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Elastic Green's function of icosahedral quasicrystals

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Abstract. The elastic theory of quasicrystals considers, in addition to the "normal" displacement field, three "phason" degrees of freedom. We present an approximative solution for the elastic Green's function of icosahedral quasicrystals, assuming that the coupling between the phonons and phasons is small.

PACS. 61.44.Br Quasicrystals – 62.20.Dc Elasticity, elastic constants

1 Introduction

The displacement field of an infinite linear elastic medium caused by external forces can be calculated immediately, when the elastic Green's function is available. Unfortunately, analytical expressions for the Green's function are known only for special cases. Lord Kelvin [1] has provided a solution for the isotropic medium, Lifshitz and Rosentsveig [2] and Kröner [3] for hexagonal crystals. Approximations have been presented by Dederichs and Leibfried [4] for cubic crystals and by Kröner [3] for arbitrary anisotropic systems.

In the case of quasicrystals [5], three additional phason degrees of freedom lead to a more general theory of elasticity [6–10]. The corresponding Green's functions for planar pentagonal (De and Pelcovits [9]), decagonal and dodecagonal (Ding *et al.* [11]) quasicrystals are known. However, the solution for icosahedral quasicrystals with five elastic constants (two for phonons, two for phasons, and one for the coupling between phonons and phasons) has not been established yet.

It is the intention of this paper to derive an analytical approximation of the elastic Green's function for icosahedral quasicrystals.

The paper is organised as follows. In Section 2 we recall the elastic theory of icosahedral quasicrystals. We present the Green's function in the case of the "spherical approximation" and for vanishing coupling between phonons and phasons. Starting from this solution and using perturbation theory as well as an invariant basis for the Green's function tensor, we derive in Section 3 an approximative solution for finite phonon-phason interactions. The last section presents the phonon and phason fields for some special cases.

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2 Elastic theory for icosahedral quasicrystals

2.1 Equations

The elastic theory of quasicrystals [7,6,8,12,13] studies, apart from the classical "phonon" displacement field $\mathbf{u}(\mathbf{x})$, also the "phason" displacement field $\mathbf{w}(\mathbf{x})$. Icosahedral quasicrystals can be described as a three-dimensional cut through a six-dimensional cubic crystal. The six-dimensional space divides into two three-dimensional subspaces, which are invariant under icosahedral symmetry operations, the "physical" or "parallel" cutting space $E^{\parallel}$ and the "perpendicular" space $E^{\perp}$. While the phonon displacement vector $\mathbf{u}$ is an element of $E^{\parallel}$, which transforms according to the icosahedral irreducible representation Γ^3, the phason displacement vector $\mathbf{w} \in E^{\perp}$ transforms according to the other three-dimensional icosahedral irreducible representation $\Gamma^{3'}$.

Both displacements only depend on the position vector $\mathbf{x} \in E^{\parallel}$. The variations of this displacement fields are described by the strain fields

$$\varepsilon^u_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \qquad \varepsilon^w_{ij} = \frac{\partial w_i}{\partial x_j} \qquad \varepsilon = \begin{bmatrix}\varepsilon^u \\ \varepsilon^w\end{bmatrix}. \quad (1)$$

In a linear theory the elastic energy is a quadratic form of the strain field:

$$F(\varepsilon) = \frac{1}{2}\mathsf{C}_{\alpha i\beta j}\varepsilon_{\alpha i}\varepsilon_{\beta j} \quad \alpha,\beta = 1\ldots 6 \quad i,j = 1\ldots 3. \quad (2)$$

Differentiation with respect to the strain $\varepsilon_{\alpha i}$ leads to Hooke's law

$$\frac{\partial F}{\partial \varepsilon_{\alpha i}} =: \sigma_{\alpha i} = \mathsf{C}_{\alpha i\beta j}\varepsilon_{\beta j}, \quad (3)$$

where σ denotes the generalized stress field. The meaning of the "phason stress" σ^w is not quite clear. According to the definition (3) it is the force conjugated to the phason strain ε^w. Phason strain is – in an atomic description – related to rearrangement of atoms on a small scale (so-called "flips"). Forces which inhibit such rearrangements might be considered as "pinning forces".

It is shown by group theoretical arguments [6] that Hooke's elastic tensor C for icosahedral symmetry contains only five independent elastic constants $(\mu_1, \ldots, \mu_5)$. From the transformation rules for $\mathbf{u}, \mathbf{x}$: Γ^3 and $\mathbf{w}$: $\Gamma^{3'}$ immediately follows [13] the transformation behaviour of the strain fields

$$\varepsilon^u : \Gamma^1 + \Gamma^5 \qquad \varepsilon^w : \Gamma^4 + \Gamma^5, \tag{4}$$

which means that they can be written in an icosahedral basis

$$\varepsilon^u \to \varepsilon^{u1} + \varepsilon^{u5} \qquad \varepsilon^w \to \varepsilon^{w4} + \varepsilon^{w5}, \tag{5}$$

where $\varepsilon^{(u/w)d}$ is a d-dimensional vector transforming according to Γ^d (see Appendix A.1 for details). In this symmetry-adjusted coordinate system for the strains ε and in an analogous way for the stresses σ Hooke's law can be written as

$$\begin{bmatrix} \sigma^{u1} \\ \sigma^{u5} \\ \sigma^{w4} \\ \sigma^{w5} \end{bmatrix} = \begin{bmatrix} \mu_1 & 0 & 0 & 0 \\ 0 & \mu_2 & 0 & \mu_3 \\ 0 & 0 & \mu_4 & 0 \\ 0 & \mu_3 & 0 & \mu_5 \end{bmatrix} \begin{bmatrix} \varepsilon^{u1} \\ \varepsilon^{u5} \\ \varepsilon^{w4} \\ \varepsilon^{w5} \end{bmatrix}. \tag{6}$$

The pure phonon elastic constants μ_1, μ_2 are related to the Lamé-constants μ, λ by

$$\mu_1 = 2\mu + 3\lambda \qquad \mu_2 = 2\mu, \tag{7}$$

expressing the fact that an icosahedral quasicrystal behaves like an isotropic medium when phason dynamics are frozen out.

μ_4 and μ_5 describe the elastic energy of pure phason strain. Contrary to the phonon case above, the phason elasticity is not isotropic, when these two constants are different. To simplify the calculations we assume in a first step that

$$\mu_4 = \mu_5 =: K_1 \tag{8}$$

is valid. We have made this assumption, because the $SO(3)$ irreducible representation $\Gamma^{l=4}$ divides under icosahedral group operations into $\Gamma^4 + \Gamma^5$, which corresponds to the splitting of the phason strain field ε^w (see Eq. (4)). If one demands not only icosahedral but spherical symmetry in the space of phason strains, the identity of the two phasonic elastic constants is necessary. Therefore we call equation (8) "spherical approximation".

Phonon and phason elasticity are coupled by μ_3. The assumption that this coupling is small,

$$\mu_3 \ll \mu_1,\ \mu_2,\ \mu_4 = \mu_5, \tag{9}$$

allows us to develop a perturbation theory with respect to μ_3.

In ideal materials (without dislocations or defects) the only sources for stress fields are external volume forces $\mathbf{f}$. Hence, the balance of forces is expressed by

$$\operatorname{div} \sigma + \mathbf{f} = 0. \tag{10}$$

Please note, that the external force $\mathbf{f} = [\mathbf{f}^u, \mathbf{f}^w]$, as the displacement $[\mathbf{u}, \mathbf{w}]$, consists of two parts – the usual phonon force $\mathbf{f}^u$ and the so-called phason force $\mathbf{f}^w$. Inserting Hooke's law (3) in the balance of stresses and forces (10) and applying the definition (1) of the strain leads to generalized elastic equations:

$$\mathsf{D}(\nabla) \begin{bmatrix} \mathbf{u} \\ \mathbf{w} \end{bmatrix} + \mathbf{f} = 0. \tag{11}$$

This system of six second order partial differential equations describes the connection between applied forces and displacement field. In this paper we provide an approximative solution by the method of Green's function.

The differential operator $\mathsf{D}(\nabla)$ is a 6×6-matrix and can be separated into four 3×3-matrices:

$$\mathsf{D}(\nabla) = \begin{bmatrix} \mathsf{D}^{u,u}(\nabla) & \mathsf{D}^{u,w}(\nabla) \\ \mathsf{D}^{w,u}(\nabla) & \mathsf{D}^{w,w}(\nabla) \end{bmatrix}. \tag{12}$$

For example, the second component of the phonon force is related to the displacements by $\mathsf{D}^{u,u}_{2i} u_i + \mathsf{D}^{u,w}_{2i} w_i + f_2 = 0$. The phonon-phonon block $\mathsf{D}^{u,u}$ is the well-known differential operator for the isotropic elastic continuum:

$$\mathsf{D}^{u,u}(\nabla) = \mu\Delta + (\mu + \lambda) \operatorname{grad} \operatorname{div}. \tag{13}$$

Applying the spherical approximation for the phason-phason-block explained above yields

$$\mathsf{D}^{w,w}(\nabla) = K_1 \Delta. \tag{14}$$

The phonon-phason coupling is described by

$$\begin{aligned} \mathsf{D}^{w,u}(\nabla) &= (\mathsf{D}^{u,w}(\nabla))^t \\ &= \frac{\mu_3}{\sqrt{6}} \begin{bmatrix} F_1(x,y,z) & F_3(x,y) & F_2(z,x) \\ F_2(x,y) & F_1(y,z,x) & F_3(y,z) \\ F_3(z,x) & F_2(y,z) & F_1(x,y,z) \end{bmatrix}. \end{aligned} \tag{15}$$

with

$$\begin{aligned} F_1(a,b,c) &= -\frac{\partial^2}{\partial a^2} - \frac{1}{\tau}\frac{\partial^2}{\partial b^2} + \tau\frac{\partial^2}{\partial c^2} \\ F_2(a,b) &= -2\frac{1}{\tau}\frac{\partial^2}{\partial a \partial b} \\ F_3(a,b) &= 2\tau\frac{\partial^2}{\partial a \partial b} \cdot \end{aligned} \tag{16}$$

2.2 Method of Green's function

The Green's function method is commonly used to solve linear inhomogenous differential equations like (11). Expressing the displacement field $[\mathbf{u}, \mathbf{w}](\mathbf{x})$ as a linear combination of the applied forces $\mathbf{f}$,

$$\begin{bmatrix} \mathbf{u} \\ \mathbf{w} \end{bmatrix}(\mathbf{x}) = \int \mathsf{G}(\mathbf{x} - \mathbf{x}')\mathbf{f}(\mathbf{x}')\mathrm{d}^3x', \tag{17}$$

leads to a system of differential equations for the "Green's function" $\mathsf{G}(\mathbf{x})$:

$$\mathsf{D}(\nabla)\mathsf{G}(\mathbf{x}) + 1\delta(\mathbf{x}) = 0. \tag{18}$$

The operator D and the Green's function G are 6×6-matrices, 1 is the six-dimensional identity operator and $\delta(\mathbf{x})$ the three-dimensional delta function.

By Fourier methods this system of differential equations can be transformed into a solvable system of algebraic equations [11]. The problem is that until now a method for Fourier back transformation has not been provided.

2.3 Solution for spherical approximation and noninteraction

If we assume that phonon elasticity is not coupled with phason elasticity ($\mu_3 = 0$), the differential equations (18) become very simple:

$$\mathsf{D}^{u,u}(\nabla)\mathsf{G}_0^{u,u}(\mathbf{x}) + 1\delta(\mathbf{x}) = 0 \tag{19}$$

$$\mathsf{D}^{w,w}(\nabla)\mathsf{G}_0^{w,w}(\mathbf{x}) + 1\delta(\mathbf{x}) = 0. \tag{20}$$

Now 1 is the three-dimensional identity operator and the Green's function matrix G is divided into four blocks by analogy with the differential operator D in (12). The solutions of these two systems are given by

$$\mathsf{G}_0^{u,u}(\mathbf{x}) = -\frac{1}{8\pi\mu(\lambda+2\mu)}\left\{(\lambda+3\mu)\frac{1}{|\mathbf{x}|} + (\lambda+\mu)\frac{\mathbf{x}\otimes\mathbf{x}}{|\mathbf{x}|^3}\right\} \tag{21}$$

$$\mathsf{G}_0^{w,w}(\mathbf{x}) = \frac{1}{4\pi K_1}1\frac{1}{|\mathbf{x}|}, \tag{22}$$

where $\mathbf{x}\otimes\mathbf{x}$ denotes the dyadic product of $\mathbf{x}$ with itself. Lord Kelvin [1] has provided solution (21). Equation (22) is mathematically equivalent to the solution for the electric potential in a given charge density (see for example Feynman [14, II 6-1]).

In the next section we develop a perturbation theory with respect to μ_3, where G_0 from (21, 22) are the solutions of zeroth order.

3 Solution for finite phonon-phason interactions

Based on the solution for vanishing coupling constant ($\mu_3 = 0$) given in the previous section we now develop an approximative solution for small but finite coupling between phonon and phason elasticity. Section 3.1 provides the perturbation of the Green's function $\mathsf{G}(\mathbf{x})$ with respect to μ_3 and yields some relations for $\mathsf{G}(\mathbf{x})$. In Section 3.2 we construct an invariant basis for the perturbative solutions, which fulfills these relations. Finally, in Section 3.3 we find the solutions up to the order 2 in μ_3.

3.1 Perturbation theory

The differential operator $\mathsf{D}(\nabla)$ defined in (12) consists of two parts

$$\mathsf{D}(\nabla) = \mathsf{D}_0(\nabla) + \mathsf{D}_1(\nabla) \tag{23}$$

with

$$\mathsf{D}_0(\nabla) = \begin{bmatrix} \mathsf{D}^{u,u}(\nabla) & 0 \\ 0 & \mathsf{D}^{w,w}(\nabla) \end{bmatrix} \tag{24}$$

$$\mathsf{D}_1(\nabla) = \begin{bmatrix} 0 & \mathsf{D}^{u,w}(\nabla) \\ \mathsf{D}^{w,u}(\nabla) & 0 \end{bmatrix}, \tag{25}$$

where the subscripts $0, 1$ denote the order of μ_3 (see (15)). Inserting (23) and the expansion of the Green's function G

$$\mathsf{G}(\mathbf{x}) = \mathsf{G}_0(\mathbf{x}) + \mathsf{G}_1(\mathbf{x}) + \mathsf{G}_2(\mathbf{x}) + \ldots \tag{26}$$

into the system of differential equations (18) and comparing the terms with the same order in μ_3 leads to

$$\mathsf{D}_0(\nabla)\mathsf{G}_0(\mathbf{x}) + 1\delta(\mathbf{x}) = 0 \tag{27}$$

$$\mathsf{D}_0(\nabla)\mathsf{G}_n(\mathbf{x}) + \mathsf{D}_1(\nabla)\mathsf{G}_{n-1}(\mathbf{x}) = 0 \quad n = 1, 2, \ldots \tag{28}$$

From the form (24, 25) of D_0 and D_1 it follows immediately that the phonon-phason-coupling blocks of the Green's function of even order vanish, while the only remaining ones are of odd order:

$$\mathsf{G}_{2i}^{u,w} = \mathsf{G}_{2i}^{w,u} = \mathsf{G}_{2i+1}^{u,u} = \mathsf{G}_{2i+1}^{w,w} = 0 \quad i = 0, 1, \ldots \tag{29}$$

Because equation (27) of zeroth order is equivalent to the noninteracting equations (19, 20), the nonvanishing part of the Green's function G_0 is given by (21, 22). It is necessary to solve (28) to obtain the Green's functions of higher order.

Let us now consider the analytic form of the solutions. Four properties result from the system of differential equations (18):

– "Homogeneity" of degree -1

$$\mathsf{G}(\alpha\mathbf{x}) = \alpha^{-1}\mathsf{G}(\mathbf{x}) \qquad \alpha \in \mathbb{R} \tag{30}$$

– "Inversion symmetry"

$$\mathsf{G}(-\mathbf{x}) = \mathsf{G}(\mathbf{x}) \tag{31}$$

– "Transposing symmetry"

$$\mathsf{G}_{ij}(\mathbf{x}) = \mathsf{G}_{ji}(\mathbf{x}) \tag{32}$$

– "Icosahedral symmetry"

$$\mathsf{G}(\mathbf{x}) = \Gamma^6(g)\mathsf{G}(\Gamma^3(g)^{-1}\mathbf{x})\Gamma^6(g)^{-1}. \tag{33}$$

The six-dimensional representation Γ^6 describes the transformation of the six-dimensional vector $[\mathbf{u}, \mathbf{w}]$. It is the sum of the two irreducible representations Γ^3 and $\Gamma^{3'}$. Each part $\mathsf{G}_n(\mathbf{x})$ of the perturbation series must have these four properties, too. The relations (30, 31) are valid for each matrix element $\mathsf{G}_{n;i,j}(\mathbf{x})$. Especially the matrix elements of the solution of zeroth order can be written as

$$\mathsf{G}_{0;ij}(\mathbf{x}) = \frac{1}{|\mathbf{x}|} \sum_{\substack{l=0 \\ l\,even}}^{l_{max}=2} \sum_{m=-l}^{l} g_{0;ij}^{l,m} Y_l^m(\mathbf{x}), \tag{34}$$

where $Y_l^m(\mathbf{x})$ are the "spherical harmonics" in Cartesian coordinates.

The solutions of higher order can be expressed in the same form with higher l_{max}. It is possible to make an ansatz with coefficients $g_{n;i,j}^{l,m}$ and to transform (28) into an algebraic system of equations. But to avoid an exploding number of coefficients, we take into account that each solution $\mathsf{G}_n(\mathbf{x})$ must be invariant under icosahedral transformations (33).

The separation of the Green's function $\mathsf{G}(\mathbf{x})$ into the four blocks $\mathsf{G}^{\alpha,\beta}(\mathbf{x})$ with $\alpha, \beta \in \{u, w\}$ transforms relations (32, 33) into

$$\mathsf{G}_{ij}^{u,u} = \mathsf{G}_{ji}^{u,u} \qquad \mathsf{G}_{ij}^{w,w} = \mathsf{G}_{ji}^{w,w} \qquad \mathsf{G}_{ij}^{w,u} = \mathsf{G}_{ji}^{u,w} \tag{35}$$

and

$$\mathsf{G}^{\alpha,\beta}(\mathbf{x}) = \Gamma^{\alpha}(g)\mathsf{G}^{\alpha,\beta}(\Gamma^3(g)^{-1}\mathbf{x})\Gamma^{\beta}(g)^{-1} \tag{36}$$

with the definition $\Gamma^u := \Gamma^3$ and $\Gamma^w := \Gamma^{3'}$. In the next section we construct icosahedral invariants for the four blocks, *e.g.* 3×3-matrix-functions, which fulfill relations (30, 31, 35) and (36).

3.2 Icosahedral invariants

Any 3×3-matrix-function can be expressed as

$$\sum_i M_i s_i(\mathbf{x}) \tag{37}$$

with 3×3-basis-matrices M_i and scalar functions $s_i(\mathbf{x})$. To achieve a basis in the space of icosahedral invariant matrix-functions it is necessary to divide the space of matrices and the space of scalar functions into icosahedral invariant subspaces, *i.e.* to construct the icosahedral irreducible bases (see for example [15]). By building the inner products of all possible combinations of irreducible bases of the matrices and the functions, where both bases belong to the same irreducible representation, we obtain a complete basis of the space of icosahedral invariant matrix-functions:

$$I_n^{\alpha,\beta}(\mathbf{x}) = \frac{1}{\sqrt{d_\gamma}} \sum_{i=1}^{d_\gamma} M_i^{\alpha,\beta;\gamma} s_i^{l;\gamma}(\mathbf{x}). \tag{38}$$

In this formula $\alpha, \beta \in \{3, 3'\}$ specify the block and γ denotes the irreducible representation Γ^γ of dimension d_γ, to which the irreducible bases $\{M_i^{\alpha,\beta;\gamma}\}_{i=1\ldots d_\gamma}$ and $\{s_i^{l;\gamma}(\mathbf{x})\}_{i=1\ldots d_\gamma}$ belong. The index n on the left hand side is a function of the representation index γ and the orbital quantum number l on the right. It is the enumeration of all possible (γ, l) combinations, ordered first by $l \in \{0, 2, 4, 6, 8\}$ and second by $\gamma \in \{1, 4, 5\}$. In the next two paragraphs we discuss the two irreducible bases.

The irreducible basis of the 3×3-matrices M can easily be calculated for all four blocks, but because of (35) it is sufficient to consider the three cases (u, u), (w, w) and (w, u). The "Clebsch-Gordan-Series" are given by

- $\Gamma^3 \otimes \Gamma^3 = \Gamma^1 \oplus \Gamma^3 \oplus \Gamma^5$
- $\Gamma^{3'} \otimes \Gamma^3 = \Gamma^4 \oplus \Gamma^5$
- $\Gamma^{3'} \otimes \Gamma^{3'} = \Gamma^1 \oplus \Gamma^{3'} \oplus \Gamma^5$.

The explicit form of the irreducible basis matrices is given in Appendix A.2. The matrices which belong to the irreducible representations Γ^3 and $\Gamma^{3'}$ are antisymmetric. We do not need them for our purpose, because the Green's function must be symmetric (32, 35).

The space of homogeneous functions of degree 0 consists of spherical invariant subspaces, denoted by the orbital quantum number l, whose bases are given by $B_l = \{Y_l^m(\mathbf{x})\}_{m=-l\ldots l}$. The inversion symmetry (31) allows us to limit the considerations to even quantum numbers l. The icosahedral group is a subgroup of the spherical group $SO(3)$. The spherical irreducible basis B_l is icosahedrally reducible for each $l > 2$. We have calculated the icosahedral irreducible bases $\{s_i^{l;\gamma}(\mathbf{x})\}_{i\ldots d_\gamma}$ from B_l for $l = 0, 2, 4, 6, 8$. They are given in Appendix A.3 for $l = 0, 2$.

Combining all possible pairs of irreducible matrices and irreducible functions using equation (38) leads to a set of icosahedral invariant matrix functions $I_n^{\alpha,\beta}(\mathbf{x})$, which shows inversion (31) and transposing (35) symmetry. These invariants are homogeneous of degree 0. By dividing them by $|\mathbf{x}|$ one obtains homogeneity of degree -1 (30).

3.3 Solution in terms of coefficients

It is possible to express the Green's function of order 0 in terms of the icosahedral invariant matrix functions calculated in the previous section. Inserting

$$1 = \sqrt{3} I_1^{3,3}(\mathbf{x}) = \sqrt{3} I_1^{3',3'}(\mathbf{x}) \tag{39}$$

$$\frac{\mathbf{x} \otimes \mathbf{x}}{\mathbf{x}^2} = \frac{1}{\sqrt{3}} I_1^{3,3}(\mathbf{x}) + \sqrt{5} I_2^{3,3}(\mathbf{x}) \tag{40}$$

in equations (21, 22) leads to

$$\mathsf{G}_0^{u,u}(\mathbf{x}) = -\frac{1}{24\pi\mu(\lambda + 2\mu)|\mathbf{x}|} \times \{2\sqrt{3}(2\lambda + 5\mu) I_1^{3,3}(\mathbf{x}) + 3\sqrt{5}(\lambda + \mu) I_2^{3,3}(\mathbf{x})\} \tag{41}$$

$$\mathsf{G}_0^{w,w}(\mathbf{x}) = \frac{\sqrt{3}}{4\pi K_1 |\mathbf{x}|} I_1^{3',3'}(\mathbf{x}). \tag{42}$$

The Green's functions of order 1 and 2 are calculated by inserting an ansatz in the invariant matrix functions into the recursion equation (28) and solving the systems of algebraic equations in the coefficients. The solutions are:

$$\mathsf{G}_1^{w,u}(\mathbf{x}) = \frac{\mu_3}{224\pi K_1 \mu(\lambda+2\mu)|\mathbf{x}|} \times \Big\{4\sqrt{5}(4\lambda+11\mu)I_1 + 7\sqrt{15}(\lambda+\mu)I_2 + 10\sqrt{21}(\lambda+\mu)I_3\Big\} \quad (43)$$

$$\begin{aligned}\mathsf{G}_2^{u,u}(\mathbf{x}) = \frac{\mu_3^2}{\pi K_1 \mu^2(\lambda+2\mu)^2|\mathbf{x}|} \times \Big\{ &-\frac{\sqrt{3}}{126}(4\lambda^2+16\lambda\mu+19\mu^2)I_1 \\ &-\frac{\sqrt{5}}{84}(2\lambda^2+8\lambda\mu+5\mu^2)I_2 \\ &-\frac{5\sqrt{21}}{16016}(43\lambda^2+242\lambda\mu+342\mu^2)I_3 \\ &+\frac{25\sqrt{7}}{672}(\lambda+\mu)(\lambda+3\mu)I_4 \\ &-\frac{5\sqrt{55}}{1056}(\lambda+\mu)(3\lambda+8\mu)I_5 \\ &+\frac{15\sqrt{1186185}}{262912}(\lambda+\mu)^2 I_6 \\ &-\frac{35\sqrt{1185}}{7584}(\lambda+\mu)^2 I_7\Big\} \end{aligned} \quad (44)$$

$$\begin{aligned}\mathsf{G}_2^{w,w}(\mathbf{x}) = \frac{\mu_3^2}{\pi K_1^2 \mu(\lambda+2\mu)|\mathbf{x}|} \times \Big\{ &-\frac{\sqrt{3}}{126}(4\lambda+11\mu)I_1 - \frac{\sqrt{5}}{42}(\lambda+3\mu)I_2 \\ &+\frac{5\sqrt{21}}{2464}(2\lambda+13\mu)I_3 \\ &+\frac{25\sqrt{7}}{672}(\lambda+\mu)I_4 + \frac{25\sqrt{55}}{1056}(\lambda+\mu)I_5\Big\}. \end{aligned} \quad (45)$$

I_n is an abbreviation for $I_n^{\alpha,\beta}(\mathbf{x})$ with appropriate $\alpha, \beta \in \{u, w\}$.

4 Results and discussion

With the help of the Green's function calculated in the previous section it is now possible to examine the displacement fields $\mathbf{u}(\mathbf{x})$ and $\mathbf{w}(\mathbf{x})$ due to a force field. Inserting the point force

$$\mathbf{f}(\mathbf{x}) = \mathbf{f}_0 \delta(\mathbf{x}) \quad (46)$$

into equation (17) leads to the displacement field

$$\begin{bmatrix}\mathbf{u}\\ \mathbf{w}\end{bmatrix}(\mathbf{x}) = \mathsf{G}(\mathbf{x})\mathbf{f}_0. \quad (47)$$

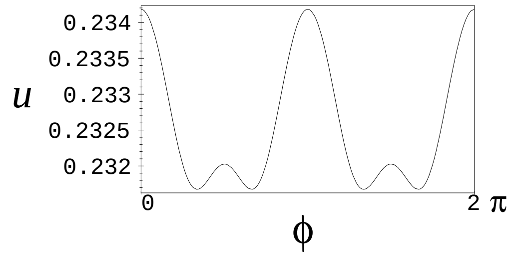

Fig. 1. Absolute value of phonon displacement $|u|$ *versus* ϕ for $\theta = \pi/4$, 2-fold axis.

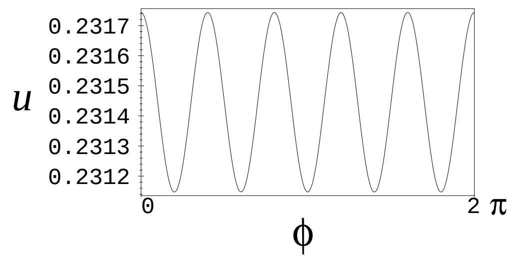

Fig. 2. Same as Figure 1, but 5-fold axis.

Because of the homogeneity of degree -1 (30) the radial behaviour is given by

$$\begin{bmatrix}\mathbf{u}\\ \mathbf{w}\end{bmatrix}(\mathbf{x}) \propto \frac{1}{|\mathbf{x}|}. \quad (48)$$

It is more interesting to examine the variation of the displacement fields on a sphere – the icosahedral symmetry should be reflected. Let us now consider a phonon force $\mathbf{f}_0^u$. The corresponding displacement fields in perturbation theory of second order

$$\mathbf{u}(\mathbf{x}) = \mathsf{G}^{u,u}(\mathbf{x})\mathbf{f}_0^u = \mathsf{G}_0^{u,u}(\mathbf{x})\mathbf{f}_0^u + \mathsf{G}_2^{u,u}(\mathbf{x})\mathbf{f}_0^u + \ldots \quad (49)$$

$$\mathbf{w}(\mathbf{x}) = \mathsf{G}^{w,u}(\mathbf{x})\mathbf{f}_0^u = \mathsf{G}_1^{w,u}(\mathbf{x})\mathbf{f}_0^u + \ldots \quad (50)$$

show, that the "isotropic" phonon displacement $\mathsf{G}_0^{u,u}(\mathbf{x})\mathbf{f}_0^u$ is corrected by a term of second order and that the phason displacement is given by a term of first order. We choose a spherical coordinate system with $\phi \in [0\ldots2\pi]$ and $\theta \in [0\ldots\pi]$, which depends on the force direction $\mathbf{f}_0^u$ in such a way, that $\mathbf{f}_0^u$ always points to the "North Pole" ($\theta = 0$).

This force breaks the full icosahedral symmetry, but nevertheless the symmetry on parallels of latitude ($\theta =$ const) is preserved: n-fold symmetry, when the force points into such a direction of the icosahedron. The figures show the absolute value of the displacement fields u (Figs. 1 and 2) and w (Fig. 3) on such a parallel with $\theta = \pi/4$. For these figures we have choosen the elastic constants as given by Jarić and Mohanty [16].

All figures reflect the deviation from the spherical symmetry but show the icosahedral symmetry: the two-fold axis in Figure 1, five-fold in Figure 2 and three-fold in Figure 3. In the case of phonon displacement this deviation is less than one percent. It is possible to examine the three components of the displacement fields or different values of θ, but the results are very similar.

It is important to note that the deviation from the spherical symmetry is present although we have made the

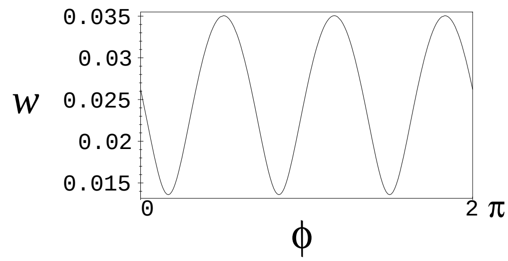

Fig. 3. Absolute value of phason displacement $|w|$ *versus* ϕ for $\theta = \pi/4$, 3-fold axis.

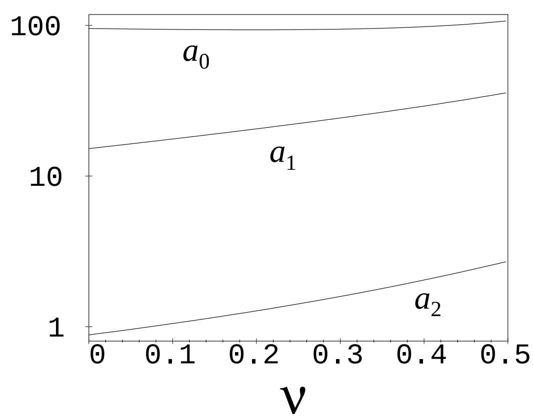

Fig. 4. Coefficients a_0, a_1, and a_2 as a function of Poisson's ratio ν.

spherical approximation in the space of phason strains. Because the space of phonon strains is isotropic by definition, this deviation is only due to the nonvashing coupling between these two spaces, depending in second order on μ_3.

We will now consider the five-fold axis (Fig. 2) in detail. The absolute value of the phonon displacement field in second order on the parallel of latitude with $\theta = \pi/4$ is given by

$$|\mathbf{u}^{(2)}(\phi)| := |\mathsf{G}_2^{u,u}(r=1, \theta = \frac{\pi}{4}, \phi)\mathbf{f}_0^u| \\ = \frac{\mu_3^2 10^{-5}}{\pi K_1 \mu^2}\sqrt{a_0\left(\frac{\lambda}{\mu}\right) + a_1\left(\frac{\lambda}{\mu}\right)\cos(5\phi) + a_2\left(\frac{\lambda}{\mu}\right)\cos(10\phi)}, \tag{51}$$

where the coefficients a_0, a_1, and a_2 are functions in the ratio λ/μ. They are plotted in Figure 4 as a function of Poisson's ratio ν, which is connected to λ and μ by

$$\frac{\lambda}{\mu} = \frac{2\nu}{1 - 2\nu}\,\cdot \tag{52}$$

In the physically interesting interval $\nu \in [0, 0.5]$ the coefficient a_0 is half an order of magnitude larger than a_1, which again is one order of magnitude larger than a_2. Therefore the maximum and the minimum of $|\mathbf{u}^{(2)}(\phi)|$ are at the same positions as the maximum and the minimum of $\cos(5\phi)$. The difference between maximum and minimum is then given by

$$|\mathbf{u}^{(2)}(0)| - |\mathbf{u}^{(2)}(\frac{\pi}{5})|. \tag{53}$$

In this paper we have discussed the theory of elasticity in icosahedral quasicrystals. We provide for the first time an approximative solution for the elastic Green's function, which reflects the deviation of the isotropy. For this approximation we made the assumption, that

- the two phason elastic constants are equal ($\mu_4 = \mu_5$) and that
- the coupling constant μ_3 is small.

Measurements of Boudard, de Boissieu *et al.* [17,18] in AlPdMn show that the first assumption is not fulfilled. The constant K_2 should be zero (see Appendix B). Nevertheless, the qualitative results of this paper remain valid, because they are based on the coupling between phonons and phasons. The component of the phason strain ε^{w5}, which is coupled to the phonon strain, is directly connected to the constant μ_5. The value of the other phason constant μ_4 does only indirectly affect this coupling.

The elastic Green's function is provided up to second order of perturbation theory in a basis of icosahedral invariants. With the help of this Green's function we examined the phonon and phason displacement fields due to a phonon point force. Although the icosahedral symmetry is close to the isotropic symmetry, the deviation from the isotropy is observable.

Appendix A: Icosahedral basis

A.1 Icosahedral irreducible strain

We have choosen the same coordinate system as in [12,13,19]. Using the golden number $\tau = (1+\sqrt{5})/2$ the icosahedral irreducible strain is given by:

$$\varepsilon^{u1} = \frac{1}{\sqrt{3}}(\varepsilon_{11}^u + \varepsilon_{22}^u + \varepsilon_{33}^u) \tag{54}$$

$$\varepsilon^{w4} = \frac{1}{\sqrt{3}}\begin{bmatrix} \varepsilon_{11}^w + \varepsilon_{22}^w + \varepsilon_{33}^w \\ \frac{1}{\tau}\varepsilon_{21}^w + \tau\varepsilon_{12}^w \\ \frac{1}{\tau}\varepsilon_{32}^w + \tau\varepsilon_{23}^w \\ \frac{1}{\tau}\varepsilon_{13}^w + \tau\varepsilon_{32}^w \end{bmatrix} \tag{55}$$

$$\varepsilon^{u5} = \begin{bmatrix} \frac{1}{2\sqrt{3}}(-\tau^2\varepsilon_{11}^u + \frac{1}{\tau^2}\varepsilon_{22}^u + (\tau + \frac{1}{\tau})\varepsilon_{33}^u) \\ \frac{1}{2}(\frac{1}{\tau}\varepsilon_{11}^u - \tau\varepsilon_{22}^u + \varepsilon_{33}^u) \\ \sqrt{2}\varepsilon_{12}^u \\ \sqrt{2}\varepsilon_{23}^u \\ \sqrt{2}\varepsilon_{31}^u \end{bmatrix} \tag{56}$$

$$\varepsilon^{w5} = \frac{1}{\sqrt{6}}\begin{bmatrix} \sqrt{3}(\varepsilon_{11}^w - \varepsilon_{22}^w) \\ \varepsilon_{11}^w + \varepsilon_{22}^w - 2\varepsilon_{33}^w \\ \sqrt{2}(\tau\varepsilon_{21}^w - \frac{1}{\tau}\varepsilon_{12}^w) \\ \sqrt{2}(\tau\varepsilon_{32}^w - \frac{1}{\tau}\varepsilon_{23}^w) \\ \sqrt{2}(\tau\varepsilon_{13}^w - \frac{1}{\tau}\varepsilon_{31}^w) \end{bmatrix}. \tag{57}$$

A.2 Icosahedral irreducible matrices

In order to write the icosahedral irreducible matrices in a compact form it is useful to define a "permutation operator"

$$P : M \mapsto P(M) \text{ with } P(M)_{i,j} := M_{i-1,j-1 \mod 3}, \quad (58)$$

which permutes the matrix indices modulo 3.

– phonon-phonon-block:

$$M_1^{3,3;1} = \frac{\sqrt{3}}{3}\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix} \qquad M_1^{3,3;3} = \frac{\sqrt{2}}{2}\begin{bmatrix}0&0&0\\0&0&1\\0&-1&0\end{bmatrix}$$

$$M_2^{3,3;3} = P(M_1^{3,3;3}) \qquad M_3^{3,3;3} = P^2(M_1^{3,3;3})$$

$$M_1^{3,3;5} = \frac{\sqrt{3}}{6}\begin{bmatrix}-\tau^2&0&0\\0&\frac{1}{\tau^2}&0\\0&0&\tau+\frac{1}{\tau}\end{bmatrix}$$

$$M_2^{3,3;5} = \frac{1}{2}\begin{bmatrix}\frac{1}{\tau}&0&0\\0&-\tau&0\\0&0&1\end{bmatrix} \qquad M_3^{3,3;5} = \frac{\sqrt{2}}{2}\begin{bmatrix}0&1&0\\1&0&0\\0&0&0\end{bmatrix}$$

$$M_4^{3,3;5} = P(M_3^{3,3;5}) \qquad M_5^{3,3;5} = P^2(M_3^{3,3;5})$$

– phason-phonon-block:

$$M_1^{3',3;4} = M_1^{3,3;1} \qquad M_2^{3',3;4} = \frac{\sqrt{3}}{3}\begin{bmatrix}0&\tau&0\\\frac{1}{\tau}&0&0\\0&0&0\end{bmatrix}$$

$$M_3^{3',3;4} = P(M_2^{3',3;4}) \qquad M_4^{3',3;4} = P^2(M_2^{3',3;4})$$

$$M_1^{3',3;5} = \frac{\sqrt{2}}{2}\begin{bmatrix}-1&0&0\\0&1&0\\0&0&0\end{bmatrix} \qquad M_2^{3',3;5} = \frac{\sqrt{6}}{6}\begin{bmatrix}-1&0&0\\0&-1&0\\0&0&2\end{bmatrix}$$

$$M_3^{3',3;5} = \frac{\sqrt{3}}{3}\begin{bmatrix}0&\frac{1}{\tau}&0\\-\tau&0&0\\0&0&0\end{bmatrix} \qquad M_4^{3',3;5} = P(M_3^{3',3;5})$$

$$M_5^{3',3;5} = P^2(M_3^{3',3;5}).$$

– The icosahedral irreducible matrices of the phason-phason-block can be generated from the matrices of the phonon-phonon-block by the substitution

$$\Gamma^3 \to \Gamma^{3'} \qquad \tau \to -\frac{1}{\tau}\,. \quad (59)$$

All matrices are normalized with respect to the quadratic vector norm, where $\{\delta_{ij}|i,j = 1\ldots3\}$ is considered to be the normalized basis of the vector space.

A.3 Icosahedral irreducible functions

$$s_1^{0;1}(\mathbf{x}) = 1 \quad (60)$$

$$s_1^{2;5}(\mathbf{x}) = \frac{\sqrt{3}}{6\mathbf{x}^2}[-\tau^2x^2 + \frac{1}{\tau^2}y^2 + (\tau+\frac{1}{\tau})z^2] \quad (61)$$

$$s_2^{2;5}(\mathbf{x}) = \frac{1}{2\mathbf{x}^2}[\frac{1}{\tau}x^2 - \tau y^2 + z^2] \quad (62)$$

$$s_3^{2;5}(\mathbf{x}) = \frac{\sqrt{2}}{\mathbf{x}^2}xy \quad s_4^{2;5}(\mathbf{x}) = \frac{\sqrt{2}}{\mathbf{x}^2}yz \quad s_5^{2;5}(\mathbf{x}) = \frac{\sqrt{2}}{\mathbf{x}^2}zx \quad (63)$$

All functions are normalized with respect to the quadratic vector norm, where $\left\{\sqrt{\frac{i!j!k!}{l!}}\frac{x^iy^jz^k}{\mathbf{x}^l}|i,j,k \geq 0, i+j+k = l\right\}$ is considered to be the normalized basis of the vector space, which is the space of all spherical harmonics to the orbital quantum number l.

Appendix B: Elastic constants

Unfortunately, the definitions of the elastic constants of icosahedral quasicrystals differ in the literature. Therefore we want to compare our definition given in (6) to others.

– Trebin, Fink, Stark [13,20]

$$\begin{matrix}\mu_1 = 3\lambda_1 & \mu_2 = \lambda_2 & \mu_3 = \lambda_3\\ \mu_4 = \lambda_4 & \mu_5 = \lambda_5. & \end{matrix} \quad (64)$$

– Shaw, Elser, Henley [21], Widom [22] and Henley [23] use the well-known Lamé-constants λ and μ, see (7). The three remaining constants are:

$$\mu_3 = K_3\sqrt{6} \quad \mu_4 = K_1 + \frac{5}{3}K_2 \quad \mu_5 = K_1 - \frac{4}{3}K_2. \quad (65)$$

Boudard, de Boissieu *et al.* [17,18] use the same elastic constants (see Ref. [19] in [18]).

– Ding *et al.* [10] also use the Lamé-constants, but the "phasonic" constants are different:

$$\mu_3 = R\sqrt{6} \qquad \mu_4 = K_1 - 2K_2 \qquad \mu_5 = K_1 + K_2. \quad (66)$$

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