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Perturbative method for solving elastic problems of one-dimensional hexagonal quasicrystals

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Abstract

A new perturbation technique for solving elastic three-dimensional problems of quasicrystals is supplied. The key idea of this technique is to simplify the equations by introducing a parameter which does not exist in the original equations, and then look for the perturbation solution for the problems of interest. To illustrate the utility of our method and for comparison, we consider the crack problem for one-dimensional hexagonal quasicrystals with point groups $6mm$, 62_h2_h, $\bar{6}m2_h$ and $6/m_hmm$, whose exact solution has been obtained by the first two authors of this paper. Only up to the order zero approximation, we get the exact expression for the stress intensity factor, which is the most important physical quantity in fracture theory. Moreover, the same procedure can be used to deal with the elastic problems for two- and three-dimensional quasicrystals. A simple review of the method is finally given.

1. Introduction

Since the discovery of three-dimensional (3D) icosahedral quasicrystals (QCs) in in Al–Mn alloys [1], 3D cubic QCs [2, 3], two-dimensional (2D) QCs [4–6] and one-dimensional (1D) QCs [7, 8] have been discovered in succession, and QCs have become the focus of theoretical and experimental studies in the physics of condensed matter. 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. Based on Landau theory, QC elasticity theory was formulated [9–12]. On the other hand, as in conventional crystals, many structural defects have already been observed experimentally in QCs. For example, some experimental results show that some 2D defects such as planar defects and cracks produced by cleavage are detected in QCs [13, 14]. Also, some macroscopic cracks or flaws inevitably exist in QC solids. So the defect problems for QCs, such as dislocation and crack problems, are studied by many authors [15–23]. However, most of the authors consider only the elastic plane or antiplane problems for QCs [15–21], i.e., they suppose that the elastic fields induced in QCs are independent of the variable z.

It is well known that the elastic equations of QCs are much more complicated than those in classical elasticity theory. The exact solutions for QC elastic equations can be obtained only in a few cases. For example, we have obtained the exact elasticity theory of 1D hexagonal QCs with point groups $6mm$, 62_h2_h, $\bar{6}m2_h$ and $6/m_hmm$ [22]. But for other QCs it seems indispensable for us to develop approximate method. In our previous work [23], we proposed the perturbation method for solving elastic 3D problems of icosahedral QCs (regarding the elastic constant R of phonon–phason coupling as a perturbation parameter). However, it is not general. For instance, it is not easily used to deal with elastic 3D problems of cubic QCs.

In this paper, we supply a new perturbation technique for solving elastic 3D problems of QCs. This method is general and can be used to deal with elastic problems for 1D, 2D and 3D QCs. To illustrate its utility and for comparison, we consider the same problem as in [22] (because its exact solution has been obtained by the first two of the authors in this paper), that is, the problem of a circular crack embedded in an infinite 1D hexagonal QC of point group $6mm$. Only up to the order zero approximation, the exact stress intensity factor expression (which is the most important physical quantity in fracture theory) for the loading of mode I is obtained. It is easy to see that the same procedure can be used to deal with the elastic problems for 2D and 3D QCs.

2. The basic equations

According to 1D QC elasticity theory [24], strain– and stress–displacement relations for 1D hexagonal QCs with point groups $6mm$, 62_h2_h, $\bar{6}m2_h$ and $6/m_hmm$, respectively, are

$$
\begin{aligned}
&\varepsilon_{ij} = (\partial_j u_i + \partial_i u_j)/2 \qquad w_{ij} = \partial_j w_i \\
&\sigma_{xx} = c_{11}\partial_x u_x + (c_{11} - 2c_{66})\partial_y u_y + c_{13}\partial_z u_z + R_1\partial_z w_z \\
&\sigma_{yy} = (c_{11} - 2c_{66})\partial_x u_x + c_{11}\partial_y u_y + c_{13}\partial_z u_z + R_1\partial_z w_z \\
&\sigma_{zz} = c_{13}\partial_x u_x + c_{13}\partial_y u_y + c_{33}\partial_z u_z + R_2\partial_z w_z \\
&\sigma_{yz} = \sigma_{zy} = c_{44}(\partial_y u_z + \partial_z u_y) + R_3\partial_y w_z \\
&\sigma_{zx} = \sigma_{xz} = c_{44}(\partial_x u_z + \partial_z u_x) + R_3\partial_x w_z \\
&\sigma_{xy} = \sigma_{yx} = c_{66}(\partial_x u_y + \partial_y u_x) \\
&H_{zz} = R_1(\partial_x u_x + \partial_y u_u) + R_2\partial_z u_z) + K_1\partial_z w_z \\
&H_{zx} = R_3(\partial_x u_z + \partial_z u_x) + K_2\partial_x w_z \\
&H_{zy} = R_3(\partial_x u_z + \partial_z u_y) + K_2\partial_x w_z.
\end{aligned} \qquad (1)
$$

The equilibrium equations in terms of displacements, in the absence of body forces, are

$$
\begin{aligned}
&(c_{11}\partial_x^2 + c_{66}\partial_y^2 + c_{44}\partial_z^2)u_x + (c_{11} - c_{66})\partial_x\partial_y u_y + (c_{13} + c_{44})\partial_x\partial_z u_z + (R_1 + R_3)\partial_x\partial_z w_z = 0 \\
&(c_{11} - c_{66})\partial_x\partial_y u_x + (c_{66}\partial_x^2 + c_{11}\partial_y^2 + c_{44}\partial_z^2)u_y + (c_{13} + c_{44})\partial_y\partial_z u_z + (R_1 + R_3)\partial_y\partial_z w_z = 0 \\
&(c_{13} + c_{44})(\partial_x\partial_z u_x + \partial_y\partial_z u_y) + (c_{44}\partial_x^2 + c_{44}\partial_y^2 + c_{33}\partial_z^2)u_z + [R_3(\partial_x^2 + \partial_y^2) + R_2\partial_z^2]w_z = 0 \\
&(R_1 + R_3)(\partial_x\partial_z u_x + \partial_y\partial_z u_y) + [R_3(\partial_x^2 + \partial_y^2) + R_2\partial_z^2]u_z + [K_2(\partial_x^2 + \partial_y^2) + K_1\partial_z^2]w_z = 0
\end{aligned} \qquad (2)
$$

where the z-axis is assumed to be the quasiperiodic axis, and the xy-plane the periodic plane of the QC, u_i, w_i phonon and phason displacements in the physical and perpendicular spaces, respectively, σ_{ij} and ε_{ij} phonon stresses and strains, H_{ij} and w_{ij} phason stresses and strains, c_{11}, c_{13}, c_{33}, c_{44}, c_{66}, K_1, K_2 the elastic constants corresponding to the phonon and phason fields and R_1, R_2, R_3 the elastic constants of phonon–phason coupling. We should keep in mind that the subscripts i, j for H_{ij}, w_{ij} cannot be exchanged according to their meanings [12]. It is very important for us to write the boundary conditions correctly.

3. The perturbation method

Introducing a dimensionless parameter δ in equations (2), then we rewrite (2) as

$$(c_{11}\partial_x^2 + c_{66}\partial_y^2 + c_{44}\partial_z^2)u_x + (c_{11} - c_{66})\partial_x\partial_y u_y + (c_{13} + c_{44})\partial_x\partial_z u_z + \delta(R_1 + R_3)\partial_x\partial_z w_z = 0$$
$$(c_{11} - c_{66})\partial_x\partial_y u_x + (c_{66}\partial_x^2 + c_{11}\partial_y^2 + c_{44}\partial_z^2)u_y + (c_{13} + c_{44})\partial_y\partial_z u_z + \delta(R_1 + R_3)\partial_y\partial_z w_z = 0$$
$$(c_{13} + c_{44})(\partial_x\partial_z u_x + \partial_y\partial_z u_y) + (c_{44}\partial_x^2 + c_{44}\partial_y^2 + c_{33}\partial_z^2)u_z + \delta[R_3(\partial_x^2 + \partial_y^2) + R_2\partial_z^2]w_z = 0$$
$$\delta(R_1 + R_3)(\partial_x\partial_z u_x + \partial_y\partial_z u_y) + \delta[R_3(\partial_x^2 + \partial_y^2) + R_2\partial_z^2]u_z + [K_2(\partial_x^2 + \partial_y^2) + K_1\partial_z^2]w_z = 0. \quad (3)$$

When $\delta = 1$, equations (3) recover (2). For equations (3) we look for the solution of the form

$$u_x = \sum_{i=0}^{\infty} \delta^i u_x^{(i)} \qquad u_u = \sum_{i=0}^{\infty} \delta^i u_y^{(i)}$$
$$u_z = \sum_{i=0}^{\infty} \delta^i u_z^{(i)} \qquad w_z = \sum_{i=0}^{\infty} \delta^i w_z^{(i)} \quad (4)$$

where $u_x^{(i)}$, $u_y^{(i)}$, $u_z^{(i)}$ and $w_z^{(i)}$ satisfy the following equations:

$$(c_{11}\partial_x^2 + c_{66}\partial_y^2 + c_{44}\partial_z^2)u_x^{(i)} + (c_{11} - c_{66})\partial_x\partial_y u_y^{(i)} + (c_{13} + c_{44})\partial_x\partial_z u_z^{(i)}$$
$$= -(R_1 + R_3)\partial_x\partial_z w_z^{(i-1)}$$
$$(c_{11} - c_{66})\partial_x\partial_y u_x^{(i)} + (c_{66}\partial_x^2 + c_{11}\partial_y^2 + c_{44}\partial_z^2)u_y^{(i)} + (c_{13} + c_{44})\partial_y\partial_z u_z^{(i)}$$
$$= -(R_1 + R_3)\partial_y\partial_z w_z^{(i-1)}$$
$$(c_{13} + c_{44})(\partial_x\partial_z u_x^{(i)} + \partial_y\partial_z u_y^{(i)}) + (c_{44}\partial_x^2 + c_{44}\partial_y^2 + c_{33}\partial_z^2)u_z^{(i)}$$
$$= -[R_3(\partial_x^2 + \partial_y^2) + R_2\partial_z^2]w_z^{(i-1)}$$
$$[K_2(\partial_x^2 + \partial_y^2) + K_1\partial_z^2]w_z^{(i)}$$
$$= -(R_1 + R_3)(\partial_x\partial_z u_x^{(i-1)} + \partial_y\partial_z u_y^{(i-1)}) - [R_3(\partial_x^2 + \partial_y^2) + R_2\partial_z^2]u_z^{(i-1)}. \quad (5)$$

From now on, the quantities with negative superscripts are taken as zero, and one can directly verify that equations (5) with $i = 0$ can be satisfied by (also see [22])

$$u_x^{(0)} = \partial_x(F_1 + F_2) - \partial_y F_3 \qquad u_y^{(0)} = \partial_y(F_1 + F_2) + \partial_x F_3$$
$$u_z^{(0)} = \partial_z(m_1 F_1 + m_2 F_2) \qquad w_z^{(0)} = F_4 \quad (6)$$

where the possible functions F_i are the solutions of

$$(\partial_x^2 + \partial_y^2 + \gamma_i^2\partial_z^2)F_i = 0 \qquad i = 1, 2, 3, 4 \quad (7)$$

where the values of m_i and γ_i are related by the following expressions:

$$\frac{c_{44} + (c_{13} + c_{44})m_i}{c_{11}} = \frac{c_{33}m_i}{c_{13} + c_{44} + c_{44}m_i} = \gamma_i^2 \qquad i = 1, 2$$
$$c_{44}/c_{66} = \gamma_3^2 \qquad K_1/k_2 = \gamma_4^2. \quad (8)$$

Substituting (4) and (6) into (1), and using (7), we have (here only a part of them is listed)

$$
\begin{aligned}
&\sigma_{zj} = \sigma_{jz} = \sum_{i=0}^{\infty} \delta^i \sigma_{zj}^{(i)} \qquad H_{zj} = \sum_{i=0}^{\infty} \delta^i H_{zj}^{(i)} \qquad (j = x, y, z) \\
&\sigma_{zz}^{(0)} = -c_{13}\partial_z^2(\gamma_1^2 F_1 + \gamma_2^2 G_2) + c_{33}\partial_z^2(m_1 F_1 + m_2 F_2) + R_2 \partial_z F_4 \\
&\sigma_{zy}^{(0)} = \sigma_{yz}^{(0)} = c_{44}\partial_y \partial_z[(m_1 + 1)F_1 + (m_2 + 1)F_2] + c_{44}\partial_x \partial_z F_3 + R_3 \partial_y F_4 \\
&\sigma_{zx}^{(0)} = \sigma_{xz}^{(0)} = c_{44}\partial_x \partial_z[(m_1 + 1)F_1 + (m_2 + 1)F_2] - c_{44}\partial_y \partial_z F_3 + R_3 \partial_y F_4 \\
&H_{zz}^{(0)} = -R_1\partial_z^2(\gamma_1^2 F_1 + \gamma_2^2 F_2) + R_2\partial_z^2(m_1 F_1 + m_2 F_2) + K_1 \partial_z F_4 \\
&H_{zx}^{(0)} = R_3 \partial_x \partial_z[(m_1 + 1)F_1 + (m_2 + 1)F_2] - R_3 \partial_y \partial_z F_3 + K_2 \partial_x F_4 \\
&H_{zy}^{(0)} = R_3 \partial_y \partial_z[(m_1 + 1)F_1 + (m_2 + 1)F_2] + R_3 \partial_x \partial_z F_3 + K_2 \partial_y F_4.
\end{aligned}
\tag{9}
$$

4. A circular crack problem

Consider an infinite 1D hexagonal QC of point group $6mm$ weakened by a flat circular crack with radius a in the plane $z = 0$, with uniform loads applied normal to the crack faces. Due to symmetry, we consider only the half-space $z \geqslant 0$. The mixed boundary conditions in the plane $z = 0$ reads

$$
\begin{aligned}
&\sigma_{zz} = -\sigma \qquad H_{zz} = -\tau \qquad 0 < r < a \\
&u_z = 0 \qquad w_z = 0 \qquad r > a \\
&\sigma_{zr} = 0 \qquad \sigma_{z\theta} = 0 \qquad r \geqslant 0.
\end{aligned}
\tag{10}
$$

Note that cylindrical polar coordinates in this case have been used (equations (4), (6) and (9) can be easily changed into those in cylindrical polar coordinates, which is omitted because of the limitation of space. Readers are referred to see [22]). Moreover, we suppose the elastic field under this loading condition to be independent of θ. We should also note that $H_{rz} = H_{\theta z} = 0$ for $r \geqslant 0$ is satisfied. After the Hankel transformation to equations (7), considering the boundary condition at infinity:

$$
\sigma_{ij} \to 0 \qquad H_{ij} \to 0 \qquad \sqrt{r^2 + z^2} \to \infty \tag{11}
$$

the solution of (7) can be expressed as

$$
F_i(r, z) = \int_0^{\infty} \xi A_i(\xi) \exp(-\xi z/\gamma_i) J_0(\xi r)\, \mathrm{d}\xi \qquad i = 1, 2, 3, 4. \tag{12}
$$

It follows from $\sigma_{z\theta} = 0$ for $r \geqslant 0$ that $F_3 = 0$. From $\sigma_{zr} = 0$ for $r \geqslant 0$, we have

$$
A_4 = \left[\frac{1 + m_1}{\gamma_1} A_1 + \frac{1 + m_2}{\gamma_2} A_2\right] \frac{c_{44}\xi}{R_3}. \tag{13}
$$

According to equations (4), (6), (9), the rest of the boundary conditions (10) and expression (13), we get

$$
\begin{cases}
\displaystyle\int_0^{\infty} \xi^3 A_1(\xi) J_0(\xi r)\, \mathrm{d}\xi = (c_2\sigma - c_4\tau)/(c_1c_4 - c_2c_3) & 0 < r < a \\
\displaystyle\int_0^{\infty} \xi^2 A_1(\xi) J_0(\xi r)\, \mathrm{d}\xi = 0 & r > a
\end{cases}
\tag{14}
$$

$$
\begin{cases}
\displaystyle\int_0^{\infty} \xi^3 A_2(\xi) J_0(\xi r)\, \mathrm{d}\xi = (c_1\sigma - c_3\tau)/(c_2c_3 - c_1c_4) & 0 < r < a \\
\displaystyle\int_0^{\infty} \xi^2 A_2(\xi) J_0(\xi r)\, \mathrm{d}\xi = 0 & r > a
\end{cases}
\tag{15}
$$

with

$$c_i = -R_1 + \frac{R_2 m_i}{\gamma_i^2} - \frac{K_1 c_{44}(1+m_i)}{\gamma_i \gamma_4 R_3} \qquad i = 1, 2$$
$$c_{j+2} = -c_{13} + \frac{c_{33} m_j}{\gamma_j^2} - \frac{R_2 c_{44}(1+m_j)}{\gamma_j \gamma_4 R_3} \qquad j = 1, 2.$$

According to the theory of dual integral equations [25, 26], from (14) and (15) we can easily obtain that (also see appendix in [22])

$$A_1(\xi) = [2(c_2\sigma - c_4\tau)/\pi(c_1c_4 - c_2c_3)]\xi^{-3}(\xi^{-1}\sin a\xi - a\cos a\xi)$$
$$A_2(\xi) = [2(c_1\sigma - c_3\tau)/\pi(c_2c_3 - c_1c_4)]\xi^{-3}(\xi^{-1}\sin a\xi - a\cos a\xi). \tag{16}$$

From the above we can calculate the most important physical quantity in fracture theory, the stress intensity factor (SIF). As in [22], for the phonon field and the phason field, respectively, we define SIFs

$$K_1^{\parallel} = \lim_{r\to a+} \sqrt{2\pi(r-a)}\sigma_{zz}(r,0) \qquad K_1^{\perp} = \lim_{r\to a+} \sqrt{2\pi(r-a)}H_{zz}(r,0). \tag{17}$$

It follows from equations (9), (12), (13) and (16) that

$$\sigma_{zz}^{(0)}(r,0) = \begin{cases} -\sigma & 0 < r < a \\ -\dfrac{2\sigma}{\pi}\left(\arcsin\dfrac{a}{r} - \dfrac{a}{\sqrt{r^2-a^2}}\right) & r > a \end{cases} \tag{18}$$

$$H_{zz}^{(0)}(r,0) = \begin{cases} -\tau & 0 < r < a \\ -\dfrac{2\tau}{\pi}\left(\arcsin\dfrac{a}{r} - \dfrac{a}{\sqrt{r^2-a^2}}\right) & r > a. \end{cases} \tag{19}$$

The substitution of (18) and (19) into (17) yields

$$K_1^{\parallel} = 2\sqrt{a/\pi}\sigma \qquad K_1^{\perp} = 2\sqrt{a/\pi}\tau. \tag{20}$$

It is of interest to see that equations (20) are the exact results which have been obtained by the first two of the authors in this paper [22].

5. Conclusions

The elastic equations of QCs are very complicated, and the exact solutions for 3D problems are scarce. As a possible approximation method, we supply a new perturbation technique for solving elastic 3D problems of QCs. Although we use it to deal with 1D hexagonal QCs with point groups $6mm$, 62_h2_h, $\bar{6}m2_h$ and $6/m_hmm$, it is obvious that the same procedure will be suitable for the elastic problems for 2D and 3D QCs. Nevertheless, are the asymptotic solutions (4) convergent? Even though equations (4) are divergent, we have also many methods to obtain their summation [27].

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