

Article

Three-Dimensional Green Tensor of One-Dimensional Hexagonal Quasicrystals

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Abstract: In this work, the elastic 4×4 Green tensor of one-dimensional quasicrystals is given and has phonon, phason and phonon–phason coupling components. Using the residue method, a closed-form expression of the elastic 4×4 Green tensor for one-dimensional hexagonal quasicrystals of Laue class 10, which possess 10 independent material constants, is derived. The 10 independent components of the obtained 4×4 Green tensor are numerically presented in contour plots, revealing features of anisotropy as well as the interesting result that the phason component of the Green tensor has the strongest contribution in comparison with all the other components. In the case of vanishing phonon–phason coupling, the phonon part of the derived Green tensor reproduces Kröner's well-known elastic 3×3 Green tensor for hexagonal crystals. The analytical closed-form expression of the derived Green tensor provides an advantage for efficient computational calculations in various applications.

Keywords: quasicrystals; Green tensor; one-dimensional hexagonal quasicrystals; residue method



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1. Introduction

Quasicrystals belong to aperiodic crystals and possess a long-range orientational order but no translational symmetry in the quasiperiodic directions [1]. Their special features provide them with unique properties such as a low friction coefficient [2], low adhesion [3] and high wear resistance [4], which are desired in various applications in technology. Nowadays, quasicrystals belong to new or novel materials enjoying the interest for their theoretical and experimental study as well as their potential use in many technological devices [5].

The basis of the continuum theory of solid quasicrystals is set up by two elementary excitations: the phonons and the phasons [6,7]. In the atomistic picture, phonons are related to the translation of atoms and phasons lead to local rearrangements of atoms in a cell. A systematic and comprehensive overview concerning the study of generalized elasticity of quasicrystals and their defects has been given by Fan [8]. There are three types of quasicrystals: one-, two- and three-dimensional quasicrystals. One-dimensional quasicrystals are an important class of quasicrystals (see [8–13]). In one-dimensional quasicrystals, there is a quasiperiodic arrangement of atoms in one direction, usually in the z -direction, and a regular periodic arrangement of atoms in the plane perpendicular to this direction, that is, in the xy -plane. One-dimensional quasicrystals are quasicrystals with crystallographic symmetries, namely, 31 point groups and 10 Laue classes [9]. One-dimensional hexagonal quasicrystals are divided into two Laue classes: Laue class 9 and Laue class 10. As it was pointed out in Agiasofitou and Lazar [14], a distinction has to be made between the two Laue classes concerning the material moduli and the constitutive relations, a fact that is often ignored in the literature concerning the elasticity theory of one-dimensional hexagonal quasicrystals. Specifically, the constitutive relations of one-dimensional hexagonal quasicrystals of Laue class 9 are different than those of one-dimensional hexagonal quasicrystals of Laue class 10, since the former possess 11 material moduli and the latter possess 10 material moduli [14]. From the point of view of the generalized elasticity of

quasicrystals, Lazar and Agiasofitou [13], using rotational transformations, have examined the corresponding isotropy condition and proved that a one-dimensional hexagonal quasicrystal of Laue class 10 is isotropic in the basal xy -plane.

Green functions are the fundamental solutions of linear partial differential equations [15–17] and play an important role in the solution of many problems in various scientific areas like applied mathematics, physics, engineering science and material science. If the differential operator entering the partial differential equation is a scalar one, then we speak of a Green function, whereas if it is a tensorial one, then we speak of a Green tensor. For isotropic materials, the elastic Green tensor was derived by Lord Kelvin [18]. For general anisotropy, Fredholm [19] deduced the form of the elastic Green tensor in terms of the roots of a sextic algebraic equation. An integral expression for the elastic Green tensor has been given by Lifshitz and Rosenzweig [20] and Synge [21] (see also [22,23]) for general anisotropy. As far as elasticity is concerned, a hexagonal medium is equivalent to a transversely isotropic medium, a fact that is important to find closed-form expressions for an elastic Green tensor. The closed-form expression for the elastic Green tensor of a hexagonal medium has been explicitly calculated by Lifshitz and Rosenzweig [20], Kröner [24] and Willis [25] (see also [26,27]). In particular, Kröner [24] used the algebraic method of Fredholm [19]. Willis [25] evaluated the elastic Green tensor from the contour integral representation given by Synge [21] for a transversely isotropic medium and pointed out some important misprints in the results of Kröner [24]. Moreover, Willis [25] gave a proof of the equivalence of the integral expression given by Synge [21] to the result of Fredholm [19] which was utilized by Kröner [24]. Note that only for isotropic and hexagonal crystals do closed-form expressions of the elastic Green tensor exist (see [20,22–24]). As a generalization of the elastic 3×3 Green tensor for hexagonal materials, the 4×4 Green tensor for hexagonal piezoelectric crystals of point group $6mm$, which is a transversely isotropic medium, has been derived by Michelitsch [28] (see also [29]) from the integral expression of the 4×4 Green tensor for general piezoelectric media given by Deeg [30], Chen [31] and Dunn [32]. Only for hexagonal piezoelectric crystals of point group $6mm$ can a closed-form expression of the 4×4 piezoelectric Green tensor be derived. In the present paper, we consider the class of one-dimensional quasicrystals, which have, in a continuum setting, a constitutive behavior analogous to that of a piezoelectric crystal of transverse isotropic symmetry (see also [14]), which are one-dimensional hexagonal quasicrystals of Laue class 10.

Concerning Green functions in quasicrystals, De and Pelcovits [33] found the two-dimensional Green functions for pentagonal quasicrystals and Ding et al. [34] found the explicit expressions of two-dimensional Green tensors for various forms of planar quasicrystals. Bachteler and Trebin [35] gave an approximative solution for the elastic Green tensor of three-dimensional icosahedral quasicrystals, assuming that the coupling between phonons and phasons is small. Lazar and Agiasofitou [36] derived the generalized three-dimensional elastic Green tensor for arbitrary quasicrystals, that is, for one-dimensional, two-dimensional and three-dimensional quasicrystals. The Green function for constrained cubic quasicrystals has been given by Zhang et al. [37]. Moreover, the generalized three-dimensional Green tensor for arbitrary piezoelectric quasicrystals has been recently given by Lazar and Agiasofitou [38]. Three-dimensional general solutions for static problems in thermo-elasticity of one-dimensional hexagonal quasicrystals have been given by Li and Li [39].

The aim of this work is to derive an analytical closed-form expression of the elastic 4×4 Green tensor for one-dimensional hexagonal quasicrystals of Laue class 10 using the integral representation of the Green tensor in Synge form given by Lazar and Agiasofitou [36] and applying the residue method. As it has been shown by Willis [25] and Michelitsch [28], the residue method is a useful tool to obtain closed-form expressions of the Green tensors in media with hexagonal symmetry. The residue calculus method can also be used for the numerical evaluation of the Green tensor and its derivatives for generally anisotropic materials as well as for piezoelectric materials (see, e.g., [40–44]).

The paper is organized as follows. In Section 2, the basic equations for one-dimensional quasicrystals are given and a suitable hyperspace notation is employed in order to derive the Green tensor for one-dimensional quasicrystals in Section 3. The 10 independent

elastic constants of one-dimensional hexagonal quasicrystals of Laue class 10, together with the conditions of positive definiteness, are given in Section 4. The Green tensor for one-dimensional hexagonal quasicrystals of Laue class 10 is derived in Section 5 with the residue method. In Section 6, the 10 components of the Green tensor for one-dimensional hexagonal quasicrystals of Laue class 10 are plotted in contour plots. Conclusions are given in Section 7. The limit of the obtained Green tensor of one-dimensional hexagonal quasicrystals of Laue class 10 to the Green tensor of hexagonal crystals is given in Appendix A.

2. Basic Equations of One-Dimensional Quasicrystals

In this section, we provide the basic equations of the generalized elasticity theory of one-dimensional quasicrystals necessary for the forthcoming calculations with focus on the hyperspace notation, which is appropriate for the representation of the phonon and phason fields in the corresponding extended field “living” in the hyperspace.

A one-dimensional quasicrystal can be generated by the projection of a four-dimensional periodic structure to the three-dimensional physical space. The four-dimensional hyperspace E^4 can be decomposed into the direct sum of two orthogonal subspaces

$$E^4 = E_{\parallel}^3 \oplus E_{\perp}^1, \quad (1)$$

where E_{\parallel}^3 is the three-dimensional physical or parallel space of the phonon fields and E_{\perp}^1 is the one-dimensional perpendicular space of the phason fields with quasiperiodicity in the z -direction. Throughout the text, phonon fields will be denoted by $(\cdot)_{\parallel}$ and phason fields by $(\cdot)_{\perp}$. Note that all quantities (phonon and phason fields) depend on the so-called material space coordinates $x \in \mathbb{R}^3$. Indices in the parallel space are denoted by small letters i, j, k, l , with $i, j, k, l = 1, 2, 3$.

In the theory of the generalized elasticity of one-dimensional quasicrystals, the *phonon displacement field* is denoted by $u_k_{\parallel} \in E_{\parallel}^3$, $k = 1, 2, 3$ and the *phason displacement field*, which is in the z -direction, is denoted by $u_3^{\perp} \in E_{\perp}^1$. That is, for one-dimensional quasicrystals, the phason displacement field is a scalar field. That is the reason that there is a mathematical analogy between one-dimensional quasicrystals and piezoelectric crystals. The *phonon and phason distortion tensors*, β_{kl}^{\parallel} and β_{3l}^{\perp} , are defined as the spatial gradients of u_k^{\parallel} and u_3^{\perp} , respectively

$$\beta_{kl}^{\parallel} = \partial_l u_k^{\parallel}, \quad (2)$$

$$\beta_{3l}^{\perp} = \partial_l u_3^{\perp}, \quad (3)$$

where $\partial_l = \partial/\partial x_l$ indicates the derivative with respect to the spatial coordinates x_l . The equilibrium conditions are of the form (see, e.g., [45,46])

$$\partial_j \sigma_{ij}^{\parallel} + f_i^{\parallel} = 0, \quad (4)$$

$$\partial_j \sigma_{3j}^{\perp} + f_3^{\perp} = 0, \quad (5)$$

where σ_{ij}^{\parallel} denotes the *phonon stress tensor*, σ_{3j}^{\perp} are the *phason stresses*, f_i^{\parallel} is the *phonon body force density* and f_3^{\perp} is the *phason body force density*. The phonon stress tensor is a symmetric tensor of rank two: $\sigma_{ij}^{\parallel} = \sigma_{ji}^{\parallel}$.

The associated linear constitutive relations between the stresses and distortions are

$$\sigma_{ij}^{\parallel} = C_{ijkl} e_{kl}^{\parallel} + D_{ij3l} \beta_{3l}^{\perp}, \quad (6)$$

$$\sigma_{3j}^{\perp} = D_{kl3j} e_{kl}^{\parallel} + E_{3j3l} \beta_{3l}^{\perp}, \quad (7)$$

where C_{ijkl} is the tensor of the elastic moduli of phonons, E_{3j3l} is the tensor of the elastic moduli of phasons and D_{ij3l} is the tensor of the elastic moduli of the phonon–phason

coupling for one-dimensional quasicrystals. The constitutive tensors possess the following *major symmetries* (see [45])

$$C_{ijkl} = C_{klij}, \quad E_{3j3l} = E_{3l3j} \quad (8)$$

and *minor symmetries*

$$C_{ijkl} = C_{jikl} = C_{ijlk}, \quad D_{ij3l} = D_{ji3l}. \quad (9)$$

Substituting Equations (6), (7), (2) and (3) into Equations (4) and (5), we obtain the *coupled inhomogeneous Navier equations for the phonon and phason displacement fields*:

$$C_{ijkl} \partial_j \partial_l u_k^{\parallel} + D_{ij3l} \partial_j \partial_l u_3^{\perp} = -f_i^{\parallel}, \quad (10)$$

$$D_{kl3j} \partial_j \partial_l u_k^{\parallel} + E_{3j3l} \partial_j \partial_l u_3^{\perp} = -f_3^{\perp}. \quad (11)$$

A major tool used in deriving the results of later sections in this article is the *hyperspace notation of quasicrystals* introduced by Lazar and Agiasofitou [36], so that the phonon and phason fields can be unified in the corresponding *extended field in the hyperspace*. The components of the extended fields will be denoted by capital letters, e.g., $I, K = 1, 2, 3, 4$. In the hyperspace notation, the following extended fields can be defined:

- The *extended displacement vector* $U_K = (u_k^{\parallel}, u_3^{\perp}) \in E_{\parallel}^3 \oplus E_{\perp}^1$

$$U_K = \begin{cases} u_k^{\parallel}, & K = 1, 2, 3, \\ u_3^{\perp}, & K = 4. \end{cases} \quad (12)$$

- The *extended elastic distortion tensor* $B_{KI} \in (E_{\parallel}^3 \oplus E_{\perp}^1) \otimes E_{\parallel}^3$

$$B_{KI} = \begin{cases} \beta_{kl}^{\parallel}, & K = 1, 2, 3, \\ \beta_{3l}^{\perp}, & K = 4. \end{cases} \quad (13)$$

- The *extended stress tensor* $\Sigma_{Ij} \in (E_{\parallel}^3 \oplus E_{\perp}^1) \otimes E_{\parallel}^3$

$$\Sigma_{Ij} = \begin{cases} \sigma_{ij}^{\parallel}, & I = 1, 2, 3, \\ \sigma_{3j}^{\perp}, & I = 4. \end{cases} \quad (14)$$

- The *extended body force vector* $F_I = (f_i^{\parallel}, f_3^{\perp}) \in E_{\parallel}^3 \oplus E_{\perp}^1$

$$F_I = \begin{cases} f_i^{\parallel}, & I = 1, 2, 3, \\ f_3^{\perp}, & I = 4. \end{cases} \quad (15)$$

- The *tensor of the extended elastic moduli* $C_{IjKI} \in (E_{\parallel}^3 \oplus E_{\perp}^1) \otimes E_{\parallel}^3 \otimes (E_{\parallel}^3 \oplus E_{\perp}^1) \otimes E_{\parallel}^3$

$$C_{IjKI} = \begin{cases} C_{ijkl}, & I = 1, 2, 3; \quad K = 1, 2, 3, \\ D_{ij3l}, & I = 1, 2, 3; \quad K = 4, \\ D_{kl3j}, & I = 4; \quad K = 1, 2, 3, \\ E_{3j3l}, & I = 4; \quad K = 4. \end{cases} \quad (16)$$

The tensor C_{IjKI} retains the *major symmetry*

$$C_{IjKI} = C_{KlIj}. \quad (17)$$

In matrix form, Equation (16) reads

$$C_{IjKl} = \begin{pmatrix} C_{ijkl} & D_{ij3l} \\ D_{kl3j} & E_{3j3l} \end{pmatrix}. \quad (18)$$

Using the hyperspace notation and the above introduced extended fields, the basic equations of one-dimensional quasicrystals can be rewritten in a “compact” form as follows. Equations (2) and (3) can be written as

$$B_{Kl} = \partial_l U_K. \quad (19)$$

The equilibrium conditions (4) and (5) read

$$\partial_j \Sigma_{Ij} + F_I = 0 \quad (20)$$

with the constitutive relations (6) and (7) to be given by

$$\Sigma_{Ij} = C_{IjKl} B_{Kl}. \quad (21)$$

Equations (10) and (11) read in terms of the extended displacement vector U_K

$$C_{IjKl} \partial_j \partial_l U_K + F_I = 0. \quad (22)$$

Equation (22) is a Navier-type partial differential equation for the extended displacement vector U_K .

3. Three-Dimensional Green Tensor for One-Dimensional Quasicrystals

In this section, we derive the three-dimensional Green tensor for one-dimensional quasicrystals in an integral form expression.

Introducing the Navier-type differential operator in the hyperspace

$$\mathcal{T}_{IK}(\nabla) = C_{IjKl} \partial_j \partial_l \quad (23)$$

with $\mathcal{T}_{IK}(\nabla) = \mathcal{T}_{KI}(\nabla)$ due to the major symmetry of C_{IjKl} , Equation (17), the field Equation (22) becomes

$$\mathcal{T}_{IK}(\nabla) U_K + F_I = 0, \quad (24)$$

where ∇ indicates the gradient operator. The symmetric 4×4 second-order differential operator $\mathcal{T}_{IK}(\nabla)$ can be written in the form

$$\mathcal{T}_{IK}(\nabla) = \begin{pmatrix} T_{ik}(\nabla) & t_i(\nabla) \\ t_k(\nabla) & \tau(\nabla) \end{pmatrix}, \quad (25)$$

where $T_{ik}(\nabla)$ is a 3×3 tensor operator given by

$$T_{ik}(\nabla) = C_{ijkl} \partial_j \partial_l, \quad (26)$$

which represents the phonon part, $t_i(\nabla)$ is a (3×1) vector operator given by

$$t_i(\nabla) = D_{ij3l} \partial_j \partial_l, \quad (27)$$

which represents the phonon–phason coupling part and τ is the (1×1) scalar operator given by

$$\tau(\nabla) = E_{3j3l} \partial_j \partial_l, \quad (28)$$

which describes the phason part.

The vector field U_K can then be represented by the elastic 4×4 Green tensor G_{KM} of one-dimensional quasicrystals according to

$$U_K(\mathbf{r}) = \int_{\mathbb{R}^3} \mathcal{G}_{KM}(\mathbf{R}) F_M(\mathbf{r}') d\mathbf{r}', \tag{29}$$

where $\mathbf{R} = \mathbf{r} - \mathbf{r}'$. The elastic 4×4 Green tensor \mathcal{G}_{KM} of one-dimensional quasicrystals is defined by

$$\mathcal{T}_{IK}(\nabla) \mathcal{G}_{KM}(\mathbf{r}) + \delta_{IM} \delta(\mathbf{r}) = 0, \tag{30}$$

where $\delta(\mathbf{r})$ is the three-dimensional Dirac delta function and δ_{IM} denotes the 4×4 unit matrix. Note that the Green tensor $G_{KM}(\mathbf{R})$ is a symmetric tensor of rank two in the hyperspace. This property follows from the symmetry of the differential operator $\mathcal{T}_{IK}(\nabla) = \mathcal{T}_{KI}(\nabla)$ in Equation (23).

The elastic 4×4 Green tensor $\mathcal{G}_{KM}(\mathbf{R})$ ($K, M = 1, 2, 3, 4$) of one-dimensional quasicrystals can be decomposed into its phonon, phason and phonon–phason coupling parts

$$\mathcal{G}_{KM}(\mathbf{R}) = \begin{pmatrix} G_{km}^{\parallel\parallel}(\mathbf{R}) & G_{k4}^{\parallel\perp}(\mathbf{R}) \\ G_{4m}^{\perp\parallel}(\mathbf{R}) & G_{44}^{\perp\perp}(\mathbf{R}) \end{pmatrix} \tag{31}$$

or, explicitly,

$$\mathcal{G}_{KM} = \begin{pmatrix} G_{11}^{\parallel\parallel} & G_{12}^{\parallel\parallel} & G_{13}^{\parallel\parallel} & G_{14}^{\parallel\perp} \\ G_{12}^{\parallel\parallel} & G_{22}^{\parallel\parallel} & G_{23}^{\parallel\parallel} & G_{24}^{\parallel\perp} \\ G_{13}^{\parallel\parallel} & G_{23}^{\parallel\parallel} & G_{33}^{\parallel\parallel} & G_{34}^{\parallel\perp} \\ G_{14}^{\perp\parallel} & G_{24}^{\perp\parallel} & G_{34}^{\perp\parallel} & G_{44}^{\perp\perp} \end{pmatrix} \tag{32}$$

and it has the following physical interpretation [36]:

$G_{km}^{\parallel\parallel}(\mathbf{R})$ is the phonon displacement at \mathbf{r} in the x_k -direction due to a unit phonon point force at \mathbf{r}' in the x_m -direction, $k, m = 1, 2, 3$;

$G_{k4}^{\parallel\perp}(\mathbf{R})$ is the phonon displacement at \mathbf{r} in the x_k -direction due to a unit phason point force at \mathbf{r}' in the x_3 -direction, $k = 1, 2, 3$;

$G_{4m}^{\perp\parallel}(\mathbf{R})$ is the phason displacement at \mathbf{r} in the x_3 -direction due to a unit phonon point force at \mathbf{r}' in the x_m -direction, $m = 1, 2, 3$;

$G_{44}^{\perp\perp}(\mathbf{R})$ is the phason displacement at \mathbf{r} in the x_3 -direction due to a unit phason point force at \mathbf{r}' in the x_3 -direction.

Using Fourier transform, the elastic 4×4 Green tensor of arbitrary anisotropic one-dimensional quasicrystals in integral form reads (at $\mathbf{r}' = 0$) [36]

$$\mathcal{G}_{KM}(\mathbf{r}) = \frac{1}{8\pi^2 r} \int_0^{2\pi} \mathcal{T}_{KM}^{-1}(\boldsymbol{\zeta}(\phi)) d\phi. \tag{33}$$

The integral is taken around the unit circle ($\boldsymbol{\zeta}^2 = 1$) in the plane normal to \mathbf{r} . $\mathcal{T}_{IK}(\boldsymbol{\zeta})$ is obtained from Equation (25) by replacing ∂_i by ζ_i ($i = 1, 2, 3$) in Equations (26)–(28) and it reads

$$\mathcal{T}_{IK}(\boldsymbol{\zeta}) = C_{Ijkl} \zeta_j \zeta_l = \begin{pmatrix} C_{ijkl} \zeta_j \zeta_l & D_{ij3l} \zeta_j \zeta_l \\ D_{kl3j} \zeta_j \zeta_l & E_{3j3l} \zeta_j \zeta_l \end{pmatrix}. \tag{34}$$

The vector $\boldsymbol{\zeta}$ can be represented as [22,28,47]

$$\boldsymbol{\zeta}(\phi) = \mathbf{e}_1 \cos \phi + \mathbf{e}_2 \sin \phi, \tag{35}$$

where the vectors \mathbf{e}_i form a useful orthonormal basis

$$\mathbf{e}_1 = \frac{1}{\rho} \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix}, \quad \mathbf{e}_2 = \frac{1}{\rho r} \begin{pmatrix} -zx \\ -zy \\ \rho^2 \end{pmatrix}, \quad \mathbf{e}_3 = \frac{1}{r} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{36}$$

with $\rho^2 = x^2 + y^2$, $r^2 = \rho^2 + z^2$ and $r = re_3$. The orientation of this coordinate system can be expressed by $e_i = \frac{1}{2}\epsilon_{ijk}e_j \times e_k$, where ϵ_{ijk} denotes the three-dimensional Levi-Civita tensor.

4. Elastic Moduli of One-Dimensional Hexagonal Quasicrystals of Laue Class 10

In this section, one-dimensional hexagonal quasicrystals of Laue class 10 are considered. Regarding the generalized elasticity of quasicrystals, a one-dimensional hexagonal quasicrystal of Laue class 10 is a transversely isotropic medium. Specifically, a one-dimensional hexagonal quasicrystal of Laue class 10 is isotropic in the basal xy -plane (see [13]). Laue class 10 consists of the following point groups [8]: 62_h2_h , $6mm$, $\bar{6}m2_h$ and $6/m_hmm$.

The one-dimensional hexagonal quasicrystals of Laue class 10 possess 10 independent elastic constants (see [9]):

- Five independent elastic moduli of phonons

$$\begin{aligned} C_{1111} = C_{2222} = C_{11}, \quad C_{1122} = C_{2211} = C_{12}, \quad C_{1133} = C_{2233} = C_{3311} = C_{3322} = C_{13}, \\ C_{3333} = C_{33}, \quad C_{2323} = C_{2332} = C_{3223} = C_{3232} = C_{1313} = C_{1331} = C_{3113} = C_{3131} = C_{44}, \\ C_{1212} = C_{1221} = C_{2112} = C_{2121} = C_{66} = (C_{11} - C_{12})/2 \end{aligned} \tag{37}$$

- Three independent elastic moduli of phonon–phason coupling

$$D_{1133} = D_{2233} = R_1, \quad D_{3333} = R_2, \quad D_{3232} = D_{2332} = D_{3131} = D_{1331} = R_3 \tag{38}$$

- Two independent elastic moduli of phasons

$$E_{3333} = K_1, \quad E_{3131} = E_{3232} = K_2. \tag{39}$$

The set of necessary and sufficient conditions for the positive definiteness of the elastic energy density of one-dimensional hexagonal quasicrystals of Laue class 10 is given by the following five inequalities imposed on the elastic constants [48]:

$$C_{11} > |C_{12}|, \quad (C_{11} + C_{12})C_{33} - 2C_{13}^2 > 0, \quad C_{44} > 0, \tag{40}$$

$$C_{44}K_2 - R_3^2 > 0, \tag{41}$$

$$[(C_{11} + C_{12})C_{33} - 2C_{13}^2]K_1 + 2(2C_{13}R_2 - C_{33}R_1)R_1 - (C_{11} + C_{12})R_2^2 > 0. \tag{42}$$

5. Three-Dimensional Green Tensor for One-Dimensional Hexagonal Quasicrystals of Laue Class 10

In this section, the main result of this article is given. The three-dimensional Green tensor for one-dimensional hexagonal quasicrystals of Laue class 10 is explicitly derived from the integral expression (33) in closed-form expression using the residue method.

In order to obtain a convenient representation of the Green tensor (33), we use an appropriate orthonormal basis to represent the 4×4 matrix $\mathcal{T}(\xi)$ and, later, $\mathcal{T}^{-1}(\xi)$ (see [28]):

$$e_b = \frac{1}{\xi_b} \begin{pmatrix} \xi_1 \\ \xi_2 \\ 0 \\ 0 \end{pmatrix}, \quad e_{b\perp} = \frac{1}{\xi_b} \begin{pmatrix} -\xi_2 \\ \xi_1 \\ 0 \\ 0 \end{pmatrix}, \quad e_c = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad e_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{43}$$

with $\xi_b = \sqrt{\xi_1^2 + \xi_2^2}$ and $\xi_c = \xi_3$. This basis represents the hexagonal symmetry. The vectors e_b and $e_{b\perp}$ are parallel to the basal plane and e_c represents the c -direction perpendicular to the basal plane and they are the suitable basis in the parallel space E_{\parallel}^3 for hexagonal symmetry. e_4 comes into play because of the phason component and is the basis in the perpendicular space E_{\perp}^1 . Using the basis (43), we obtain the following expression:

$$\begin{aligned} \mathcal{T}(\xi) = & T_{b\perp} \mathbf{e}_{b\perp} \otimes \mathbf{e}_{b\perp} + T_b \mathbf{e}_b \otimes \mathbf{e}_b + T_{bc} (\mathbf{e}_b \otimes \mathbf{e}_c + \mathbf{e}_c \otimes \mathbf{e}_b) + T_c \mathbf{e}_c \otimes \mathbf{e}_c \\ & + t_{b4} (\mathbf{e}_b \otimes \mathbf{e}_4 + \mathbf{e}_4 \otimes \mathbf{e}_b) + t_{c4} (\mathbf{e}_c \otimes \mathbf{e}_4 + \mathbf{e}_4 \otimes \mathbf{e}_c) + \tau \mathbf{e}_4 \otimes \mathbf{e}_4. \end{aligned} \quad (44)$$

The scalar quantities $T_{b\perp}$, T_b , T_{bc} , T_c , t_{b4} , t_{c4} and τ correspond to the tensors T , t and τ from Equations (26), (27) and (28), respectively (\otimes indicates dyadic multiplication). They are obtained as

$$T_{b\perp} = C_{66} \xi_b^2 + C_{44} \xi_c^2, \quad (45)$$

$$T_b = C_{11} \xi_b^2 + C_{44} \xi_c^2, \quad (46)$$

$$T_{bc} = (C_{13} + C_{44}) \xi_b \xi_c, \quad (47)$$

$$T_c = C_{44} \xi_b^2 + C_{33} \xi_c^2, \quad (48)$$

$$t_{b4} = (R_1 + R_3) \xi_b \xi_c, \quad (49)$$

$$t_{c4} = R_3 \xi_b^2 + R_2 \xi_c^2, \quad (50)$$

$$\tau = K_2 \xi_b^2 + K_1 \xi_c^2. \quad (51)$$

Here, and in what follows, the elastic constant $C_{66} = (C_{11} - C_{12})/2$ is used instead of C_{12} , since it provides more elegant expressions. The inverse 4×4 matrix $\mathcal{T}^{-1}(\xi)$ is given by

$$\mathcal{T}^{-1}(\xi) = \frac{\Lambda(\xi)}{f(\xi)}, \quad (52)$$

where $\Lambda(\xi) = \text{adj } \mathcal{T}(\xi)$ is the adjoint of the 4×4 matrix $\mathcal{T}(\xi)$, which are polynomials of degree 6 in ξ , and $f(\xi) = \det \mathcal{T}(\xi)$ is the determinant of the 4×4 matrix $\mathcal{T}(\xi)$, which is a polynomial of degree 8 in ξ . Using Equation (44), Λ can be written as follows:

$$\begin{aligned} \Lambda(\xi) = & \Lambda_{b\perp} \mathbf{e}_{b\perp} \otimes \mathbf{e}_{b\perp} + \Lambda_b \mathbf{e}_b \otimes \mathbf{e}_b + \Lambda_{bc} (\mathbf{e}_b \otimes \mathbf{e}_c + \mathbf{e}_c \otimes \mathbf{e}_b) + \Lambda_c \mathbf{e}_c \otimes \mathbf{e}_c \\ & + \Lambda_{b4} (\mathbf{e}_b \otimes \mathbf{e}_4 + \mathbf{e}_4 \otimes \mathbf{e}_b) + \Lambda_{c4} (\mathbf{e}_c \otimes \mathbf{e}_4 + \mathbf{e}_4 \otimes \mathbf{e}_c) + \Lambda_4 \mathbf{e}_4 \otimes \mathbf{e}_4, \end{aligned} \quad (53)$$

where

$$\Lambda_{b\perp} = \tau (T_b T_c - T_{bc}^2) - (t_{c4}^2 T_b - 2t_{c4} t_{b4} T_{bc} + t_{b4}^2 T_c), \quad (54)$$

$$\Lambda_b = T_{b\perp} (T_c \tau - t_{c4}^2), \quad (55)$$

$$\Lambda_{bc} = -T_{b\perp} (T_{bc} \tau - t_{b4} t_{c4}), \quad (56)$$

$$\Lambda_c = T_{b\perp} (T_b \tau - t_{b4}^2), \quad (57)$$

$$\Lambda_{b4} = T_{b\perp} (T_{bc} t_{c4} - T_c t_{b4}), \quad (58)$$

$$\Lambda_{c4} = -T_{b\perp} (T_b t_{c4} - T_{bc} t_{b4}), \quad (59)$$

$$\Lambda_4 = T_{b\perp} (T_b T_c - T_{bc}^2). \quad (60)$$

The determinant $f(\xi)$ of \mathcal{T} can be written as

$$f(\xi) = \det \mathcal{T}(\xi) = T(\xi)_{b\perp} \Lambda_{b\perp}(\xi). \quad (61)$$

Substituting Equations (45)–(51) and Equation (54) into Equation (61) shows that only terms proportional to $\xi_b^{2n} \xi_c^{8-2n}$ ($n = 0, 1, 2, 3, 4$) appear. This is a unique property of the hexagonal medium. It is the central property that is needed to solve the integration problem (33). Thus, Equation (54) is a polynomial of degree 3 in a if we put $a = \xi_b^2 / \xi_c^2$. We then can write

$$\Lambda_{b\perp} = P(a) \xi_c^6, \quad (62)$$

where $P(a)$ is a polynomial of degree 3 in a and takes the form

$$P(a) = Aa^3 + Ba^2 + Ca + D \quad (63)$$

and the coefficients A, B, C, D are given by

$$A = C_{11} \left(K_2 C_{44} - R_3^2 \right), \quad (64)$$

$$B = K_1 C_{11} C_{44} + K_2 \left(C_{11} C_{33} - 2C_{13} C_{44} - C_{13}^2 \right) - C_{44} R_3^2 - 2C_{11} R_3 R_2 + 2(C_{13} + C_{44}) R_3 (R_1 + R_3) - C_{44} (R_1 + R_3)^2, \quad (65)$$

$$C = K_1 \left(C_{11} C_{33} - 2C_{13} C_{44} - C_{13}^2 \right) + K_2 C_{33} C_{44} - 2R_3 R_2 C_{44} - R_2^2 C_{11} + 2R_2 (R_1 + R_3) (C_{13} + C_{44}) - C_{33} (R_1 + R_3)^2, \quad (66)$$

$$D = C_{44} \left(K_1 C_{33} - R_2^2 \right). \quad (67)$$

The determinant f can be factorized according to

$$f(\xi) = \xi_c^8 C_{66} A (a + A_1) (a + A_2) (a + A_3) (a + A_4) \quad (68)$$

with $T(a)_{b\perp} = C_{66} (a + A_1) \xi_c^2$, $A_1 = C_{44} / C_{66}$ and

$$P(a) = A (a + A_2) (a + A_3) (a + A_4). \quad (69)$$

The subdeterminant (54) gives with $a = \xi_b^2 / \xi_c^2$ and $\xi_c^2 = 1$

$$\Lambda_{b\perp}(a) = P(a) = Aa^3 + Ba^2 + Ca + D. \quad (70)$$

The numbers A_2, A_3, A_4 are the roots of the cubic equation

$$Aa^3 - Ba^2 + Ca - D = 0 \quad (71)$$

with the coefficients A, B, C, D given in Equations (64)–(67). The $A_l, l = 1, 2, 3, 4$ are material quantities and fully determined by the elastic moduli C, D, E . Furthermore, the subdeterminants (55)–(60) give with $a = \xi_b^2 / \xi_c^2$ and $\xi_c^2 = 1$

$$\Lambda_b(a) = (C_{66}a + C_{44}) \left[(K_2a + K_1)(C_{44}a + C_{33}) - (R_3a + R_2)^2 \right], \quad (72)$$

$$\Lambda_{bc}(a) = \sqrt{a} (C_{66}a + C_{44}) [(R_1 + R_3)(R_3a + R_2) - (K_2a + K_1)(C_{13} + C_{44})], \quad (73)$$

$$\Lambda_c(a) = (C_{66}a + C_{44}) \left[(K_2a + K_1)(C_{11}a + C_{44}) - a(R_1 + R_3)^2 \right], \quad (74)$$

$$\Lambda_{b4}(a) = \sqrt{a} (C_{66}a + C_{44}) [(C_{13} + C_{44})(R_3a + R_2) - (C_{44}a + C_{33})(R_1 + R_3)], \quad (75)$$

$$\Lambda_{c4}(a) = -(C_{66}a + C_{44}) [(C_{11}a + C_{44})(R_3a + R_2) - a(C_{13} + C_{44})(R_1 + R_3)], \quad (76)$$

$$\Lambda_4(a) = (C_{66}a + C_{44}) \left[a^2 C_{11} C_{44} + a \left(C_{11} C_{33} - 2C_{13} C_{44} - C_{13}^2 \right) + C_{33} C_{44} \right]. \quad (77)$$

Note that the dependence on a in Equations (54)–(60) is obtained by inserting $\xi_b = \sqrt{a}$ and $\xi_c = 1$ in Equations (45)–(51).

Furthermore, we use the property

$$\Lambda(\xi\lambda) = \lambda^6 \Lambda(\xi), \quad (78)$$

where λ denotes an arbitrary scalar number. The components of the adjoint Λ are homogeneous functions of degree 6 and the determinant f is homogeneous of degree 8

$$f(\xi\lambda) = \lambda^8 f(\xi). \quad (79)$$

Therefore, it yields

$$\mathcal{T}^{-1}(\xi) = \lambda^2 \frac{\Lambda(\lambda\xi)}{f(\lambda\xi)}. \tag{80}$$

We introduce the complex vector [47]

$$\gamma(\phi) = 2e^{i\phi}\xi(\phi) \tag{81}$$

with $\xi(\phi)$ given by Equation (35) (i denotes the imaginary unit). Equation (81) can be written

$$\gamma(s) = \mathbf{h}^*s + \mathbf{h} \tag{82}$$

with the complex variable

$$s = e^{2i\phi} \tag{83}$$

and

$$\mathbf{h} = \mathbf{e}_1 + i\mathbf{e}_2. \tag{84}$$

Using $\lambda = 2e^{i\phi}$, Equation (80) can be written as

$$\mathcal{T}^{-1}(\xi) = 4s \frac{\Lambda(\gamma(s))}{f(\gamma(s))}. \tag{85}$$

Note that

$$ds = 2is d\phi. \tag{86}$$

The integral (33) can be transformed into an integral over the unit circle as follows:

$$\mathcal{G}(r) = \frac{1}{8\pi^2r} \oint_{|s|=1} \frac{4\Lambda(\gamma(s))}{f(\gamma(s))} \frac{ds}{i}. \tag{87}$$

Using the residue theorem, the integral (87) can be rewritten as

$$\mathcal{G}(r) = \frac{1}{8\pi^2r} 2\pi i \sum \text{Res} \left(\frac{4\Lambda(\gamma(s))}{if(\gamma(s))} \right). \tag{88}$$

In order to compute Equation (88), one has to find all roots of $f(\gamma(s))$, which are located within the unit circle. $f(\gamma(s))$ is a polynomial of degree 8 in s . Thus, there exist eight roots s_j of f . It is assumed that f has no multiple roots s_j and this excludes the degenerate cases. Analytically, such a case is well captured by the present approach by adding a small $\epsilon > 0$ to one or more multiple roots in order to make them different and, thereby, removing the degeneracy.

Following Michelitsch and Wunderlin [47], we conclude that there are four pairs of roots s_l, \bar{s}_l ($l = 1, 2, 3, 4$) having the property $|s_l\bar{s}_l| = 1$. There are only four roots s_l that are located within the unit circle, four roots \bar{s}_l lie outside the unit circle and the roots can be written in the form [47]

$$s_l = e^{2i\Phi_l}e^{-2\psi_l}, \tag{89}$$

$$\bar{s}_l = e^{2i\Phi_l}e^{+2\psi_l}, \tag{90}$$

where $\psi_l > 0$ ($l = 1, 2, 3, 4$). Here, the degenerate case $|s_l| = |\bar{s}_l|$ is excluded by the assumption of no multiple roots. Only the residues corresponding to the four roots (89) lying within the unit circle contribute to Equation (88). We obtain

$$\text{Res} \left(\frac{4\Lambda(\gamma(s))}{if(\gamma(s))} \right) \Big|_{s=s_l} = \frac{4\Lambda(\gamma(s_l))}{i \frac{df(\gamma(s))}{ds} \Big|_{s=s_l}}. \tag{91}$$

Finally, the Green tensor (33) reduces to

$$\mathcal{G}(\mathbf{r}) = \frac{1}{4\pi r} \sum_{l=1}^4 \frac{4\Lambda(\gamma(s_l))}{\left. \frac{df(\gamma(s))}{ds} \right|_{s=s_l}}. \tag{92}$$

The roots s_l of $f(\gamma(s))$ within the unit circle yield

$$s_l = \frac{\sqrt{A_l \rho^2 + z^2} - r}{\sqrt{A_l \rho^2 + z^2} + r}. \tag{93}$$

To obtain Equation (93), Equation (68) together with Equations (82) and (84) have been used. Evaluating Equation (92), the Green tensor takes the form

$$\mathcal{G}(\mathbf{r}) = \frac{1}{4\pi A C_{66}} \sum_{l=1}^4 \frac{\Lambda(\xi^{(l)})}{\sqrt{A_l \rho^2 + z^2} \prod_{j=1, (j \neq l)}^4 (A_j - A_l)}, \tag{94}$$

where $\xi^{(l)}$ ($l = 1, 2, 3, 4$) are the solutions of the equations

$$f(\xi) = 0 \tag{95}$$

or

$$\xi_1^2 + \xi_2^2 + A_l \xi_3^2 = 0 \tag{96}$$

and

$$\xi \mathbf{r} = \xi_1 x + \xi_2 y + \xi_3 z = 0 \tag{97}$$

with $\xi_3^{(l)} = 1$. Equations (95) and (97) have the solutions ($l = 1, 2, 3, 4$)

$$\xi_1^{(l)} = \frac{1}{\rho^2} \left[-zx + iy \sqrt{A_l \rho^2 + z^2} \right], \tag{98}$$

$$\xi_2^{(l)} = \frac{1}{\rho^2} \left[-zy - ix \sqrt{A_l \rho^2 + z^2} \right], \tag{99}$$

where

$$\rho = \sqrt{x^2 + y^2}. \tag{100}$$

Note that this formulation is in complete analogy to the result obtained by Kröner [24] for the elastic Green tensor of a hexagonal crystal using Fredholm’s method [19].

Using Equation (94), the Cartesian representation of the *elastic* 4×4 Green tensor for *one-dimensional hexagonal quasicrystals of Laue class 10* is given by

$$\mathcal{G}(\mathbf{r}) = \sum_{l=1}^4 \frac{1}{\sqrt{A_l \rho^2 + z^2}} \begin{pmatrix} \mathcal{G}_{11}^{(l)} & \mathcal{G}_{12}^{(l)} & \mathcal{G}_{13}^{(l)} & \mathcal{G}_{14}^{(l)} \\ \mathcal{G}_{12}^{(l)} & \mathcal{G}_{22}^{(l)} & \mathcal{G}_{23}^{(l)} & \mathcal{G}_{24}^{(l)} \\ \mathcal{G}_{13}^{(l)} & \mathcal{G}_{23}^{(l)} & \mathcal{G}_{33}^{(l)} & \mathcal{G}_{34}^{(l)} \\ \mathcal{G}_{14}^{(l)} & \mathcal{G}_{24}^{(l)} & \mathcal{G}_{34}^{(l)} & \mathcal{G}_{44}^{(l)} \end{pmatrix} \tag{101}$$

with the abbreviations

$$g_{11}^{(l)} = \frac{1}{\mathcal{E}_l} \left[-\Gamma_b(-A_l) \frac{x^2 z^2 - y^2 (A_l \rho^2 + z^2)}{\rho^4} + \Lambda_{b\perp}(-A_l) \right], \quad (102)$$

$$g_{22}^{(l)} = \frac{1}{\mathcal{E}_l} \left[-\Gamma_b(-A_l) \frac{y^2 z^2 - x^2 (A_l \rho^2 + z^2)}{\rho^4} + \Lambda_{b\perp}(-A_l) \right], \quad (103)$$

$$g_{12}^{(l)} = \frac{1}{\mathcal{E}_l} \left[-\Gamma_b(-A_l) \frac{xy(A_l \rho^2 + 2z^2)}{\rho^4} \right], \quad (104)$$

$$g_{13}^{(l)} = \frac{1}{\mathcal{E}_l} \left[-\Gamma_{bc}(-A_l) \frac{xz}{\rho^2} \right], \quad (105)$$

$$g_{23}^{(l)} = \frac{1}{\mathcal{E}_l} \left[-\Gamma_{bc}(-A_l) \frac{yz}{\rho^2} \right], \quad (106)$$

$$g_{33}^{(l)} = \frac{1}{\mathcal{E}_l} \Lambda_c(-A_l), \quad (107)$$

$$g_{14}^{(l)} = \frac{1}{\mathcal{E}_l} \left[-\Gamma_{b4}(-A_l) \frac{xz}{\rho^2} \right], \quad (108)$$

$$g_{24}^{(l)} = \frac{1}{\mathcal{E}_l} \left[-\Gamma_{b4}(-A_l) \frac{yz}{\rho^2} \right], \quad (109)$$

$$g_{34}^{(l)} = \frac{1}{\mathcal{E}_l} \Lambda_{c4}(-A_l), \quad (110)$$

$$g_{44}^{(l)} = \frac{1}{\mathcal{E}_l} \Lambda_4(-A_l). \quad (111)$$

Here, we have introduced the abbreviation

$$\mathcal{E}_l = 4\pi C_{66} A \prod_{j=1, (j \neq l)}^4 (A_j - A_l) \quad (112)$$

and the quantities

$$\Gamma_b(a) = \frac{1}{a} [\Lambda_{b\perp}(a) - \Lambda_b(a)], \quad (113)$$

$$\Gamma_{bc}(a) = \frac{1}{\sqrt{a}} \Lambda_{bc}(a), \quad (114)$$

$$\Gamma_{b4}(a) = \frac{1}{\sqrt{a}} \Lambda_{b4}(a), \quad (115)$$

together with Equation (70) and Equations (72)–(77).

Equation (101) together with Equations (102)–(111) gives the 10 independent components of the Green tensor in closed form. In particular, Equation (101) together with Equations (102)–(107) gives the six phonon components of the Green tensor, Equation (101) together with Equations (108)–(110) gives the three phonon–phason coupling components of the Green tensor and Equation (101) together with Equation (111) gives the one phason component of the Green tensor (see also Equation (32)). Due to the closed-form expression of the Green tensor (101), it is straightforward to calculate its first and second gradients if they are needed for further applications. This can be done without any numerical tool, revealing one of the main advantages of the present approach. In the piezoelectric framework, the first and second gradients of the corresponding Green tensor are explicitly calculated in the context of the inclusion problem in Michelitsch and Levin [29].

It is interesting to note that the closed-form expression of the 4×4 Green tensor for one-dimensional hexagonal quasicrystals of Laue class 10 given in Equation (101) with Equations (102)–(111) is analogous to the closed-form expression of the 4×4 Green tensor for hexagonal piezoelectric crystals of point group $6mm$ given by Michelitsch [28], due to

the analogy in the constitutive setting between one-dimensional hexagonal quasicrystals of Laue class 10, which possess 10 elastic moduli, and hexagonal piezoelectric crystals of point group $6mm$, which possess 10 material moduli. Of course, this analogy is only formal, since quasicrystals and piezoelectric materials are different materials from the physical point of view.

It should be pointed out that the procedure used in this paper for the derivation of closed-form expressions cannot be applied, for example, in one-dimensional hexagonal quasicrystals of Laue class 9, which possess 11 elastic moduli and correspond to piezoelectric crystals of point group 6, which possess 11 material moduli, since these are not transversal isotropic materials (see [13,49]). That is also another reason that the distinction between the two Laue classes of one-dimensional hexagonal quasicrystals has to be respected (see [14]).

6. Numerical Results for One-Dimensional Hexagonal Quasicrystals of Laue Class 10

In this section, the 10 independent components of the 4×4 Green tensor (101) of one-dimensional hexagonal quasicrystals of Laue class 10 are presented numerically in contour plots.

The elastic constants of one-dimensional hexagonal quasicrystals of Laue class 10, which are used for the numerical computation, are tabulated in Table 1 by referring to Li et al. [50]. Since there are no values for the elastic constants of one-dimensional hexagonal quasicrystals of Laue class 10 based on experiments or ab-initio calculations, it is crucial to check that the above values fulfil the conditions of positive definiteness of the elastic energy density. It is easy to check that the elastic constants given in Table 1 fulfil the conditions of positive definiteness of one-dimensional hexagonal quasicrystals of Laue class 10 given in Equations (40)–(42).

Table 1. Elastic constants of one-dimensional hexagonal quasicrystals of Laue class 10 given in GPa (see [50]).

Phonon:	$C_{11} = 150$	$C_{12} = 100$	$C_{13} = 90$	$C_{33} = 130$	$C_{44} = 50$
Phason:	$K_1 = 0.18$	$K_2 = 0.30$			
Phonon–phason:	$R_1 = -1.50$	$R_2 = 1.20$	$R_3 = 1.20$		

The phonon components of the Green tensor, Equation (101) with Equations (102)–(107), are plotted in Figure 1. The phason and phonon–phason coupling components of the Green tensor, Equation (101) with Equations (108)–(111), are plotted in Figure 2. Using the elastic constants given in Table 1, it can be seen that the phason component $G_{44}^{\perp\perp}$, Figure 2a, gives the strongest contribution in comparison with all the other components of the Green tensor. The anisotropy is visible in the diagonal phonon components $G_{11}^{\parallel\parallel}$, $G_{22}^{\parallel\parallel}$, $G_{33}^{\parallel\parallel}$, Figure 1a–c and in the phonon–phason coupling component, $G_{34}^{\parallel\perp}$, Figure 2b. One can further observe that the phonon components $G_{13}^{\parallel\parallel}$ and $G_{23}^{\parallel\parallel}$, Figure 1e,f, have the same contour form. This reflects the transverse isotropic symmetry in the basal plane (see Equations (105) and (106)). The same holds for the phonon–phason coupling components $G_{14}^{\parallel\perp}$ and $G_{24}^{\parallel\perp}$, Figure 2c,d (see Equations (108) and (109)).

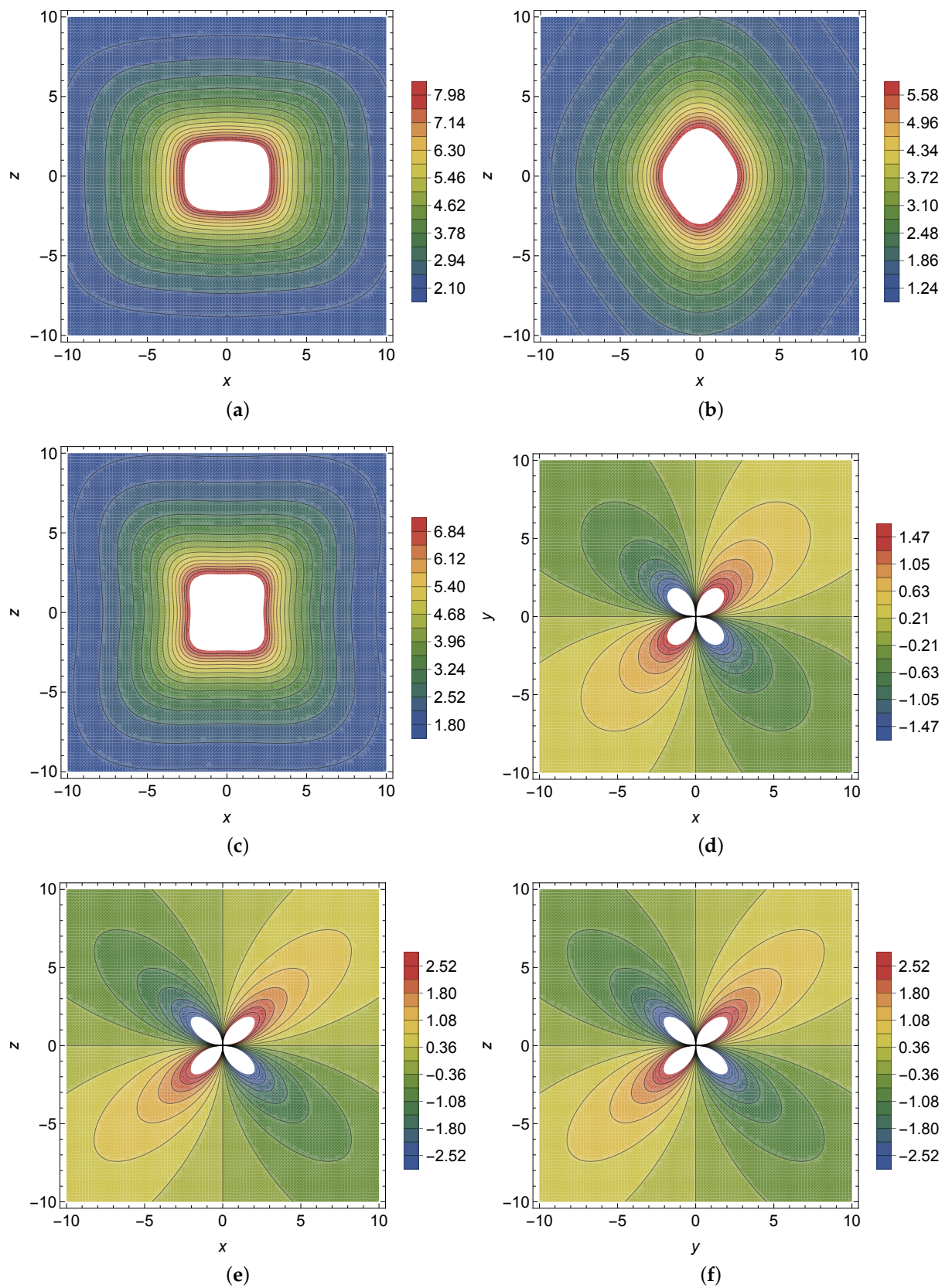


Figure 1. Phonon components of the Green tensor: (a) $G_{11}^{\parallel\parallel\parallel} \times 10^4$, (b) $G_{22}^{\parallel\parallel\parallel} \times 10^4$, (c) $G_{33}^{\parallel\parallel\parallel} \times 10^4$, (d) $G_{12}^{\parallel\parallel\parallel} \times 10^4$, (e) $G_{13}^{\parallel\parallel\parallel} \times 10^4$, (f) $G_{23}^{\parallel\parallel\parallel} \times 10^4$.

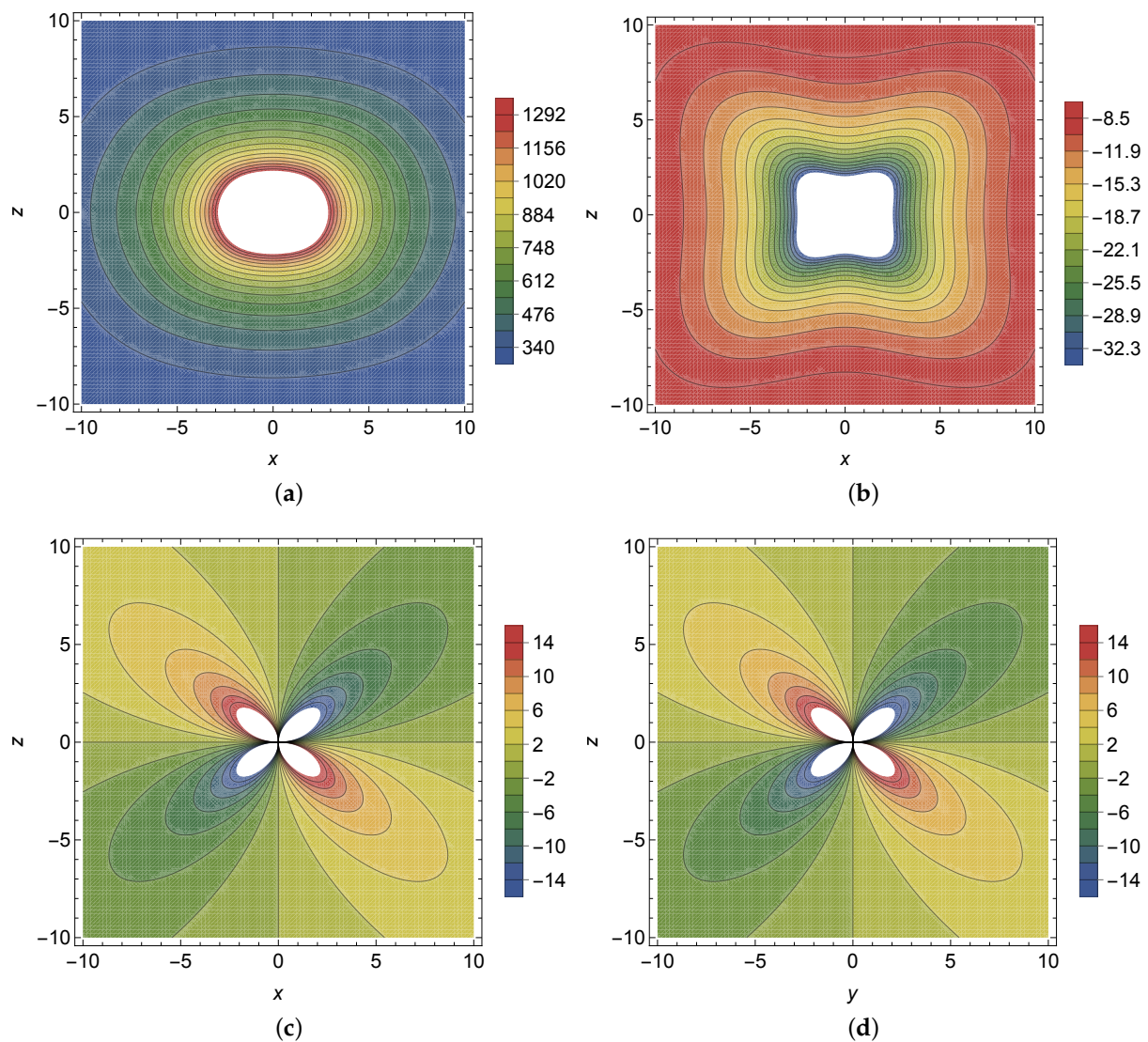


Figure 2. Phason and phonon–phason coupling components of the Green tensor: (a) $G_{44}^{\perp\perp} \times 10^4$, (b) $G_{34}^{\perp\perp} \times 10^4$, (c) $G_{14}^{\perp\perp} \times 10^4$, (d) $G_{24}^{\perp\perp} \times 10^4$.

7. Conclusions

In this paper, starting from an integral form expression of the elastic 4×4 Green tensor valid for one-dimensional quasicrystals, a closed-form representation of the 4×4 Green tensor for one-dimensional hexagonal quasicrystals of Laue class 10 is derived using the residuum theorem. Contour plots of the 10 independent components of the obtained elastic 4×4 Green tensor of one-dimensional hexagonal quasicrystals of Laue class 10 have been given to show their main characteristics. It is interesting to see that the phason component of the Green tensor has the strongest contribution in comparison with all the other components. The fact that the derived solution is in closed form can drastically reduce the computational cost in any application, making the present result a powerful tool for the implementation into numerical schemes, for instance, solving boundary value problems. In general, the Green tensor derived in the present paper allows to solve a wide range of problems in one-dimensional hexagonal quasicrystals of Laue class 10 such as the Eshelby inclusion problem, Eshelby tensor, dislocation loops and other problems of micromechanics.

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Appendix A. Limit to the Three-Dimensional Green Tensor of Hexagonal Crystals

In this appendix, we show that in the case of vanishing phonon–phason coupling $D_{ij3l} = 0$, the Green tensor (101) of one-dimensional hexagonal quasicrystals of Laue class 10 yields well-known results. Specifically, the phonon part $\mathcal{G}_{ij} = G_{ij}^{\parallel\parallel}$, $i, j = 1, 2, 3$ provides Kröner’s elastic Green tensor of a hexagonal crystal [24], the phason part $\mathcal{G}_{44} = G_{44}^{\perp\perp}$ provides the Green function of a “hexagonal” Poisson equation and the phonon–phason coupling part $\mathcal{G}_{j4} = G_{j4}^{\parallel\perp}$, $j = 1, 2, 3$ vanishes.

We consider the case of vanishing phonon–phason coupling ($D_{ij3l} = 0$ or $R_1 = R_2 = R_3 = 0$). In this case, Equations (49) and (50) become

$$t_{b4} = t_{c4} = 0. \tag{A1}$$

The determinant f (Equation (61)) simplifies to

$$f(a) = \det \mathcal{T}(a) = \tau(a) T_{b\perp}(a) \left(T_b(a) T_c(a) - T_{bc}^2(a) \right) \tag{A2}$$

and can be written as

$$f(a) = K_2 C_{11} C_{44} C_{66} (a + a_1)(a + a_2)(a + a_3)(a + a_4), \tag{A3}$$

where $a_l = A_l$ denote the roots of $f(-a)$ in the decoupled case. In addition,

$$a_1 = \frac{C_{44}}{C_{66}} \tag{A4}$$

represents the root of $T_{b\perp}(-a)$. Moreover, $a_{2,3}$ are the roots of the quadratic equation

$$T_b(-a) T_c(-a) - T_{bc}^2(-a) = C_{11} C_{44} a^2 + \left(C_{13}^2 + 2C_{13} C_{44} - C_{11} C_{33} \right) a + C_{33} C_{44} = 0 \tag{A5}$$

and they read

$$a_{2,3} = \frac{1}{2C_{11} C_{44}} \left(- \left(C_{13}^2 + 2C_{13} C_{44} - C_{11} C_{33} \right) \pm \sqrt{\left[\left(C_{13}^2 + 2C_{13} C_{44} - C_{11} C_{33} \right)^2 - 4C_{11} C_{33} C_{44}^2 \right]} \right). \tag{A6}$$

Moreover, a_4 is given by

$$a_4 = \frac{K_1}{K_2} \tag{A7}$$

and represents the root of $\tau(-a)$. Using Equations (70)–(77) together with Equations (113)–(115), we find

$$\Lambda_{b\perp}(a = -a_l) = K_2 C_{11} C_{44} (a_2 - a_l)(a_3 - a_l)(a_4 - a_l), \quad (\text{A8})$$

$$\Lambda_b(a = -a_l) = K_2 C_{66} (C_{33} - a_l C_{44})(a_1 - a_l)(a_4 - a_l), \quad (\text{A9})$$

$$\Gamma_b(a = -a_l) = -K_2 (a_4 - a_l) \left[(C_{66} - C_{11})(C_{33} - a_l C_{44}) + (C_{13} + C_{44})^2 \right], \quad (\text{A10})$$

$$\Gamma_{bc}(a = -a_l) = -K_2 C_{66} (C_{13} + C_{44})(a_1 - a_l)(a_4 - a_l), \quad (\text{A11})$$

$$\Lambda_c(a = -a_l) = K_2 C_{66} (C_{44} - a_l C_{11})(a_1 - a_l)(a_4 - a_l) \quad (\text{A12})$$

and

$$\Gamma_{b4}(a = -a_l) = \Lambda_{c4}(a = -a_l) = 0, \quad (\text{A13})$$

obtaining $\mathcal{G}_{j4} = 0, j = 1, 2, 3$ and

$$\Lambda_4(a = -a_l) = C_{11} C_{44} C_{66} (a_1 - a_l)(a_2 - a_l)(a_3 - a_l). \quad (\text{A14})$$

For $l = 1, 2, 3$,

$$\mathcal{E}_l = K_2 (a_4 - a_l) E_l \quad (\text{A15})$$

with

$$E_l = 4\pi C_{11} C_{44} C_{66} \prod_{j=1, (j \neq l)}^3 (a_j - a_l). \quad (\text{A16})$$

The terms (A16) coincide with Kröner's (corrected) "E_l". The terms E_l defined in Kröner [24] have been corrected by a prefactor $-C_{11} C_{44} C_{66}$ providing the correct result for the elastic Green tensor (see [25–27]).

For $l = 4$,

$$\mathcal{E}_4 = 4\pi K_2 C_{11} C_{44} C_{66} (a_1 - a_4)(a_2 - a_4)(a_3 - a_4) = 4\pi K_2 \Lambda_4(-a_4). \quad (\text{A17})$$

We observe, from Equations (A8)–(A12), the following properties:

$$\frac{\Lambda_{b\perp}(a = -a_4)}{\mathcal{E}_4} = \frac{\Lambda_b(a = -a_4)}{\mathcal{E}_4} = \frac{\Gamma_b(a = -a_4)}{\mathcal{E}_4} = \frac{\Gamma_{bc}(a = -a_4)}{\mathcal{E}_4} = \frac{\Lambda_c(a = -a_4)}{\mathcal{E}_4} = 0 \quad (\text{A18})$$

($\mathcal{E}_4 \neq 0$, Equation (A17)). Thus, the term $l = 4$ in the sum (101) does not contribute to the elastic phonon components $\mathcal{G}_{ij}, i, j = 1, 2, 3$. Using Equations (A14) and (A15) together with Equation (A16), we obtain for $l = 1, 2, 3$ that

$$\frac{\Lambda_4(a = -a_l)}{\mathcal{E}_l} = 0, \quad (\text{A19})$$

which means there are no contributions to the sum (101) for $l = 1, 2, 3$ to the phason part \mathcal{G}_{44} . For $l = 4$, we find from Equations (A14) and (A17) that

$$\frac{\Lambda_4(a = -a_4)}{\mathcal{E}_4} = \frac{1}{4\pi K_2}. \quad (\text{A20})$$

Note that Equation (A20) is independent of the elastic moduli C_{ijkl} , which is a consequence of $D_{ij3l} = 0$. Thus, the phason part \mathcal{G}_{44} of the Green tensor (101) gives

$$\mathcal{G}_{44}(r) = \frac{\Lambda_4(a = -a_4)}{\mathcal{E}_4} \frac{1}{\sqrt{a_4 \rho^2 + z^2}} = \frac{1}{4\pi K_2 \sqrt{a_4 \rho^2 + z^2}} \quad (\text{A21})$$

with a_4 to be given by Equation (A7). It can be seen that the phason part \mathcal{G}_{44} of the Green tensor (101), Equation (A21), is the fundamental solution of the following “hexagonal” Poisson equation:

$$\tau(\nabla)\mathcal{G}_{44}(\mathbf{r}) + \delta^3(\mathbf{r}) = 0 \quad (\text{A22})$$

with

$$\tau(\nabla) = \left[K_2 \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + K_1 \frac{\partial^2}{\partial z^2} \right]. \quad (\text{A23})$$

Let us consider the cases $l = 1, 2, 3$. From Equations (A8)–(A12) together with Equation (A15), we obtain the following:

- These terms coincide with Kröner’s “ \mathcal{A}_l ” in [24]

$$-\frac{\Gamma_b(a = -a_l)}{\mathcal{E}_l} = \mathcal{A}_l = \frac{(C_{66} - C_{11})(C_{33} - a_l C_{44}) + (C_{13} + C_{44})^2}{E_l}. \quad (\text{A24})$$

- These terms coincide with Kröner’s “ \mathcal{B}_l ” in [24]

$$\frac{\Lambda_{b\perp}(a = -a_l)}{\mathcal{E}_l} = \mathcal{B}_l = \frac{C_{11}C_{44}a_l^2 + (C_{13}^2 + 2C_{13}C_{44} - C_{11}C_{33})a_l + C_{33}C_{44}}{E_l}. \quad (\text{A25})$$

- These terms coincide with Kröner’s “ \mathcal{C}_l ” in [24]

$$-\frac{\Gamma_{bc}(a = -a_l)}{\mathcal{E}_l} = \mathcal{C}_l = \frac{(C_{44} - a_l C_{66})(C_{13} + C_{44})}{E_l}. \quad (\text{A26})$$

- These terms coincide with Kröner’s “ \mathcal{D}_l ” from [24]

$$\frac{\Lambda_c(a = -a_l)}{\mathcal{E}_l} = \mathcal{D}_l = \frac{(C_{44} - a_l C_{66})(C_{44} - a_l C_{11})}{E_l}. \quad (\text{A27})$$

Because of the property (A18), the elastic phonon part of the Green tensor \mathcal{G}_{ij} ($i, j = 1, 2, 3$), by inserting Equations (A24)–(A27) into Equation (101) and by using the abbreviations (102)–(107), yields Kröner’s Green tensor G_{ij} for hexagonal crystals [24]:

$$\mathbf{G}(\mathbf{r}) = \sum_{l=1}^3 \frac{1}{\sqrt{a_l \rho^2 + z^2}} \times \begin{pmatrix} \mathcal{A}_l \frac{x^2 z^2 - y^2 (a_l \rho^2 + z^2)}{\rho^4} + \mathcal{B}_l \mathcal{A}_l \frac{xy(a_l \rho^2 + 2z^2)}{\rho^4} & C_l \frac{xz}{\rho^2} \\ \mathcal{A}_l \frac{xy(a_l \rho^2 + 2z^2)}{\rho^4} & \mathcal{A}_l \frac{y^2 z^2 - x^2 (a_l \rho^2 + z^2)}{\rho^4} + \mathcal{B}_l C_l \frac{yz}{\rho^2} \\ C_l \frac{xz}{\rho^2} & C_l \frac{yz}{\rho^2} & \mathcal{D}_l \end{pmatrix}. \quad (\text{A28})$$

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