Stability conditions for quasicrystals

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The stability conditions for quasicrystals may, depending on the symmetry of the quasicrystals, include properties which do not appear in the equations of mechanics.

The stability conditions in the mechanics of solids (the vector displacement field), liquid crystals (the nematic rotation field), and magnetic materials (the spin-flip field) are usually expressed in terms of constants which appear in the dynamic equations. In the cases of liquid crystals and magnetic materials, a stability analysis reduces to the requirement that the energy of nonuniform states be positive definite. The equivalent condition in elastic theory is that the squares of sound velocities be positive (§22 in Ref. 1). The latter condition is weaker than the condition for stability with respect to uniform deformations (§4 in Ref. 1). In quasicrystals, on the other hand, there may be special cases in which new properties appear in the stability conditions.

Following the general procedure for constructing a mechanics of quasicrystals,[2] we will demonstrate this effect in the simplest possible quasicrystal structure: a 2D quasicrystal with an eightfold axis. The symmetry of the structure is determined by the set of Fourier components of the spatial modulation of the density function $\rho(\vec{r})$:

$$\rho(\vec{r}) = \rho_0 + \Sigma|\rho_{\vec{k}}|e^{i(\vec{k}\vec{r}-\varphi_{\vec{k}})}. \qquad (1)$$

Small deformations of the quasicrystal are described in this case by the four phase fields φ_1, φ_2, φ_3, and φ_4, which correspond to the fundamental modes, with the wave vectors of minimum magnitude, oriented at angles of $\pi/2$ and $\pi/4$ with respect to each other (since the density is real we have $\varphi_{\vec{k}} = -\varphi_{-\vec{k}}$).

We introduce the complex field

$$u_x + iu_y = \frac{a}{2\pi}(\varphi_1 + e^{i\pi/4}\varphi_2 + e^{i2\pi/4}\varphi_3 + e^{i3\pi/4}\varphi_4), \qquad (2)$$

which is transformed by a vector representation of the point symmetry group of the quasicrystal, C_{8v} (a quasicrystal class):

$$C_8(u_x + iu_y) = e^{i\pi/4}(u_x + iu_y); \quad \sigma_v(u_x + iu_y) = u_x - iu_y. \qquad (3)$$

Here a is the quasicrystal period, and σ_v is a reflection. The field

$$\xi + i\chi = \frac{a}{2\pi}(\varphi_1 + +e^{i3\pi/4}\varphi_2 + e^{i6\pi/4}\varphi_3 + e^{i9\pi/4}\varphi_4) \quad (4)$$

transforms in accordance with

$$C_8(\xi + i\chi) = e^{i3\pi/4}(\xi + i\chi); \quad \sigma_v(\xi + i\chi) = \xi - i\chi. \quad (5)$$

The components u_x and u_y constitute the displacement vector of the quasicrystal as a hole, while the quantities ξ and χ correspond to an internal motion. The energy of the elastic and phase deformation of the quasicrystal is

$$\begin{aligned} &\frac{\lambda}{2}u_{ii}^2 + \mu u_{ik}^2 + \lambda_1(\partial_x + i\partial_y)(\xi + i\chi)(\partial_x - i\partial_y)(\xi - i\chi) \\ &\qquad +\lambda_2(\partial_x + i\partial_y)(\xi - i\chi)(\partial_x - i\partial_y)(\xi + i\chi) \\ &+\lambda_3\{(\partial_x + i\partial_y)(\xi + i\chi)(\partial_x + i\partial_y)(\xi + i\chi) + \text{c.c.}\} \\ &+\lambda_4\{(\partial_x + i\partial_y)(u_x + iu_y)(\partial_x + i\partial_y)(\xi - i\chi) + \text{c.c.}\}. \end{aligned} \quad (6)$$

The two terms of a purely phase deformation (λ_1 and λ_2) differ by the invariant

$$\partial_x\xi\partial_y\chi - \partial_y\xi\partial_x\chi,$$

which reduces to a total derivative, so only the parameter $\lambda_1 + \lambda_2$ appears in the equations of mechanics of the quasicrystal. Nevertheless, a different combination appears in the boundary conditions and also in the energy of uniform deformations. Under conditions of stability with respect to nonuniform deformations, the combination of constants $\lambda_1 - \lambda_2$ does not appear. The actual stability conditions, found through a consideration of the energy of uniform deformations (in which case the quantities u_{ik}, $\partial_i\xi$, and $\partial_i\chi$ are constant), reduce to the system of inequalities

$$\lambda + \mu > 0: \quad \mu > 0; \quad \lambda_1 + 2\lambda_3 > 0; \quad \lambda_1 - 2\lambda_3 > 0; \quad \lambda_2 > 0; \quad \lambda_2\mu > 2\lambda_4^2.$$

The effect which we are discussing here also occurs in a crystal with a tenfold axis, which was analyzed in Ref. 2. Instead of the conditions given there, the following inequalities must hold:

$$\lambda + \mu > 0; \quad \mu > 0; \quad k_1 + k_2 > 0; \quad k_1 - k_2 > 0; \quad \mu(k_1 + k_2) > 2(k_3^2 + k_4^2).$$

In an icosahedral quasicrystal there are no invariants which reduce to a total derivative.

[1]L. D. Landau and E. M. Lifshitz, *Theory of Elasticity*, Pergamon, New York, 1970.
[2]D. Levin, T. C. Lubensky, S. Ostlund, *et al.*, Phys. Rev. Lett. **54**, 1520 (1985).

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