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LETTER TO THE EDITOR

A study on the specific heat of a one-dimensional hexagonal quasicrystal

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Abstract. Extending the Debye approach for studying the specific heat of a crystal to a quasicrystal, this study gives the formula of the specific heat of a one-dimensional hexagonal quasicrystal.

Since a quasicrystal was observed first by Shechtman *et al* (1984), the electronic structure and the optic, magnetic, thermal and mechanical properties of the material have been extensively investigated. This letter reports a study on the specific heat of a quasicrystal. It is well known that the understanding of the specific heat of a quasicrystal depends upon the knowledge on the lattice vibration of the solid. Because there is a lack of this knowledge, one can study the specific heat of a quasicrystal only based on phenomenological versions at present. Among them, the Debye (1912) continuous medium model for studying the specific heat of an ordinary crystal is one of the useful models, which can be extended to analysing the specific heat of a quasicrystal. Even taking the phenomenological continuous medium model, the problem presents a fundamental difficulty due to the complexity of the basic equations of the elasticity of quasicrystals. To overcome the difficulty, this letter suggests a simple model, that is, the three-dimensional elastic field of a one-dimensional hexagonal quasicrystal is simplified approximately as a superposition of a plane field and an anti-plane field, in which the phonon and phason parameters are coupled in the anti-plane field. This model extremely simplifies the basic equations of the elasticity of the quasicrystal. Particularly, only in this way is the analytic formulation of the specific heat of the material available.

Soon after the discovery of the quasicrystal, Bak (1985) developed the theory of elasticity of quasicrystals based on the Landau–Lifshitz (1968) phenomenological theory of elementary excitation of condensed matter. In Bak's theory there are two lower frequency excitations such as phonon $\boldsymbol{u}$ and phason $\boldsymbol{w}$. The introduction of the phason, which is an essential difference between the theories of elasticity of quasicrystals and crystals, gives a macro-description of the quasiperiodicity of the new solid phases. Corresponding to the phonon and phason parameters, there are two strain fields u_{ij} and w_{ij} in the theory of elasticity of quasicrystals, in which the former describes the change in the shape and volume of the unit cell and the latter describes the local rearrangement of the unit cell in the quasicrystal, while the local rearrangement is indistinguishable in a crystal. Either the phonon or the phason is considered as a continuous medium field variable under the frame of the present theory of elasticity of quasicrystals. The Bak theory is the basis of the present study.

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Consider a one-dimensional hexagonal quasicrystal with the Laue class $6/m_h mm$; (x_1, x_2, x_3) represents the rectilinear coordinate system. Assume the atom arrangement along the axis x_3 is quasiperiodic, and the atom arrangement along the x_1–x_2 plane is periodic in the quasicrystal. In this case, there are phonon displacement components u_1, u_2, u_3 and phason displacement component w_3 (and $w_1 = w_2 = 0$).

For simplicity of mathematical treatment, assume approximately the field quantities are independent of x_3, i.e.,

$$u_i = u_i(x_1, x_2, t) \qquad (i = 1, 2, 3) \qquad w_3 = w_3(x_1, x_2, t) \tag{1}$$

in which x_1, x_2 are the spatial coordinates measured above, and t the time.

Under the assumption (1), the stress–strain relations originating with Wang *et al* (1997) will be reduced to the following

$$\begin{aligned} \sigma_{11} &= C_{11}\varepsilon_{11} + C_{12}\varepsilon_{22} \\ \sigma_{22} &= C_{12}\varepsilon_{11} + C_{11}\varepsilon_{22} \\ \sigma_{12} &= \sigma_{21} = 2C_{66}\varepsilon_{12} \\ \sigma_{33} &= C_{13}(\varepsilon_{11} + \varepsilon_{22}) \\ H_{33} &= R_3(\varepsilon_{11} + \varepsilon_{22}) \end{aligned} \tag{2}$$

$$\begin{aligned} \sigma_{23} &= \sigma_{32} = 2C_{44}\varepsilon_{23} + R_3 w_{32} \\ \sigma_{31} &= \sigma_{13} = 2C_{44}\varepsilon_{31} + R_3 w_{31} \\ H_{23} &= 2R_3\varepsilon_{23} + K_2 w_{32} \\ H_{31} &= 2R_3\varepsilon_{31} + K_2 w_{31} \end{aligned} \tag{3}$$

where ε_{ij} are the strain components associated with the phonon field, w_{ij} the strain components associated with the phason field and

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \qquad w_{ij} = \frac{\partial w_i}{\partial x_j}. \tag{4}$$

σ_{ij} are the stress components similar to those in a conventional crystal, H_{ij} the stress components due to the existence of the phason field, C_{ij} the elastic constants of the phonon field, K_i the elastic constants of the phason field and R_i the phonon–phason coupling elastic constants.

The corresponding equations of motion are

$$\frac{\partial\sigma_{11}}{\partial x_1} + \frac{\partial\sigma_{12}}{\partial x_2} = \rho\frac{\partial^2 u_1}{\partial t^2} \qquad \frac{\partial\sigma_{21}}{\partial x_1} + \frac{\partial\sigma_{22}}{\partial y} = \rho\frac{\partial^2 u_2}{\partial t^2} \tag{5}$$

$$\frac{\partial\sigma_{31}}{\partial x_1} + \frac{\partial\sigma_{32}}{\partial x_2} = \rho\frac{\partial^2 u_3}{\partial t^2} \qquad \frac{\partial H_{31}}{\partial x_1} + \frac{\partial H_{32}}{\partial x_2} = \rho\frac{\partial^2 w_3}{\partial t^2} \tag{6}$$

in which ρ is the mass density of the quasicrystal.

It is evident that the field described by equations (2) and (5) is a plane phonon field, and the field described by equations (3) and (6) represents an anti-plane coupling phonon–phason field.

If we introduce displacement potentials F, G and ϕ, ψ such that

$$u_1 = \frac{\partial F}{\partial x_1} + \frac{\partial G}{\partial x_2} \qquad u_2 = \frac{\partial F}{\partial x_2} - \frac{\partial G}{\partial x_1} \tag{7}$$

$$u_3 = \alpha\phi - R_3\psi \qquad w_3 = R_3\phi + \alpha\psi \tag{8}$$

where

$$\alpha = \left[C_{44} - K_2 + \sqrt{(C_{44} - K_2)^2 + 4R_3^2} \right] / 2 \tag{9}$$

then (2)–(6) are reduced to the following wave equations

$$\nabla^2 F = \frac{1}{c_1^2} \frac{\partial^2 F}{\partial t^2} \qquad \nabla^2 G = \frac{1}{c_2^2} \frac{\partial^2 G}{\partial t^2} \tag{10}$$

$$\nabla^2 \phi = \frac{1}{s_1^2} \frac{\partial^2 \phi}{\partial t^2} \qquad \nabla^2 \psi = \frac{1}{s_2^2} \frac{\partial^2 \psi}{\partial t^2} \tag{11}$$

in which $\nabla^2 = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2$, and

$$\begin{aligned} c_1 &= \sqrt{C_{11}/\rho} \qquad c_2 = \sqrt{(C_{11} - C_{12})/2\rho} \\ s_1 &= \sqrt{\varepsilon_1/\rho} \qquad s_2 = \sqrt{\varepsilon_2/\rho} \\ \varepsilon_1 &= \left(C_{44} + K_2 + \sqrt{(C_{44} - K_2)^2 + 4R_3^2} \right) / 2 \\ \varepsilon_2 &= \left(C_{44} + K_2 - \sqrt{(C_{44} - K_2)^2 + 4R_3^2} \right) / 2. \end{aligned} \tag{12}$$

Equations (10) and (11) describe the propagation of vibration in the medium of a one-dimensional hexagonal quasicrystal with the Laue class $6/m_h mm$ and c_1, c_2, s_1 and s_2 are the speeds of the wave propagation.

Debye (1912) considered that a solid may be seen as a continuous elastic medium, which can propagate the waves of elastic vibration. We now extend the Debye hypothesis to a quasicrystal. That is we consider the one-dimensional hexagonal quasicrystal to be a continuous elastic medium, in which the elastic vibration and the wave propagation have been discussed in the proceeding section. Denoting by ν 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 by N the number of atoms then the total number of degrees of freedom should be

$$\int_0^\infty g(\nu)\,\mathrm{d}\nu = 3N. \tag{13}$$

Extending the Debye model (1912) for a crystal to a quasicrystal to cover the phonon as well as the phason we have

$$g(\nu)\,\mathrm{d}\nu = B\nu^2\,\mathrm{d}\nu \tag{14}$$

in which

$$B = 4\pi V \left(\frac{1}{c_1^3} + \frac{1}{c_2^3} + \frac{1}{s_1^3} + \frac{1}{s_2^3} \right) \tag{15}$$

V represents the volume of the material and c_1, c_2, s_1 and s_2 are defined by (12) respectively.

As a special case, i.e. where the phason field is absent, $K_i = R_i = 0$, and the material reduces to conventional isotropic matter, $C_{11} = \lambda + 2\mu$, $C_{11} - C_{12} = 2\mu$, $C_{44} = \mu$ in which λ and μ are the Lamé constants, then $s_1 = c_2$, $s_2 = 0$, the relevant vibration component with s_2 does not exist, in this case, c_1 and c_2 are the speeds of the longitudinal and transverse waves of the conventional crystal, then equation (15) reduces to that corresponding to the classical Debye model (1912), i.e.,

$$B = B' \equiv 4\pi V \left(\frac{1}{c_1^3} + \frac{2}{c_2^3} \right). \tag{16}$$

This check shows that the result of the present work is in exact agreement with those of the well known Debye model in the classical case.

Considering the total number of degrees of freedom should be finite, there is a maximum frequency ν_D, i.e., (13) will be rewritten as

$$\int_0^{\nu_D} g(\nu)\,\mathrm{d}\nu = 3N. \tag{17}$$

Substituting (14) into the above formula leads to

$$\nu_D^3 = 9N/B. \tag{18}$$

The lattice vibration of the quasicrystal is assumed to be quantized and an effective average energy $\epsilon(\nu)$ corresponding to frequency ν introduced; then the total energy is

$$E = E_0 + \sum \bar{\epsilon}(\nu) = E_0 + \int_0^{\nu_D} \bar{\epsilon}(\nu) g(\nu)\,\mathrm{d}\nu \tag{19}$$

where E_0 is a constant and

$$\bar{\epsilon}(\nu) = \frac{h\nu}{\mathrm{e}^{h\nu/kT} - 1} \tag{20}$$

h and k are the Planck constant and Boltzmann constant, T the absolute temperature, respectively.

According to the definition of specific heat

$$c_V = (\partial E/\partial T)_V$$

and formulae (19), (20) and (14) we obtain

$$\frac{c_V}{k} = B \int_0^{\nu_D} \left(\frac{h}{kT}\right)^2 \frac{\mathrm{e}^{h\nu/kT} \nu^4\,\mathrm{d}\nu}{(\mathrm{e}^{h\nu/kT} - 1)^2} \tag{21}$$

in which B is given by (15). Formula (21) gives the analytic interpretation of the specific heat of a one-dimensional hexagonal quasicrystal, which can also be written as

$$\frac{c_V}{3Nk} = 4D(x) - \frac{3x}{\mathrm{e}^x - 1} \tag{22}$$

where

$$D(x) = \frac{3}{x^3} \int_0^x \frac{y^3\,\mathrm{d}y}{\mathrm{e}^y - 1} \tag{23}$$

is the Debye function and

$$x = \frac{h\nu_D}{kT} = \frac{\Theta}{T} \qquad \Theta = \frac{h\nu_D}{k} \qquad y = \frac{h\nu}{kT}. \tag{24}$$

Here Θ is understood as the generalized Debye characteristic temperature for a quasicrystal, which can be evaluated as follows

$$\Theta = \frac{h}{k}\nu_D = \frac{h}{k}\left(\frac{9N}{B}\right)^{1/3} = \frac{h}{k}\left(\frac{9N}{4\pi V}\right)^{1/3} \frac{1}{\chi^{1/3}} \tag{25}$$

with

$$\chi = \frac{1}{c_1^3} + \frac{1}{c_2^3} + \frac{1}{s_1^3} + \frac{1}{s_2^3} = \rho^{3/2} \left\{ \frac{1}{(C_{11})^{3/2}} + \frac{1}{[(C_{11} - C_{12})/2]^{3/2}} + \frac{1}{\varepsilon_1^{3/2}} + \frac{1}{\varepsilon_2^{3/2}} \right\}. \tag{26}$$

The preceding result on the specific heat of a one-dimensional hexagonal quasicrystal is an extension of the Debye theory of crystals. It is well known that the Debye theory of specific heat of crystals is based on the elastic continuous model, which is a phenomenological theory;

it does not involve any concrete crystal structure. The basic parameters in the Debye formula connected with the crystal elasticity are only the speeds c_1 and c_2 of the elastic longitudinal and transverse waves of the medium. The scope of this study lies in extending the Debye phenomenological model to include certain contributions from the quasiperiodicity of the material to the specific heat. The generalized Debye formula (21) (or (22)) contains speeds c_1, c_2, s_1 and s_2, which reflect the behaviours of the elastic vibration and wave propagation of a one-dimensional hexagonal quasicrystal; these are quite different from those of crystals.

We emphasize once again that in the sense of the continuous medium model frame this letter has taken into account the contribution of the phason field and the coupling between the phonon field and phason field to the specific heat i.e., the effect of the quasiperiodicity of the material has been considered. Of course, it is a phenomenological and approximate theory, because the Debye theory is also a phenomenological and approximate theory even for the simple crystal structure.

The assumption of $\partial()/\partial x_3 = 0$ implied in formula (1) in this paper is only a mathematical simplification; this does not eliminate the effect of quasiperiodicity. If we do not make this assumption, the mathematical manipulation is quite complicated, which is not necessary in understanding the specific heat of quasicrystals.

This letter to some extent is an application of the elastodynamics of a one-dimensional hexagonal quasicrystal developed by the author and his coworkers (Fan *et al* 1999) to a thermal property of the solid. The results on thermodynamics of the material connected with the present study will be reported in another paper (Fan 1999).

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