 & 0 \\
0 & 1 & 0 \\
\end{array} \right) \\
\Gamma^3' \equiv 3' & \left( \begin{array}{ccc}
1 - \tau & -\tau & -1 \\
-\tau & 1 & \tau \\
1 & \tau - 1 & -\tau \\
\end{array} \right) & \left( \begin{array}{ccc}
0 & 0 & 1 \\
1 & 0 & 0 \\
0 & 1 & 0 \\
\end{array} \right) \\
\Gamma^4 \equiv 4 & \left( \begin{array}{ccc}
-1 & \sqrt{5} & \sqrt{5} \\
-\sqrt{5} & 1 & -3 \\
\sqrt{5} & 3 & 1 \\
\end{array} \right) & \left( \begin{array}{ccc}
1 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0 \\
\end{array} \right) \\
\Gamma^5 \equiv 5 & \frac{1}{4} \left( \begin{array}{ccc}
1 & \sqrt{3} & -\sqrt{6} \\
\sqrt{3} & -1 & -\sqrt{2} \\
\sqrt{6} & 2 & 0 \\
\end{array} \right) & \frac{1}{4} \left( \begin{array}{ccc}
-1 & \sqrt{3} & 0 \\
\sqrt{3} & 1 & 0 \\
0 & 0 & 2 \\
\end{array} \right) \\
\hline
\end{array}
$$

$$
I_2^{uww} = \frac{1}{60} \sqrt{30} \left[ (\eta)^2 \eta^w + (\eta^w)^2 \eta^w - 2 (\eta^w)^2 \eta^w + 2 \eta^w \eta^w \eta^w + 2 \eta^w \eta^w \eta^w + 3 (\eta^w)^2 \eta^w \\
-3 (\eta^w)^2 \eta^w - 4 \eta^w \eta^w \eta^w + 6 \eta^w \eta^w \eta^w + 4 \sqrt{2} \eta^w \eta^w \eta^w + 4 \sqrt{2} \eta^w \eta^w \eta^w \\
+4 \sqrt{2} \eta^w \eta^w \eta^w + \sqrt{3} (\eta^w)^2 \eta^w - \sqrt{3} (\eta^w)^2 \eta^w + 2 \sqrt{3} \eta^w \eta^w \eta^w \\
-2 \sqrt{3} \eta^w \eta^w \eta^w \right].
$$

$$
I_3^{uww} = \frac{1}{20} \sqrt{10} \left[ (\eta)^2 \eta^w - (\eta^w)^2 \eta^w - (\eta^w)^2 \eta^w - (\eta^w)^2 \eta^w + 2 (\eta^w)^2 \eta^w - 2 \eta^w \eta^w \eta^w + 2 \eta^w \eta^w \eta^w + \sqrt{3} (\eta^w)^2 \eta^w - \sqrt{3} (\eta^w)^2 \eta^w \\
+2 \sqrt{3} \eta^w \eta^w \eta^w - 2 \sqrt{3} \eta^w \eta^w \eta^w \right].
$$

$$
I_4^{uww} = \frac{1}{5} \sqrt{10} \eta^w \left[ (\eta)^2 \eta^w + (\eta^w)^2 \eta^w + (\eta^w)^2 \eta^w + (\eta^w)^2 \eta^w \right],
$$

$$
I_1^{uww} = \frac{1}{2} \eta^w \left[ (\eta)^2 + (\eta^w)^2 + (\eta^w)^2 \right],
$$

$$
I_2^{uww} = \frac{1}{5} \sqrt{5} \eta^w \left[ (\eta)^2 \eta^w + (\eta^w)^2 \eta^w + (\eta^w)^2 \eta^w + (\eta^w)^2 \eta^w \right],
$$

$$
I_3^{uww} = \frac{1}{60} \sqrt{30} \left[ \eta^w \eta^w \eta^w + 2 \eta^w \eta^w \eta^w - 2 \eta^w \eta^w \eta^w + 2 \eta^w \eta^w \eta^w + 2 \eta^w \eta^w \eta^w + 3 \eta^w \eta^w \eta^w \\
-3 \eta^w \eta^w \eta^w - 4 \eta^w \eta^w \eta^w + 6 \eta^w \eta^w \eta^w + 4 \sqrt{2} \eta^w \eta^w \eta^w + 4 \sqrt{2} \eta^w \eta^w \eta^w \\
+4 \sqrt{2} \eta^w \eta^w \eta^w - \sqrt{3} \eta^w \eta^w \eta^w + \sqrt{3} \eta^w \eta^w \eta^w - 2 \sqrt{3} \eta^w \eta^w \eta^w \\
+2 \sqrt{3} \eta^w \eta^w \eta^w \right],
$$

$$
I_4^{uww} = \frac{1}{20} \sqrt{10} \left[ \eta^w \eta^w \eta^w + \eta^w \eta^w \eta^w - \eta^w \eta^w \eta^w - \eta^w \eta^w \eta^w + 2 \eta^w \eta^w \eta^w - 2 \eta^w \eta^w \eta^w + 2 \eta^w \eta^w \eta^w + \sqrt{3} \eta^w \eta^w \eta^w - \sqrt{3} \eta^w \eta^w \eta^w \\
-2 \eta^w \eta^w \eta^w - 2 \eta^w \eta^w \eta^w + 4 \eta^w \eta^w \eta^w + \sqrt{3} \eta^w \eta^w \eta^w - \sqrt{3} \eta^w \eta^w \eta^w \right].
$$
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\[ I_5^{uvw} = \frac{1}{30} \sqrt{15} \left[ 2 \eta_3^{uv} \eta_4^{uw} + 2 \eta_3^{uv} \eta_4^{uw} + 2 \eta_3^{uv} \eta_4^{uw} + \sqrt{2} \eta_3^{uv} (\eta_3^{uv})^2 + \sqrt{2} \eta_3^{uv} (\eta_3^{uv})^2 \right] \]

\[ -2 \sqrt{2} \eta_3^{uv} (\eta_3^{uv})^2 + 2 \sqrt{5} \eta_5^{uv} \eta_6^{uw} + 2 \sqrt{5} \eta_5^{uv} \eta_6^{uw} + 2 \sqrt{5} \eta_5^{uv} \eta_6^{uw} + \sqrt{6} \eta_5^{uv} (\eta_5^{uv})^2 + \sqrt{6} \eta_5^{uv} (\eta_5^{uv})^2 \]

\[ + \sqrt{6} \eta_5^{uv} (\eta_5^{uv})^2 - \sqrt{6} \eta_5^{uv} (\eta_5^{uv})^2 \]

\[ I_6^{uvw} = \frac{1}{60} \sqrt{15} \left( 4 \eta_3^{uv} \eta_4^{uw} + 4 \eta_3^{uv} \eta_4^{uw} + 4 \eta_3^{uv} \eta_4^{uw} - 6 \eta_2^{uv} \eta_7^{uw} - 6 \eta_2^{uv} \eta_7^{uw} \right. \]

\[ + 2 \sqrt{5} \eta_5^{uv} \eta_6^{uw} + 2 \sqrt{5} \eta_5^{uv} \eta_6^{uw} + 2 \sqrt{5} \eta_5^{uv} \eta_6^{uw} + 2 \sqrt{5} \eta_5^{uv} \eta_6^{uw} \]

\[ + 2 \sqrt{5} \eta_5^{uv} \eta_6^{uw} - \sqrt{10} \eta_5^{uv} \eta_6^{uw} - \sqrt{10} \eta_5^{uv} \eta_6^{uw} \]

\[ - \sqrt{10} \eta_5^{uv} \eta_6^{uw} - \sqrt{10} \eta_5^{uv} \eta_6^{uw} + 2 \sqrt{10} \eta_3^{uv} \eta_2^{uw} + 2 \sqrt{10} \eta_3^{uv} \eta_2^{uw} \]

\[ - \sqrt{30} \eta_3^{uv} \eta_2^{uw} - \sqrt{30} \eta_3^{uv} \eta_2^{uw} + \sqrt{30} \eta_3^{uv} \eta_2^{uw} \]

\[ \left. \right) \]

\[ I_7^{uvw} = \frac{1}{20} \sqrt{10} \left( \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} + \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} - \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} + 2 \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} + 2 \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} \right. \]

\[ - \sqrt{3} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} + \sqrt{3} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} - \sqrt{3} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} + \sqrt{3} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} \]

\[ + \sqrt{6} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} - \sqrt{6} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} - \sqrt{6} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} + \sqrt{6} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} \]

\[ + \sqrt{6} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} - \sqrt{6} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} - \sqrt{6} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} + \sqrt{6} \eta_3^{uv} \eta_4^{uw} \eta_5^{uw} \]

\[ \left. \right) \]

\[ I_1^{uvw} = \frac{1}{4} \sqrt{3} \left[ (\eta_1^{uw})^3 - \eta_1^{uw} (\eta_4^{uw})^2 - \eta_1^{uw} (\eta_4^{uw})^2 + 2 \sqrt{5} \eta_2^{uw} \eta_3^{uw} \eta_4^{uw} \right], \]

\[ I_2^{uvw} = \frac{1}{20} \sqrt{30} \left[ (\eta_1^{uw})^3 + \eta_1^{uw} (\eta_4^{uw})^2 - \eta_1^{uw} (\eta_4^{uw})^2 + 2 \eta_1^{uw} (\eta_4^{uw})^2 \right. \]

\[ + 4 \sqrt{2} \eta_7^{uw} \eta_8^{uw} + \sqrt{3} \eta_5^{uw} (\eta_5^{uw})^2 - \sqrt{3} \eta_5^{uw} (\eta_5^{uw})^2 \]

\[ \left. \right) \]

\[ I_3^{uvw} = \frac{1}{20} \sqrt{10} \left[ (\eta_1^{uw})^3 - \eta_1^{uw} (\eta_4^{uw})^2 + \eta_1^{uw} (\eta_4^{uw})^2 + 2 \eta_1^{uw} (\eta_4^{uw})^2 \right. \]

\[ + 3 \sqrt{3} \eta_6^{uw} (\eta_6^{uw})^2 - 3 \sqrt{3} \eta_6^{uw} (\eta_6^{uw})^2 \]

\[ \left. \right) \]

\[ I_4^{uvw} = \frac{1}{10} \sqrt{10} \left[ (\eta_1^{uw})^3 + (\eta_4^{uw})^2 (\eta_4^{uw})^2 - 2 (\eta_4^{uw})^2 (\eta_4^{uw})^2 + \sqrt{2} \eta_2^{uw} \eta_3^{uw} \eta_6^{uw} + \sqrt{2} \eta_2^{uw} \eta_3^{uw} \eta_6^{uw} \right. \]

\[ + \sqrt{2} \eta_2^{uw} \eta_3^{uw} \eta_6^{uw} + \sqrt{2} \eta_2^{uw} \eta_3^{uw} \eta_6^{uw} - \sqrt{3} (\eta_5^{uw})^2 \eta_5^{uw} - \sqrt{3} (\eta_5^{uw})^2 \eta_5^{uw} + \sqrt{10} \eta_1^{uw} \eta_4^{uw} \eta_5^{uw} \]

\[ \left. \right] \]

\[ I_5^{uvw} = \frac{1}{20} \sqrt{10} \left[ (\eta_1^{uw})^3 - \eta_1^{uw} (\eta_4^{uw})^2 + \eta_1^{uw} (\eta_4^{uw})^2 - 3 \eta_1^{uw} (\eta_4^{uw})^2 + 3 \eta_1^{uw} (\eta_4^{uw})^2 \right. \]

\[ + 2 \sqrt{5} \eta_2^{uw} \eta_3^{uw} \eta_6^{uw} + 2 \sqrt{5} \eta_2^{uw} \eta_3^{uw} \eta_6^{uw} + \sqrt{10} \eta_1^{uw} \eta_4^{uw} \eta_5^{uw} \]

\[ \left. \right] \]

\[ \left( B.3 \right) \]

The invariants comprise strain components of irreducible representations as displayed in table B.1. Note that the following pairs have exactly the same structure: \( I_2^{uvw} / I_4^{uvw}, I_3^{uvw} / I_5^{uvw}, I_4^{uvw} / I_2^{uvw}, I_5^{uvw} / I_3^{uvw}, I_2^{uvw} / I_3^{uvw}, I_3^{uvw} / I_4^{uvw}, I_4^{uvw} / I_5^{uvw}, I_5^{uvw} / I_2^{uvw} \). Furthermore, \( 3 I_3^{uvw} \) is obtained from \( I_2^{uvw} \) by replacing only the phason \( \Gamma_5 \)-components in the manner described above.

\( \sqrt{6} I_5^{uvw} \) follows from \( I_5^{uvw} \) by replacing only the phason \( \Gamma_5 \)-components in the manner described above.
be combined to

\[ \{ \text{det}(\eta) \} \mid \{ \text{tr}(\eta^3) \} \mid \{ \text{tr}((\eta^*)^2) \} \mid \{ \text{tr}((\eta^*)^2) \} \mid \{ \text{det}(\eta^w) \} \]

In (C.1), index \( s \) denotes that \( \eta_{ij}^s \) must be replaced by \( \frac{1}{2}(\eta_{ij}^s + \eta_{ji}^s) \). Some of our third-order invariants are just proportional to \( \eta_{ij}^s \) times one of the second-order, invariant scalar products given in Section 3. Note that \( \text{tr}(\eta^w) \) is not invariant. Our invariants \( I_1^{uuu} \) and \( I_1^{uuu} \) are also \( O(3) \)-invariants, while \( I_2^{uuu} \) and \( I_3^{uuu} \) must be combined to give a linearly independent third \( O(3) \)-invariant. In the degenerate case of phononic isotropy, our elastic constants \( C_{ij}^{uuu} \) can be expressed by sets of classical third-order elastic constants already in use: \( C_1^{uuu} = \sqrt{3}(l + \frac{1}{3} n), C_2^{uuu} = \frac{1}{3} \sqrt{30} n, C_3^{uuu} = -\frac{\sqrt{6}}{6} n, C_4^{uuu} = \sqrt{5}(m - \frac{1}{3} n) \)

\( I_1^{uuu} = \sqrt{3}(\frac{1}{2} \nu_1 + \nu_2 + \frac{\gamma}{2} \nu_3), C_2^{uuu} = \frac{1}{3} \sqrt{30} \nu_3, C_3^{uuu} = -\frac{\sqrt{6}}{6} \nu_3, C_4^{uuu} = \sqrt{5}(\nu_2 + \frac{\gamma}{4} \nu_3) \).

Up to normalisation factors, the phason third-order invariants \( I_5, I_5, J \) and \( J' \) of Ishii \([14]\) are transformed into our \( I_2^{uuw}, I_3^{uuw}, I_4^{wuu} \) and \( I_5^{wuuw} \), respectively, by the substitutions \( \eta_{ij}^5 \to -\frac{1}{4}(\sqrt{10} \eta_{ij}^5 + \sqrt{6} \eta_{ij}^6) \) and \( \eta_{ij}^5 \to \frac{1}{4}(-\sqrt{6} \eta_{ij}^5 + \sqrt{10} \eta_{ij}^6) \). This is necessary because in \([14]\) other irreducible components are used than in \([21]\).

**References**

[1] Levine D, Lubensky T C, Ostlund S, Ramaswamy S, Steinhardt P J and Toner J 1985 *Phys. Rev. Lett.* 54 1520

[2] Bak P 1985 *Phys. Rev. B* 32 5764

[3] Katz A and Gratias D 1994 *Lectures on Quasicrystals (Aussois, France)*, edited by Hippert F and Gratias D (Les Ulis: Les Editions de Physique) pp 187

**Table B1.** Powers of irreducible representation components \( \eta_{ij}^{\alpha} \) in third-order invariants. Possible combinations are: \( \alpha = 1, i = 1; \alpha = 5, i = 2,3,4; \alpha = 5, i = 5,6,7,8,9 \) (\( \alpha = w \)).

| \( (a, \alpha) \) | \( (u,1) \) | \( (u,5) \) | \( (w,4) \) | \( (w,5) \) | \( (u,1) \) | \( (u,5) \) | \( (w,4) \) | \( (w,5) \) |
|---|---|---|---|---|---|---|---|---|
| \( I_1^{uuu} \) | 3 | \( I_1^{uuu} \) | 1 | 2 |
| \( I_1^{uuu} \) | 3 | \( I_1^{uuu} \) | 1 | 2 |
| \( I_1^{uuu} \) | 3 | \( I_1^{uuu} \) | 1 | 2 |
| \( I_1^{uuu} \) | 2 | 1 | \( I_1^{uuu} \) | 1 | 1 |
| \( I_1^{uuu} \) | 2 | 1 | \( I_1^{uuu} \) | 1 | 1 |
| \( I_1^{uuu} \) | 1 | \( I_1^{uuu} \) | 3 |
| \( I_1^{uuu} \) | 1 | \( I_1^{uuu} \) | 3 |
| \( I_1^{uuu} \) | 1 | \( I_1^{uuu} \) | 2 |
| \( I_1^{uuu} \) | 1 | \( I_1^{uuu} \) | 2 | 1 |
| \( I_1^{uuu} \) | 1 | \( I_1^{uuu} \) | 2 | 1 |
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[4] Boudard M, de Boissieu M, Janot C, Heger G, Beeli C, Nissen H-U, Vincent H, Ibberson R, Audier M and Dubois J M 1992 J. Phys. Cond. Mat. 4 10149

[5] Spoor P S, Maynard J D and Kortan A R 1995 Phys. Rev. Lett. 75 3462

[6] Kerber A and Scharf T 1987 J. Math. Phys. 28 2323

[7] Duquesne J-Y and Perrin B 2000 Phys. Rev. Lett. 85 4301

[8] Birch F 1947 Phys. Rev. 71 809

[9] Murnaghan F D 1951 Finite Deformation of an Elastic Solid (New York: John Wiley and Sons)

[10] Chen L C, Ebalard S, Goldman L M, Ohashi W, Park B and Spaepen F 1986 J. Appl. Phys. 60 2638. Erratum 1994 76 2001. We agree with the authors of [7] that the erratum still contains a misprint and that the right relation for $C_{456}$ is $C_{456} = -\frac{1}{2}C_{144} - \frac{1}{2}(\tau - 1)C_{155} + \frac{1}{2}\tau C_{166}$.

[11] Fradkin M A 1992 Comput. Phys. Commun. 73 197

[12] Rama Mohana Rao K and Hemagiri Rao P 1993 J. Phys. Cond. Mat. 5 5513

[13] Goshen S Y and Birman J L 1994 J. Phys. I France 4 1077

[14] Ishii Y 1990 Quasicrystals, vol 93 of Springer Series in Solid-State Sciences, edited by Fujiwara T and Ogawa T (Berlin, Heidelberg: Springer) pp 129

[15] Ricker M, Bachteler J and Trebin H-R 2001 Eur. Phys. J. B 23 351

[16] Brugger K 1964 Phys. Rev. 133 A1611

[17] Gähler F 2000 Private communication

[18] Yang W, Ding D, Hu C and Wang R 1994 Phys. Rev. B 49 12656

[19] Bachteler J and Trebin H-R 1998 Eur. Phys. J. B 4 299

[20] Cornwell J F 1984 Group Theory in Physics vol 1, vol 7 of Techniques of Physics, edited by March N H and Daglish H N (London: Academic Press)

[21] Ishii Y 1989 Phys. Rev. B 39 11862

[22] Trebin H-R, Fink W and Stark H 1991 J. Phys. I France 1 1451

[23] Toupin R A and Bernstein B 1961 J. Acoust. Soc. Am. 33 216