The partition function and state equation of the point group 12mm two-dimensional dodecagonal quasicrystal

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Abstract. This study extends the analysis of the vibrational spectrum of the one-dimensional hexagonal quasicrystal to the two-dimensional quasicrystal with the 12mm point group. Several thermodynamic functions and the state equation of the material are shown.

The study of the vibrational spectrum of a quasicrystal is an acknowledged problem. At present, there is a lack of knowledge of the lattice vibrations for quasicrystals, which leads to a fundamental difficulty in studying their spectra. For this reason the Debye [1] hypothesis presented the approximation that a solid may be seen as an elastic medium which can propagate elastic vibration to describe approximately the lattice vibration. This treatment is reasonable at least in the case of low temperatures and longwave length. The Debye approximation for crystals has been a considerable success and the theoretical predications of his specific heat formula for crystals are in excellent agreement with experimental results for a wide temperature range. Fan [2] extended the Debye approximation to study the energy distribution problem for a one-dimensional hexagonal quasicrystal and gave a very simple and quantitative description of the specific heat of the quasicrystal.

In this paper we extend the model and the method suggested by Fan [2] for a one-dimensional quasicrystal to the two-dimensional quasicrystal case. It is well known that the structure and elasticity of a two-dimensional quasicrystal are considerably more complicated than those of a one-dimensional quasicrystal. Up to now people have observed four kinds of quasicrystals with five-fold, eight-fold, ten-fold and twelve-fold symmetries, which are also called as pentagonal, octagonal, decagonal and dodecagonal quasicrystals respectively. Among them the elasticity of the dodecagonal quasicrystal is the simplest. At first, the vibration and wave propagation for the quasicrystal with a

12mm point group symmetry were studied. Fortunately, the elastic vibration equations for this two-dimensional quasicrystal can be exactly reduced to some standard wave equations, thus providing the opportunity to: (1) determine some exact thermal properties (under the longwave length approximation), (2) to find some exact solutions for the dislocation and crack dynamics for the dodecagonal quasicrystal and (3) to extend the description of dynamic equations to other two-dimensional quasicrystals, etc. Here we discuss only for the first problem.

1 The generalized Debye model for quasicrystals

We assume that a quasicrystal may be seen as a continuous elastic medium with phonon and phason parameters, which can propagate elastic vibration waves, and we take the vibration of the medium to describe approximately the lattice vibration of the quasicrystal. Meanwhile the energy of lattice vibration of the solid is quantized, *i.e.*, the energy distribution follows the Planck formula.

2 Vibration and wave propagation in the two-dimensional dodecagonal quasicrystal

The key step in employing the Debye approach to discuss the energy distribution of the quasicrystal lies in the

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description of vibration and wave propagation in the material.

Consider a 12mm point group for a two-dimensional quasicrystal, and (x_1, x_2, x_3) stands for the rectilinear coordinate system. Assume the atom arrangement along the axis x_3 is periodic, and the atom arrangement along the $x_1 - x_2$ plane is quasiperiodic in the quasicrystal. In this case, there are phonon displacement components u_1, u_2, u_3, and phason displacement components w_1, w_2, and $w_3 = 0$.

For simplicity of mathematical treatment, suppose approximately that the field quantities are independent from x_3, $i.e.$

$$u_i = u_i(x_1, x_2, t) \quad (i = 1, 2, 3),$$
$$w_i = w_i(x_1, x_2, t) \quad (i = 1, 2) \qquad (1)$$

where x_1, x_2 are the spatial coordinates mentioned above, and t the time.

Under the condition (1), the generalized Hooke's law for a two-dimensional dodecagonal quasicrystal with twelve-fold symmetry, see $e.g.$ Hu $et\ al.$ [3] and Fan [4] is as follows

$$\sigma_{11} = C_{12}(\varepsilon_{11} + \varepsilon_{22}) + (C_{11} - C_{12})\varepsilon_{11}$$
$$\sigma_{22} = C_{12}(\varepsilon_{11} + \varepsilon_{22}) + (C_{11} - C_{12})\varepsilon_{22}$$
$$\sigma_{12} = \sigma_{21} = (C_{11} - C_{12})\varepsilon_{12}$$
$$\sigma_{13} = \sigma_{31} = 2C_{44}\varepsilon_{13}$$
$$\sigma_{23} = \sigma_{32} = 2C_{44}\varepsilon_{23}$$
$$H_{11} = K_1 w_{11} + K_2 w_{22}$$
$$H_{22} = K_1 w_{22} + K_2 w_{11}$$
$$H_{12} = (K_1 + K_2 + K_3)w_{12} + K_3 w_{21}$$
$$H_{21} = (K_1 + K_2 + K_3)w_{21} + K_3 w_{12} \qquad (2)$$

in which σ_{ij} denotes the stress tensors associated with the phonon, H_{ij} the stress tensor associated with the phason, and ε_{ij} and w_{ij} the strain tensors defined by

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad w_{ij} = \frac{\partial w_i}{\partial x_j} \qquad (3)$$

C_{ij} the elastic constants of the phonon field, and K_i the elastic constants of the phason field, respectively. For the two-dimensional quasicrystal with twelve-fold symmetry, the phonon and phason are decoupled, so the coupling elastic constants $R_{ij} = 0$.

The related equations of motion are

$$\frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{12}}{\partial x_2} = \rho\frac{\partial^2 u_1}{\partial t^2}, \quad \frac{\partial \sigma_{21}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} = \rho\frac{\partial^2 u_2}{\partial t^2},$$

$$\frac{\partial \sigma_{31}}{\partial x_1} + \frac{\partial \sigma_{32}}{\partial x_2} = \rho\frac{\partial^2 u_3}{\partial t^2},$$

$$\frac{\partial^2 H_{11}}{\partial x_1} + \frac{\partial H_{12}}{\partial x_2} = \rho\frac{\partial^2 w_1}{\partial t^2} \quad \frac{\partial H_{21}}{\partial x_1} + \frac{\partial H_{22}}{\partial x_2} = \rho\frac{\partial^2 w_2}{\partial t^2}$$
$$(4)$$

in which ρ represents the mass density of the material.

If we introduce the following displacement potentials such as

$$u_1 = \frac{\partial F}{\partial x_1} + \frac{\partial G}{\partial x_2}, \qquad u_2 = \frac{\partial F}{\partial x_2} - \frac{\partial G}{\partial x_1}$$

$$w_1 = \frac{\partial P}{\partial x_1} + \frac{\partial Q}{\partial x_2}, \qquad w_2 = -\frac{\partial P}{\partial x_2} + \frac{\partial Q}{\partial x_1} \qquad (5)$$

then the basic equations (2, 3, 4) are reduced to the following wave equations

$$\nabla^2 F = \frac{1}{c_1^2}\frac{\partial^2 F}{\partial t^2}, \quad \nabla^2 G = \frac{1}{c_2^2}\frac{\partial^2 G}{\partial t^2}, \quad \nabla^2 u_3 = \frac{1}{c_3^2}\frac{\partial^2 u_3}{\partial t^2},$$

$$\nabla^2 P = \frac{1}{d_1^2}\frac{\partial^2 P}{\partial t^2}, \quad \nabla^2 Q = \frac{1}{d_2^2}\frac{\partial^2 Q}{\partial t^2}, \quad (6)$$

where $\nabla^2 = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2$ and

$$c_1 = \sqrt{C_{11}/\rho}, \quad c_2 = \sqrt{(C_{11} - C_{12})/2\rho}, \quad c_3 = \sqrt{C_{44}/\rho}$$

$$d_1 = \sqrt{K_1/\rho}, \quad d_2 = \sqrt{(K_1 + K_2 + K_3)/\rho} \qquad (7)$$

are wave speeds of the propagation of the vibration in the quasicrystal.

The justification of the above procedure can be confirmed via direct substitution, $i.e.$, substituting (5) into (3), then into (2) and then into (4), one finds that the wave equations (6) must be satisfied.

If the phason field is absent, then $K_i = 0$, so $d_1 = d_2 = 0$, and if the medium is isotropic, we have

$$C_{11} = \lambda + 2\mu, \quad \frac{C_{11} - C_{12}}{2} = \mu, \quad C_{44} = \mu$$

in which λ and μ are the Lamé constants, and c_1 and $c_2 = c_3$ will be the speeds of the longitudinal and transverse waves of the materials. Equations (6) will then be reduced to the classical elastic wave equations.

Equations (6) give a macro-description of vibration and wave propagation in the two-dimensional quasicrystal with twelve-fold symmetry. The discovery of the last two equations of (6) is a fortunate, similar to the case of the one-dimensional hexagonal quasicrystal, see $e.g.$ Fan [2,4]. Apart from these two cases, one cannot obtain the standard wave equations for other quasicrystal systems via this simple approach. Due to the complexity of the elasticity of quasicrystals, there is no possibility to find the general and universal forms of the elastic wave equations suitable for all other quasicrystals. But the present results are significant in their ability to describe elastic vibration and wave propagation approximately for other two-dimensional quasicrystals.

3 Partition function and state equation of the dodecagonal quasicrystal

Denoting ν to be the atom vibration frequency and $g(\nu)$ the frequency distribution function, then

$$g(\nu)\mathrm{d}\nu$$

will be the number of simple harmonic vibrations between ν and $\nu + \mathrm{d}\nu$, and denoting N to be the number of atoms then the total number of degrees of freedom is given by

$$\int_0^\infty g(\nu)\mathrm{d}\nu = 3N. \qquad (8)$$

Extending the model for the one-dimensional hexagonal quasicrystal given by Fan [2] to the two-dimensional quasicrystal of 12mm point group symmetry, we have

$$g(\nu)\mathrm{d}\nu = B\nu^2\mathrm{d}\nu, \qquad (9)$$

with

$$B = 4\pi V \left(\frac{1}{c_1^3} + \frac{1}{c_2^3} + \frac{1}{c_3^3} + \frac{1}{d_1^3} + \frac{1}{d_2^3} \right), \qquad (10)$$

where V stands for the volume of the material, and c_1, c_2, c_3, d_1 and d_2 are defined by (7).

As a special case, where the phason field is absent, so d_1 and d_2 and the vibrational components corresponding to d_1 and d_2 do not exist and furthermore that the material is isotropic, then $C_{11} = \lambda + 2\mu$, $C_{11} - C_{12} = 2\mu$, $C_{44} = \mu$, and formula (10) reduces to the classical Debye [1] formula, i.e.,

$$B = B' \equiv 4\pi V \left(\frac{1}{c_1^3} + \frac{2}{c_2^3} \right). \qquad (11)$$

This shows that the present result is in exact agreement with that of the well-known Debye model in the classical limit case.

Considering that the total number of degrees of freedom should be finite, there is a maximum frequency ν_D (which is named as Debye frequency), i.e., (8) should be rewritten as

$$\int_0^{\nu_D} g(\nu)\mathrm{d}\nu = 3N \qquad (12)$$

with (substituting (9) into (12))

$$\nu_D^3 = 9N/B \cdot \qquad (13)$$

Based on (9, 10) and the energy quantization assumption, we can find the energy E due to the lattice vibration

$$E = E_0 + \sum \bar{\bar{\in}}(\nu) = E_0 + \int_0^{\nu_D} \bar{\bar{\in}}(\nu)g(\nu)\mathrm{d}\nu, \qquad (14)$$

with

$$\bar{\bar{\in}}(\nu) = \frac{h\nu}{\mathrm{e}^{h\nu/kT} - 1}, \qquad (15)$$

and the partition function Φ

$$\Psi = \ln\Phi = -\frac{E_0}{kT} + \int_0^{\nu_D} g(\nu)\ln\left(\frac{1}{1 - \mathrm{e}^{-h\nu/kT}}\right)\mathrm{d}\nu \qquad (16)$$

for the quasicrystal, in which E_0 is a constant, h and k are Planck's constant and Boltzman's constant respectively, T the absolute temperature and ν_D is given by (13) and (10) (the mathematical details are omitted here).

From (14) one can obtain the specific heat of the materials, refer to Fan [2]. From (16) we find the state equation of the solid

$$p = kT\frac{\partial\Psi}{\partial V} = -\frac{\partial E_0}{\partial V} - \frac{E - E_0}{\Theta}\frac{\partial\Theta}{\partial V} \qquad (17)$$

in which p stands for the pressure and

$$\Theta = \frac{h\nu_D}{k} \qquad (18)$$

is understood to be the generalized Debye characteristic temperature of a two-dimensional quasicrystal with twelve-fold symmetry.

Denoting α as the expansion coefficient and as the compression coefficient of the material

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p, \qquad \kappa = \frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T \qquad (19)$$

respectively, then one finds that

$$\frac{\alpha}{\kappa} = \left(\frac{\partial p}{\partial T}\right)_V = -\frac{1}{\Theta}\frac{\partial\Theta}{\partial V}\left(\frac{\partial E}{\partial T}\right)_V = -\frac{1}{\Theta}\frac{\partial\Theta}{\partial V}c_V \qquad (20)$$

where c_V is the specific heat of the material given by $c_V = (\partial E/\partial T)_V$ in which E is defined by (14) with (9) and (10). Equation (20) is the generalized Grueneisen law for the quasicrystlal.

References

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