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Computation of the time-dependent Green's function of three dimensional elastodynamics in 3D quasicrystals

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Abstract: The time-dependent differential equations of elasticity for 3D quasicrystals are considered in the paper. These equations are written in the form of a vector partial differential equation of the second order with symmetric matrix coefficients. The Green's function is defined for this vector partial differential equation. A new method of the numerical computation of values of the Green's function is proposed. This method is based on the Fourier transformation and some matrix computations. Computational experiments confirm the robustness of our method for the computation of the time-dependent Green's function in icosahedral quasicrystals.

Keywords: Three-dimensional quasicrystals, equations of elastodynamics, Green's function, analytical method, simulation.

1 Introduction

Quasicrystalline materials are clearly fascinating materials: crystal structures and properties are surprising and could be remarkably useful. Most of these properties combine effectively to give technologically interesting applications which have been protected recently by several patents [Blaaderen (2009); Dubois (2005)]. For instance, the combination of such kind of properties as high hardness, low friction and corrosive resistance of quasicrystals (QCs) gives almost ideal material for motor-car engines. The application of QCs in motor-car engines would be undoubtedly result in reduced air pollution and increase engines lifetimes. The same set of associated properties (hardness, low friction, corrosive resistance) combined with bio-compatibility is also very promising for introducing QCs in surgical applications as parts used for bone repair and prosthetic applications [Blaaderen (2009); Dubois (2005); Dubois (2000)]

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The quasicrystal as a new structure of solids has been first discovered in 1984 by [Shechtman, Blech, Gratias, and Cahn (1984)]. The physical properties, such as the structural, electronic, magnetic, optical and thermal properties, of QCs have been investigated intensively. Elasticity is one of the interesting properties of QCs.

1D, 2D and 3D QCs are defined as three dimensional bodies with the special atom arrangements. The atom arrangement of 1D QC is quasi-periodic in direction and periodic in the plane which is orthogonal to this direction. The atom arrangement of 2D QC is quasi-periodic in a plane and periodic in the orthogonal direction. The atom arrangement of 3D QC is quasi-periodic in three dimensions without periodic direction. Three-dimensional QCs such as icosahedral QCs (e.g. Al-Cu-Fe and Al-Li-Cu) are quasiperiodic in three dimensions, without periodic direction. They play a central role in the study of QCs.

The fundamental theory based on the motion of the continuum model to describe the elastic behavior of QCs is well known (see, for example, [Ding, Yang, Hu, and Wang (1993); Hu, Wang, and Ding (2000); Gao and Zhao (2006); Rochal1 and Lorman (2002)]. The elastic equations in 3D elasticity of QCs are more complicated than those of classical elasticity. In QCs a phason displacement field exits in addition to a phonon displacement. All existing models of QC elastodynamics are given by partial differential equations and explain main features of phonon-phason motion but none of them have been completely checked on the consistency with all experimental data [Rochal1 and Lorman (2002)]. Verification of the consistency of models, given by partial differential equations, can be done by comparison the values of solutions for these equations with experimental data. But it is more difficult to obtain solutions of elastodynamic equations for QCs than for crystals. Besides that computation of values of solutions of elastodynamic equations for 3D QCs are more complicated than those for 1D and 2D QCs. Because of the complexities of the solution of elastodynamic equations most authors consider only elastic plane problems for QCs [Ding, Yang, Hu, and Wang (1993); Akmaz and Akinci (2009); Fan and Mai (2004)] i.e. they suppose that the elastic fields induced in QCs are independent of the variable z.

The plane elasticity problems of 3D and 2D quasicrystals have been studied for the static case in [Ding, Wang, Yang, and Hu (1995)]. The general solution of the plane elasticity problems of icosahedral quasicrystals based on the stress potential function has been studied for static case in [Lian-He and Tian-You (2006)]. Gao (2009) has established general solutions for plane elastostatic of cubic quasicrystals using the operator method. [Fan and Guo (2005)] has developed the potential function theory for plane elastostatic of three-dimensional icosahedral quasicrystals. The dynamic plane elastic problems in 2D QCs with dodecagonal, pentagonal and decagonal structures have been studied in [Akmaz and Akinci (2009)]. The time-dependent elastic problems in QCs have been studied in [Fan and Mai (2004); Wang (2006); Akmaz and Akinci (2009); Akmaz (2009); Yakhno and Yaslan (2011)]. 2D dynamic problems for 1D and 2D hexagonal QCs have been solved in [Fan and Mai (2004)] using decomposition and superposition procedures. Wang (2006) has found a general solution for 3D dynamic problem in 1D hexagonal QCs. 3D elastic problems in 3D QCs have been solved in [Akmaz (2009)] using PS method related with the polynomial presentation of data. A method for the derivation of the time-dependent fundamental solution with three space variables in 2D QCs with arbitrary system of anisotropy has been proposed in [Yakhno and Yaslan (2011)].

In the present paper a new method for the numerical computation of the time-dependent Green's function of three-dimensional elastodynamics in 3D QCs is suggested. This method consists of the following. The dynamic equations of the motion for 3D QCs are written in terms of the Fourier transform with respect to space variables as a vector ordinary differential equation with matrix coefficients depending on the Fourier parameters. Applying the matrix transformations and properties of matrix coefficients a solution of the vector ordinary differential equation is computed. Finally, the Green's function (GF) is computed numerically by the inverse Fourier transform. Computational experiments confirm the robustness of our method for the numerical computation of the values of the time-dependent Green's function of three-dimensional elastodynamics in 3D QCs.

Green's functions for equations of mathematical physics can be considered as a useful tool for different methods in the presentation of acoustic, electromagnetic, elastic and other fields, in particular, for the method of moments and boundary element method (see for example, [Tewary (1995);Tewary (2004); Ting (2005); Yang and Tewary. (2008); Gu, Young, and Fan (2009); Chen, Ke, and Liao (2009)]. When the dyadic Green's functions can be constructed it leads to the significant simplification of modelling electromagnetic waves and allows engineers to overcome calculational difficulties [Tewary, Bartolo, and Powell (2002)].

The paper is organized as follows. The basic equations of elastodynamics for 3D QCs are written in Section 2. The Green's function (GF) of elastodynamics in 3D QCs and vector partial differential equation for GF columns are given in Section 3. The method of computing GF columns is described in the Section 4. Computational examples with the description of input data and results of computations are written in Section 5. The conclusion, appendix and a collection of computational images of phonon and phason displacements for anisotropic QCs with icosahedral structure are given at the end of the paper.

2 Time-dependent GF of elastodynamics in 3D QCs

2.1 The basic equations of elastodynamics for 3D QCs

Let $x = (x_1, x_2, x_3) \in R^3$ be a space variable, $t \in R$ be a time variable. The generalized Hooke's laws of the elasticity problem of 3D QCs are given by (see, for example, [Ding, Yang, Hu, and Wang (1993); Hu, Wang, and Ding (2000); Gao and Zhao (2006)])

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} + R_{ijkl}w_{kl}, \tag{1}$$

$$H_{ij} = R_{klij}\varepsilon_{kl} + K_{ijkl}w_{kl}, \tag{2}$$

where ε_{kl} and w_{kl} are defined as follows

$$\varepsilon_{kl} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right),\ w_{kl} = \frac{\partial w_k}{\partial x_l},\ k,l = 1,2,3. \tag{3}$$

Here u_k and $w_k, k = 1,2,3$ are the phonon and phason displacements; $\varepsilon_{kl}(x,t)$, $w_{kl}(x,t),\ k,l = 1,2,3$ are phonon and phason strains.

C_{ijkl} are the phonon elastic constants, K_{ijkl} are the phason elastic constants, R_{ijkl} are the phonon-phason coupling elastic constants. Moreover, they satisfy the following symmetric properties (see, for example, [Ding, Yang, Hu, and Wang (1993); Hu, Wang, and Ding (2000); Gao and Zhao (2006)])

$$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij},\ K_{ijkl} = K_{klij},\ R_{ijkl} = R_{jikl}. \tag{4}$$

The positivity of elastic strain energy density requires the elastic constant tensors C_{ijkl}, K_{ijkl}, R_{ijkl} to be positive definite. Namely, when the strain tensors ε_{ij}, w_{ij} are not zero entirely, the elastic constant tensors satisfy the following inequality (see, for example [Gao and Zhao (2006)])

$$\sum_{i,j,k,l=1}^{3} C_{ijkl}\varepsilon_{ij}\varepsilon_{kl} > 0,\ \sum_{i,j,k,l=1}^{3} K_{ijkl}w_{ij}w_{kl} > 0,\ \sum_{i,j,k,l=1}^{3} R_{ijkl}\varepsilon_{ij}w_{kl} > 0. \tag{5}$$

The dynamic equilibrium equations can be written in the following form

$$\rho\frac{\partial^2 u_i(x,t)}{\partial t^2} = \sum_{j=1}^{3}\frac{\partial \sigma_{ij}(x,t)}{\partial x_j} + f_i(x,t), \tag{6}$$

$$\rho\frac{\partial^2 w_i(x,t)}{\partial t^2} = \sum_{j=1}^{3}\frac{\partial H_{ij}(x,t)}{\partial x_j} + g_i(x,t), \tag{7}$$

where the constant $\rho > 0$ is the density; $f_i(x,t)$ and $g_i(x,t), i = 1,2,3$ are body forces densities for the phonon and phason displacements, respectively; σ_{ij} and $H_{ij},\ i,j = 1,2,3$ are phonon and phason stresses (see, for example, [Ding, Yang, Hu, and Wang (1993); Hu, Wang, and Ding (2000); Gao and Zhao (2006); Yang, Wang, Ding, and Hu (1993)]).

Using (1)-(3), equations (6), (7) can be presented in the form

$$\rho \frac{\partial^2 u_i(x,t)}{\partial t^2} = \sum_{j,k,l=1}^{3} C_{ijkl} \frac{\partial^2 u_k(x,t)}{\partial x_j \partial x_l} + \sum_{j,l=1}^{3} R_{ijkl} \frac{\partial^2 w_k(x,t)}{\partial x_j \partial x_l} + f_i(x,t), \tag{8}$$

$$\rho \frac{\partial^2 w_i(x,t)}{\partial t^2} = \sum_{j,k,l=1}^{3} R_{klij} \frac{\partial^2 u_k(x,t)}{\partial x_j \partial x_l} + \sum_{j,l=1}^{3} K_{ijkl} \frac{\partial^2 w_i(x,t)}{\partial x_j \partial x_l} + g_i(x,t). \tag{9}$$

Denoting $\mathbf{V} = (u_1,u_2,u_3,w_1,w_2,w_3)$, $\mathbf{F} = (f_1,f_2,f_3,g_1,g_2,g_3)$ equations (8)-(9) can be written as one vector partial differential equation of the following form

$$\rho \frac{\partial^2 \mathbf{V}}{\partial t^2} = \sum_{j,l=1}^{3} \mathbf{P}_{jl} \frac{\partial^2 \mathbf{V}}{\partial x_j \partial x_l} + \mathbf{F}(x,t), \tag{10}$$

where matrices $\mathbf{P}_{jl}$ are defined by

$$\mathbf{P}_{jl} = \frac{1}{2} \times$$

$$\begin{bmatrix} C_{1j1l}+C_{1l1j} & C_{1j2l}+C_{1l2j} & C_{1j3l}+C_{1l3j} & R_{1j1l}+R_{1l1j} & R_{1j2l}+R_{1l2j} & R_{1j3l}+R_{1l3j} \\ C_{2j1l}+C_{2l1j} & C_{2j2l}+C_{2l2j} & C_{2j3l}+C_{2l3j} & R_{2j1l}+R_{2l1j} & R_{2j2l}+R_{2l2j} & R_{2j3l}+R_{2l3j} \\ C_{3j1l}+C_{3l1j} & C_{3j2l}+C_{3l2j} & C_{3j3l}+C_{3l3j} & R_{3j1l}+R_{3l1j} & R_{3j2l}+R_{3l2j} & R_{3j3l}+R_{3l3j} \\ R_{1j1l}+R_{1l1j} & R_{2j1l}+R_{2l1j} & R_{3j1l}+R_{3l1j} & K_{1j1l}+K_{1l1j} & K_{1j2l}+K_{1l2j} & K_{1j3l}+K_{3l1j} \\ R_{1j2l}+R_{1l2j} & R_{2j2l}+R_{2l2j} & R_{3j2l}+R_{3l2j} & K_{2j1l}+K_{2l1j} & K_{2j2l}+K_{2l2j} & K_{2j3l}+K_{2l3j} \\ R_{1j3l}+R_{1l3j} & R_{2j3l}+R_{2l3j} & R_{3j3l}+R_{3l3j} & K_{3j1l}+K_{3l1j} & K_{3j2l}+K_{3l2j} & K_{3j3l}+K_{3l3j} \end{bmatrix}.$$

2.2 GF of elastodynamics in 3D QCs

The time-dependent GF of elastodynamics in 3D QCs is a 6×6 matrix whose mth column is a vector function

$$\mathbf{V}^m(x,t) = (u_1^m(x,t), u_2^m(x,t), u_3^m(x,t), w_1^m(x,t), w_2^m(x,t), w_3^m(x,t))$$

satisfying

$$\rho \frac{\partial^2 \mathbf{V}^m}{\partial t^2} = \sum_{j,l=1}^{3} \mathbf{P}_{jl} \frac{\partial^2 \mathbf{V}^m}{\partial x_j \partial x_l} + \mathbf{E}^m \delta(x)\delta(t), \tag{11}$$

$$\mathbf{V}^m(x,t)\ |_{t<0} = 0. \tag{12}$$

Here $\delta(x) = \delta(x_1)\delta(x_2)\delta(x_3)$ is the Dirac delta function of the space variable concentrated at $x_1 = 0,\ x_2 = 0,\ x_3 = 0$; $\delta(t)$ is the Dirac delta function of the time variable concentrated at $t = 0$; $m = 1,...,6$; $\mathbf{E}^m = (\delta_1^m, \delta_2^m, \delta_3^m, \delta_4^m, \delta_5^m, \delta_6^m)$, δ_n^m is the Kronecker symbol i.e. $\delta_n^m = 1$ if $n = m$ and $\delta_n^m = 0$ if $n \neq m$, $n = 1,...,6$. $\mathbf{P}_{jl}$ are matrices defined above.

The computation of mth column for the time-dependent GF in 3D QCs is the main problem of this paper. This problem is related with finding a vector function $\mathbf{V}^m(x,t)$ satisfying (11) and (12).

3 Computation of *m*th column for the GF of elastodynamics in 3D QCs

The method of deriving $\mathbf{V}^m(x,t)$ satisfying (11) and (12) consists of the following. In the first step equations (11) and (12) are written in terms of the Fourier transform with respect to $x \in R^3$. In the second step, a solution of the obtained initial value problem is derived by matrix transformations and the ordinary differential equations technique. In the last step, an explicit formula for mth column of the GF is found by the inverse Fourier transform.

3.1 Equations for m th column of GF in terms of Fourier images

Let $\tilde{\mathbf{V}}^m(\nu,t) = (\tilde{u_1}^m, \tilde{u_2}^m, \tilde{u_3}^m, \tilde{w_1}^m, \tilde{w_2}^m, \tilde{w_3}^m)$ be the Fourier image of $\mathbf{V}^m(x,t)$ with respect to $x = (x_1,x_2,x_3) \in R^3$ (see, for example Vladimirov (1971)), i.e. $\tilde{V_j}^m(\nu,t) = \int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} V_j^m(x,t)e^{ix\cdot\nu}dx_1dx_2dx_3$, $\nu = (\nu_1, \nu_2, \nu_3) \in R^3$, $x \cdot \nu = x_1\nu_1 + x_2\nu_2 + x_3\nu_3$, $i^2 = -1$, $j = 1,...,6$.

The problem of finding a vector function $\mathbf{V}^m(x,t)$ satisfying (11) and (12) can be written in terms of $\tilde{\mathbf{V}}^m(\nu,t)$ as follows

$$\rho\frac{\partial^2\tilde{\mathbf{V}}^m}{\partial t^2} + \mathbf{A}(\nu)\tilde{\mathbf{V}}^m = \mathbf{E}^m\delta(t), \tag{13}$$

$$\tilde{\mathbf{V}}^m(\nu,t)|_{t<0} = 0. \tag{14}$$

Here $\nu = (\nu_1, \nu_2, \nu_3) \in R^3, t \in R$ and

$$\mathbf{A}(\nu) = \sum_{j,l=1}^{3} \mathbf{P}_{jl}\nu_j\nu_l, \tag{15}$$

where $\mathbf{P}_{jl}$ are matrices defined after (10).

3.2 The derivation of a solution of (13), (14)

3.2.1 Diagonalization of the matrix $\mathbf{A}(\nu)$

Using the positivity of elastic constant tensors $C_{ijkl},\ R_{ijkl},\ K_{ijkl}$ we obtain that the matrix $\mathbf{A}(\nu)$, defined by (15), is symmetric positive semi-definite (see Appendix). For the matrix $\mathbf{A}(\nu)$ we construct an orthogonal matrix $\mathscr{T}(\nu)$ and a diagonal matrix $D(\nu) = diag(D_k(\nu),\ k = 1,2,3,4,5,6)$ with nonnegative elements such that

$$\mathscr{T}^*(\nu)\mathbf{A}(\nu)\mathscr{T}(\nu) = D(\nu), \tag{16}$$

where $\mathscr{T}^*(\nu)$ is the transposed matrix to $\mathscr{T}(\nu)$. We note that values of $\mathscr{T}(\nu)$, $\mathscr{T}^*(\nu)$, $\mathscr{D}(\nu)$ can be computed in MATLAB. MATLAB code of these computations is given below:

> `Input:` $C_{ijkl},\ R_{ijkl},\ K_{ijkl}$
> $\nu_1\ \nu_2\ \nu_3$ `real;`
> $[EigVecA(\nu), EigValA(\nu)] = eig(A(\nu));$
> $\mathscr{T}(\nu) = EigVecA(\nu);$
> $\mathbf{D}(\nu) = EigValA(\nu);$
> `Output:` $\mathbf{T}(\nu),\ \mathbf{T}^*(\nu),\ \mathbf{D}(\nu).$

3.2.2 Formula for a solution of (13), (14)

Let values of $\mathscr{T}(\nu)$ and $D(\nu) = diag(D_k(\nu),\ k = 1,2,3,4,5,6)$ be computed. Let

$$\tilde{\mathbf{V}}^m(\nu,t) = \mathscr{T}(\nu)\mathbf{Y}^m(\nu,t), \tag{17}$$

where $\mathbf{Y}^m(\nu,t)$ is unknown vector function. Substituting (17) into (13), (14) and then multiplying the obtained equations by $\mathscr{T}^*(\nu)$ and using (16) we find

$$\rho\frac{\partial^2\mathbf{Y}^m}{\partial t^2} + D(\nu)\mathbf{Y}^m = \mathscr{T}^*(\nu)\mathbf{E}^m\delta(t), \tag{18}$$

$$\mathbf{Y}^m(\nu,t)|_{t<0} = 0. \tag{19}$$

Using the ordinary differential equations technique, a solution of the initial value problem (18)-(19) is given by

$$\mathbf{Y}^m_k(\nu,t) = \theta(t)\frac{(\mathscr{T}^*(\nu)\mathbf{E}^m)_k}{\sqrt{\rho D_k(\nu)}}\sin(t\frac{\sqrt{D_k(\nu)}}{\sqrt{\rho}}),\ for\ D_k(\nu) > 0, \tag{20}$$

$$\mathbf{Y}_k^m(\nu,t) = \theta(t)\frac{(\mathscr{T}^*(\nu)\mathbf{E}^m)_k}{\rho}t,\ for\ D_k(\nu) = 0, \tag{21}$$

where $k = 1,2,3,4,5,6$; $\theta(t)$ is the Heaviside function, i.e. $\theta(t) = 1$ for $t \geq 0$ and $\theta(t) = 0$ for $t < 0$. Finally, a solution of (13), (14) is determined by (17).

3.3 Formula for mth column for the time-dependent GF of elastodynamics in 3D QCs

We note that values of $\mathbf{V}^m(x,t)$, $\tilde{\mathbf{V}}^m(\nu,t)$, $\mathscr{T}(\nu)$ and $D(\nu) = diag(D_k(\nu),\ k = 1,2,3,4,5,6)$ are real. Therefore, applying the inverse Fourier transform to (17) (see, for example [Vladimirov (1971)]), we find that a solution of (11), (12) is given by

$$\begin{aligned}\mathbf{V}^m(x,t) &= \frac{\theta(t)}{(2\pi)^3} Re\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathscr{T}(\nu)\mathbf{Y}^m(\nu,t)\exp(\nu\cdot x)d\nu_1 d\nu_2 d\nu_3\right] \\ &= \frac{\theta(t)}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathscr{T}(\nu)\mathbf{Y}^m(\nu,t)\cos(\nu\cdot x)d\nu_1 d\nu_2 d\nu_3. \end{aligned} \tag{22}$$

4 Computational experiments

Three-dimensional icosahedral QC Al-Cu-Li (see, for example, Li, Fan, and Wu (2009)) has been taken for our computational experiment. The values of phonon, phason and phonon-phason coupling elastic constants are given by the following relations (see, for example Ding, Yang, Hu, and Wang (1993); Hu, Wang, and Ding (2000); Akmaz (2009)):

$$C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{jl}\delta_{ik} + \delta_{il}\delta_{jk}),$$

$\lambda = 30.4,\ \mu = 40.9(GPa)$;

$$\begin{aligned}
K_{1111} &= K_{2222} = K_{1212} = K_{2121} = 300(MPa),\\
K_{1131} &= K_{1113} = K_{2213} = K_{2312} = -K_{2231} = -K_{2321} = -K_{1232} = -K_{3221} = 150(MPa),\\
K_{3333} &= 450(MPa),\ K_{2323} = K_{3131} = K_{3232} = K_{1313} = 150(MPa),\\
R_{1111} &= R_{1122} = R_{1133} = R_{1113} = R_{2233} = R_{2332} = R_{3111} = R_{3131} = R_{1221} = 0.8(GPa),\\
R_{2211} &= R_{2222} = R_{2213} = R_{2312} = R_{2321} = R_{3122} = R_{1223} = R_{1212} = -0.8(GPa),\\
R_{3333} &= -1.6(GPa).
\end{aligned}$$

The conditions (4), (5) are satisfied for 3D QC Al-Cu-Li. The density ρ has been chosen as $\rho = 1(10^3 kg/m^3)$.

The aim of the computational experiment is to derive values of elements for the time-dependent GF of elastodynamics in 3D QC Al-Cu-Li and present results in the form of 3D graphs. Using the method of Section 4 we have computed a solution $\mathbf{V}^m(x,t) = (V_1^m(x,t), V_2^m(x,t), V_3^m(x,t), V_4^m(x,t), V_5^m(x,t), V_6^m(x,t))$ of (11), (12) for each $m = 1,2,...,6$. The computed vector-functions $\mathbf{V}^m(x,t)$ are columns of the GF of elastodynamics in Al-Cu-Li. We note that the first three components of the vector function $\mathbf{V}^m(x,t)$ are the phonon displacement $\mathbf{u}^m(x,t) = (u_1^m(x,t), u_2^m(x,t), u_3^m(x,t))$ and the last three components of $\mathbf{V}^m(x,t)$ are the phason displacement $\mathbf{w}^m(x,t) = w_1^m(x,t), w_2^m(x,t), w_3^m(x,t))$ arising in QC from forces $\mathbf{f}(x,t) = (f_1, f_2, f_3)$, $\mathbf{g}(x,t) = (g_1, g_2, g_3)$ whose components defined as follows

$$f_k(x,t) = \delta_k^m \delta(x_1)\delta(x_2)\delta(x_3)\delta(t), \;\; g_k(x,t) = \delta_{k+3}^m \delta(x_1)\delta(x_2)\delta(x_3)\delta(t),$$

where $m = 1,2,...,6; k = 1,2,3$; δ_k^m is the Kronecker symbol.

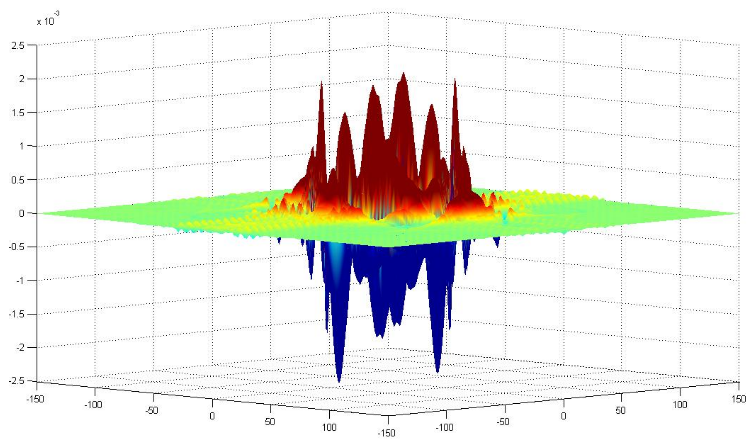

Figure 1: 3D surface $z = V_1^6(x_1, x_2, 0, t)$ for $t = 0.15$ in QC Al-Cu-Li.

The result of the computational experiment is presented in Figures 1-6. Figure 1 presents the graph of the 3-D surface $V_1^6(x_1, x_2, t)$ for $t = 0.15$. Here the horizontal axes are x_1 and x_2. The vertical axis is the magnitude of $V_1^6(x_1, x_2, 0, 0.15)$. Figure 2 presents a view from the top of the magnitude axis V_1^6 (i.e. the view of the surface $z = V_1^6(x_1, x_2, 0, 0.15)$). Similar, Figures 3, 5 present the graph of the 3-D surfaces $V_6^6(x_1, x_2, 0, t)$ for $t = 0.02,\ 0.15$, respectively. Here the horizontal axes are x_1 and x_2. The vertical axis is the magnitude of $V_6^6(x_1, x_2, 0, t)$. Figures 4, 6 present a view from the top of the magnitude axis $V_6^6(x_1, x_2, 0, t)$ (i.e. the view of the surface $z = V_6^6(x_1, x_2, 0, t)$) for time $t = 0.02, 0.15$.

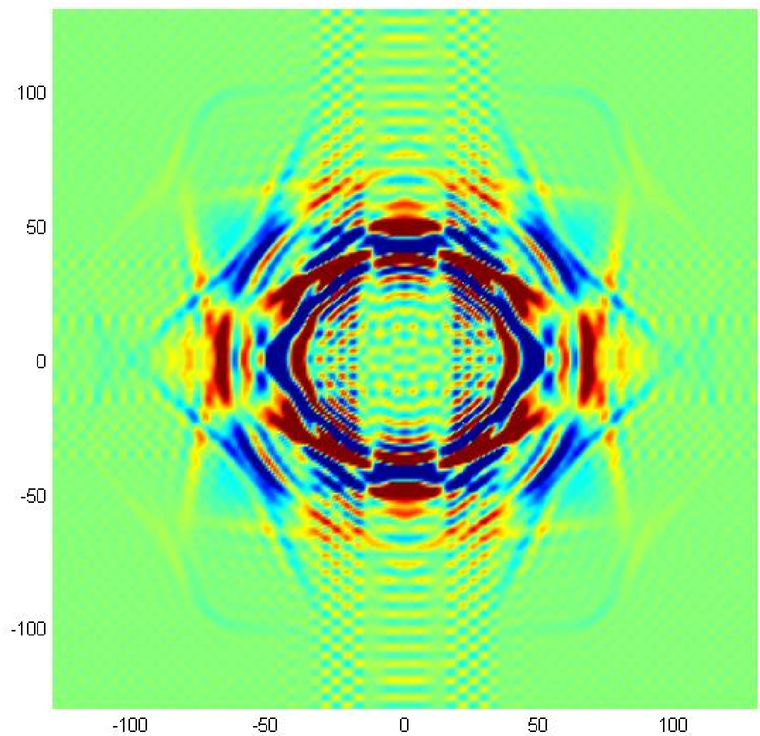

Figure 2: The map surface plot (plan) of 3D surface $z = V_1^6(x_1, x_2, 0, 0.15)$ in QC Al-Cu-Li.

5 Conclusion

The paper has described the method which allows us to derive the formula of the time-dependent GF of elastodynamics in 3D QCs by the matrix transformations, solutions of some ordinary differential equations depending on the Fourier parameters and the inverse Fourier transform. The formula for the GF of elastodynamics in 3D QCs has been presented in the form convenient for computation of the transient phonon and phason displacement fields. Computational experiments confirm the robustness of our method for the computation of the time-dependent Green's function in icosahedral quasicrystals. Using our method the simulation of phonon and phason displacement field in 3D QCs has been made. The results of simulation give a possibility to observe and analyze the elastic wave propagation arising from pulse point sources.

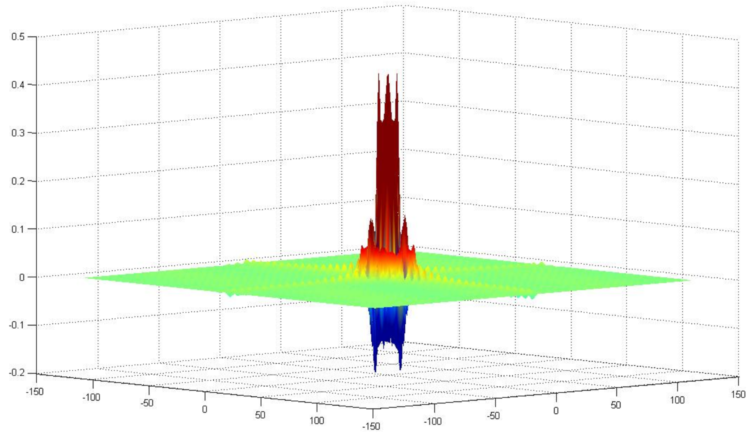

Figure 3: 3D surface $z = V_6^6(x_1, x_2, 0, t)$ for $t = 0.02$ in QC Al-Cu-Li.

6 Appendix

The matrix $\mathbf{A}(\nu)$, defined by (15), is symmetric with real valued elements. Let us show that $\mathbf{A}(\nu)$ is positive-definite for any nonzero (ν_1, ν_2, ν_3) from R^3, i.e. the matrix $\mathbf{A}(\nu)$ has to satisfy

$$\mathbf{V}^*\mathbf{A}(\nu)\mathbf{V} > 0 \tag{23}$$

for arbitrary nonzero vectors $\mathbf{V} = (u_1, u_2, u_3, w_1, w_2, w_3) \in R^6$ and $(\nu_1, \nu_2, \nu_3) \in R^3$. We assume in Section 2 that $C_{ijkl},\ R_{ijkl},\ K_{ijkl}$ satisfy conditions (5) for any symmetric matrix $(\varepsilon_{ij})_{3\times 3}$ and any matrix $(w_{ij})_{3\times 3}$.
The relations (5) can be written in the form

$$\sum_{j,l,i,k=1}^{3} C_{ijkl} u_i u_k \nu_j \nu_l > 0, \sum_{i,j,k,l=1}^{3} R_{ijkl} u_i w_k \nu_j \nu_l > 0, \sum_{i,j,k,l=1}^{3} K_{ijkl} w_i w_k \nu_j \nu_l > 0, \tag{24}$$

when

$$\varepsilon_{ij} = \frac{1}{2}(u_i \nu_j + u_j \nu_i),\ \ w_{kl} = \nu_l w_k,$$

here $\nu_1,\ \nu_2,\ \nu_3, u_1,\ u_2,\ u_3, w_1,\ w_2,\ w_3$ are arbitrary nonzero real numbers.

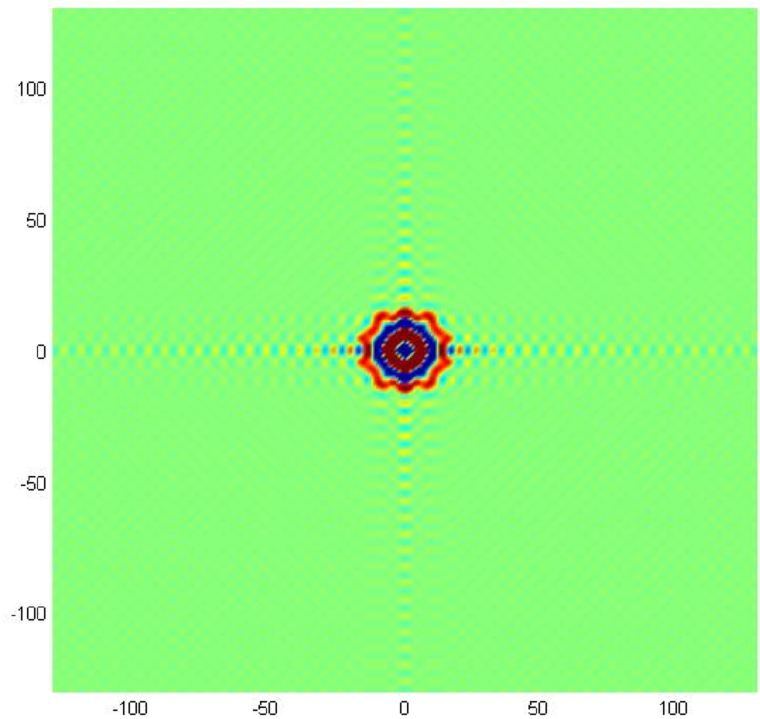

Figure 4: The map surface plot (plan) of 3D surface $z = V_6^6(x_1, x_2, 0, 0.02)$ in QC Al-Cu-Li.

Using (15) we find

$$\mathbf{V}^*\mathbf{A}(v)\mathbf{V} = \frac{1}{2}\sum_{j,l,i,k=1}^{3}(C_{ijkl}+C_{ilkj})u_iu_kv_jv_l$$

$$+ \sum_{j,l,i,k=1}^{3}(R_{ijkl}+R_{ilkj})u_iw_kv_jv_l + \frac{1}{2}\sum_{j,l,i,k=1}^{3}(K_{ijkl}+K_{ilkj})w_iw_kv_jv_l, \tag{25}$$

where $\mathbf{V} = (u_1, u_2, u_3, w_1, w_2, w_3) \in R^6$ and $(v_1, v_2, v_3) \in R^3$ are arbitrary nonzero vectors.

The inequality (23) follows from (24) and (25) for all nonzero $\mathbf{V} = (u_1, u_2, u_3, w_1, w_2, w_3) \in R^6$ and $(v_1, v_2, v_3) \in R^3$.

Remark: For all $(v_1, v_2, v_3) \in R^3$ the matrix $\mathbf{A}(v)$ defined by (15) is positive semi

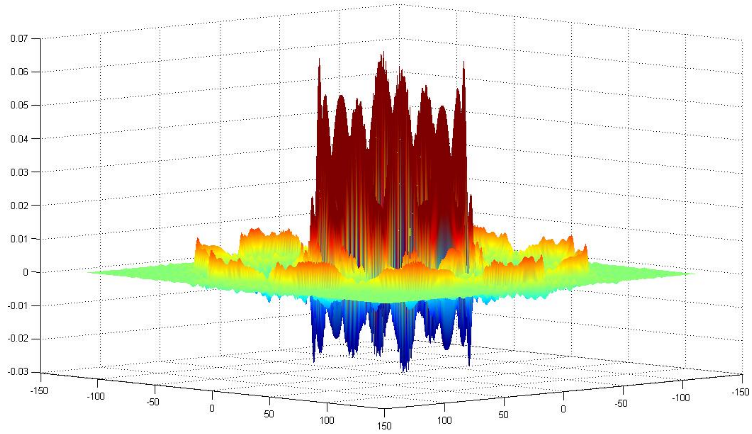

Figure 5: 3D surface $z = V_6^6(x_1, x_2, 0, t)$ for $t = 0.15$ in QC Al-Cu-Li.

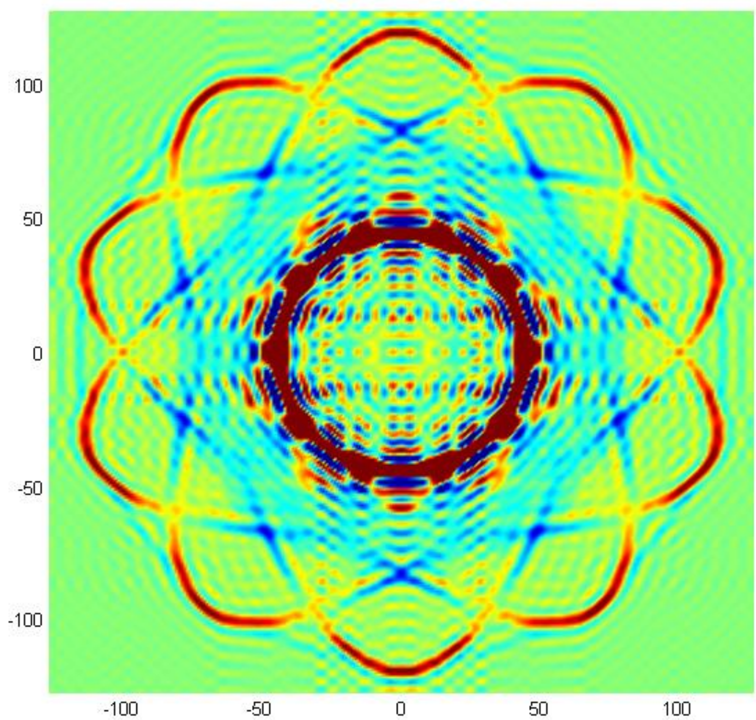

Figure 6: The map surface plot (plan) of 3D surface $z = V_6^6(x_1, x_2, 0, 0.15)$ in QC Al-Cu-Li.

definite matrix.

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