Elasticity and Dislocations in Pentagonal and Icosahedral Quasicrystals

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Theories for elasticity and dislocation defects in two-dimensional pentagonal and three-dimensional icosahedral quasicrystals are presented.

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Though regular periodic crystals with pentagonal symmetry in dimension $d=2$ and icosahedral symmetry in dimension $d=3$ cannot exist, there are both theoretical[1] and experimental[2] reasons to believe that "quasicrystals" with such symmetries can. In this paper, we identify the hydrodynamic variables describing low-energy, long-wavelength fluctuations about these ideal ordered quasicrystalline states and characterize their topological defects (dislocations). We also compute the elastic energy associated with the hydrodynamic variables. From the form of the elastic energy, we conclude that, just as in conventional crystals, the Debye-Waller factor is nonzero in three dimensions and vanishes as an inverse power of the size of the system in two dimensions. We find that topological excitations analogous to dislocations do exist in quasicrystals. The Burgers-vector lattice is, however, a $2\times d$ dimensional lattice which is distinct from the d-dimensional real-space lattice of atomic positions.

Quasicrystals, as opposed to conventional crystals, are materials with two or more incommensurate length scales. As defined in Ref. 1, quasicrystals fall into two classes. In the first class, which includes the pentagonal and icosahedral examples, the rotational symmetry corresponds to a disallowed crystal symmetry and determines a unique ratio of incommensurate length scales that defines the structure. In the second case, the rotational symmetry corresponds to an allowed crystal symmetry, and many different sets of incommensurate length scales are possible. We will reserve the term quasicrystal for the former case and the more conventional term "incommensurate crystal" for the latter. In pentagonal and icosahedral quasicrystals, as in incommensurate crystals with two length scales, there are twice as many hydrodynamic variables as in conventional crystals. In quasicrystals, as distinct from incommensurate crystals, however, the additional variables cannot be interpreted as displacements or relative displacements of any of the incommensurate sublattices. A physical consequence is that a dislocation cannot be interpreted as the insertion (or removal) of a layer of atoms.

The density $\rho(\mathbf{r})$ of any of these translationally ordered phases P can be expanded in a Fourier series

$$\rho(\mathbf{r})=\sum_{\mathbf{G}\in L_R}\rho_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{r}}, \tag{1}$$

where L_R is the reciprocal lattice associated with P. Because the vector $\mathbf{G}_\alpha+\mathbf{G}_\beta$ is in L_R if $\mathbf{G}_\alpha$ and $\mathbf{G}_\beta$ are, there is a minimal set containing N_R vectors $\mathbf{G}_\alpha$ from which L_R can be constructed. In periodic crystals, $N_R=d$. In quasicrystals and incommensurate crystals, $N_R=n_i d$, where n_i is the number of relatively incommensurate lengths. Each $\rho_{\mathbf{G}}$ is a complex number with an amplitude $|\rho_{\mathbf{G}}|$ and a phase $\phi_{\mathbf{G}}$. Since $\rho(\mathbf{r})$ is real, $\rho^*_{\mathbf{G}}=\rho_{-\mathbf{G}}$ and, hence, $\phi_{\mathbf{G}}=-\phi_{-\mathbf{G}}$. The phase P is characterized by nonvanishing $|\rho_{\mathbf{G}}|$. Thus P and phase transitions to and from it can be described in terms of a phenomenological Landau free energy F that can be expanded in a power series in $\rho(\mathbf{r})$.[3] In the expansion of F in the phase P, the kth power of $\rho(\mathbf{r})$ gives rise to terms of the form

$$\prod_{a=1}^{k}\rho_{\mathbf{G}_a}+\text{c.c.}\sim\cos\Big(\sum_{a=1}^{k}\phi_{\mathbf{G}}\Big),$$

where $\sum_{a=1}^{k}\mathbf{G}_a=0$. Minimization of F with respect to all $\phi_{\mathbf{G}}$'s leads to a minimum-energy state with constraints among the $\phi_{\mathbf{G}}$'s. These constraints leave unspecified N_R $\phi_{\mathbf{G}}$'s which are the hydrodynamic variables of the theory. Once an appropriate representation for these $\phi_{\mathbf{G}}$'s has been found, elastic distortions and dislocations in the lattice can be discussed in terms of spatially varying phases $\phi_{\mathbf{G}}(\mathbf{r})$.

Before considering systems with pentagonal symmetry, let us review briefly the more familiar case of hexagonal symmetry. In this case, the six vectors $\mathbf{G}_n=G[\cos(2\pi n/6),\sin(2\pi n/6)]$ determine the sixfold symmetry and generate the reciprocal lattice. G which has units of inverse length, sets the unique length scale of the system. By the reality constraint on ρ, we can restrict our attention to the three vectors $\mathbf{G}_n=G[\cos(2\pi n/3),\sin(2\pi n/3)]$, $n=0,1,2$. These vectors are not, however, independent because $\sum_n\mathbf{G}_n=0$, and any two of them can be used to con-

struct L_R. Thus, in the minimum-energy state, the phases ϕ_n associated with $\mathbf{G}_n$ satisfy $\sum_n \phi_n = \gamma = \text{const}$, leaving two ($n_i = 1$, $N_R = d = 2$) independent components of ϕ_n which can be parametrized by the two-component vector $\mathbf{u}$ via

$$\phi_n = \mathbf{G}_n \cdot \mathbf{u} + \gamma/3. \tag{2}$$

$\mathbf{u}$ is a hydrodynamic variable whereas γ is not.

The Burgers-vector lattice is the lattice of displacements $\mathbf{u}$ that leave the ϕ_n's invariant modulo 2π. It can be obtained from the reciprocal lattice by constructing vectors $\mathbf{R}_n = R[-\sin(2\pi n/3), \cos(2\pi n/3)]$ that are perpendicular to $\mathbf{G}_n$. The length R is then chosen so that $\mathbf{G}_n \cdot \mathbf{R}_m$ is zero if $n = m$, 2π if $m = \langle n+1 \rangle_3$, and -2π if $m = \langle n-1 \rangle_3$. (Here and in what follows, we will use the symbol $\langle n \rangle_p$ to mean n mod p.) From this we obtain $R = 2\pi/[G\sin(2\pi/3)]$. The set of vectors formed from arbitrary linear combinations (with integer coefficients) of the $\mathbf{R}_n$'s form the Burgers-vector lattice. Here, in the case of all conventional crystal lattices, the Burgers-vector lattice constructed in this way is equivalent to the direct (real-space) lattice. As we shall see, this will not be true in the cases studied below.

The extension of the above treatment to lattices with pentagonal symmetry is straightforward. (Note that the reciprocal lattice must have tenfold symmetry.) In place of the three vectors of the hexagonal lattice, there are now five vectors, $\mathbf{G}_n = G \times [\cos(2\pi n/5), \sin(2\pi n/5)]$, $n = 0, \ldots, 4$, and associated phases ϕ_n. This lattice is fundamentally incommensurate because the ratio of the magnitudes of the collinear vectors $\mathbf{G}_0$ and $\mathbf{G}_1 + \mathbf{G}_4$ is not rational. As in the hexagonal case, $\sum_n \mathbf{G}_n = 0$ and $\sum_n \phi_n = \gamma$. We can parametrize the four ($n_i = 2$, $N_R = 2d = 4$) independent components of ϕ_n with two two-component fields $\mathbf{u} = (u_x, u_y)$ and $\mathbf{v} = (v_x, v_y)$ via

$$\phi_n = \mathbf{G}_n \cdot \mathbf{u} + a\mathbf{G}_{\langle 3n \rangle_5} \cdot \mathbf{v} + \gamma/5, \tag{3}$$

where a is an arbitrary scale factor to be chosen later. Note that a cyclic permutation $\phi_n \rightarrow \phi_{\langle n+1 \rangle_5}$ is equivalent to a rotation of $\mathbf{u}$ by $2\pi/5$ and $\mathbf{v}$ by $6\pi/5$. As usual, a spatially constant $\mathbf{u}$ describes uniform translations of the lattice whereas a constant $\nabla \times \mathbf{u}$ describes uniform rotations of the lattice. A spatially uniform $\mathbf{v}$ destroys the tenfold symmetry of the origin as can be seen in Fig. 1.

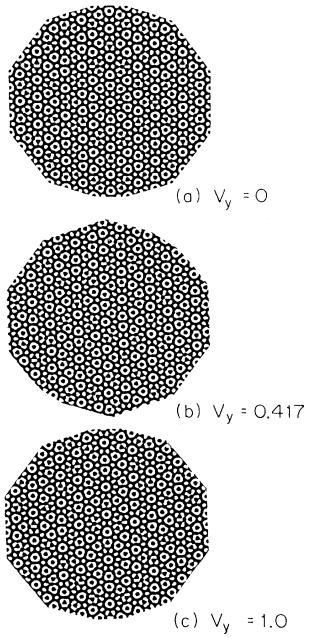

FIG. 1. A sequence of figures (a)–(c) illustrates the effect of adding a phase determined by $(u, v) = (0, 0, 0, v_y)$. For small values of v_y, the tenfold symmetry of the origin is destroyed, and no new center of symmetry is produced. When v_y attains R, the pattern becomes symmetric about a new symmetry center, displaced from the original center. To see that tenfold symmetry has been destroyed in (b), it is useful to look at the sequence of fivefold star patterns away from any apparent center of symmetry.

Since there are four independent ϕ_n's, it is natural to introduce a four-dimensional lattice B_R^4 spanned by the vectors $\tilde{\mathbf{G}}_n \equiv \mathbf{G}_n \oplus a\mathbf{G}_{\langle 3n \rangle_5}$ with components $(\tilde{\mathbf{G}}_n)_\alpha$, $\alpha = 1, \ldots, 4$. Then

$$\phi_n = \tilde{\mathbf{G}}_n \cdot \tilde{\mathbf{u}} + \gamma/5, \tag{4}$$

where $\tilde{\mathbf{u}} = \mathbf{u} \oplus \mathbf{v}$. The vectors $\tilde{\mathbf{G}}_n$ satisfy $\sum_n \tilde{\mathbf{G}}_{n\alpha} \cdot \tilde{\mathbf{G}}_{n\beta} \sim \delta_{\alpha\beta}$. Associated with B_R^4 is a Burgers-vector lattice B^4 constructed in analogy with the hexagonal case. First define the vectors $\mathbf{R}_n = R[-\sin(2\pi n/5), \cos(2\pi n/5)]$ orthogonal to the vectors $\mathbf{G}_n$, and from these construct the four-dimensional vector $\tilde{\mathbf{R}}_n \equiv \mathbf{R}_n \oplus b\mathbf{R}_{\langle 3n \rangle_5}$, where b is an arbitrary scale factor. Then we have

$$\phi_{n,m} \equiv \tilde{\mathbf{G}}_n \cdot \tilde{\mathbf{R}}_m = GR\{\sin[2\pi(n-m)/5] + ab\sin[6\pi(n-m)/5]\}. \tag{5}$$

By construction, $\phi_{n,n} = 0$. R, a, and b are determined by requiring $\phi_{n,(n+2)} = -\phi_{n,(n+3)} = 2\pi$ and $\phi_{n,(n+1)} = \phi_{n,(n+4)} = 0$. This yields

$$GR = 8\pi\sin(4\pi/5)/5, \quad ab = \sin(2\pi/5)/\sin(4\pi/5). \tag{6}$$

Thus the length R is fixed by G but only the product ab is fixed. Different values of a and b subject to the constraint (6) can be chosen. For the present purpose, we wish to make the Burgers-vector lattice as simple as possi-

ble, and so we choose $b=1$. In this case, the vectors $\tilde{\mathbf{R}}_n$ point to the five vertices of a simplex inscribed in a sphere of radius $\sqrt{2}R$ in four dimensions as can be seen by calculating $\tilde{\mathbf{R}}_n \cdot \tilde{\mathbf{R}}_m = R^2(5\delta_{nm} - 1)/2$. Since there are four independent $\tilde{\mathbf{R}}_n$'s in a four-dimensional space, it is clear that L_R is a regular periodic lattice with a Wigner-Seitz unit cell constructed in the usual way. For this choice of b, the vectors $\tilde{\mathbf{G}}_n$ do not point to the vertices of a simplex in reciprocal space so that the unit cells in B^4 and B_R^4 are not equivalent. The Burgers-vector lattice and the direct quasicrystal lattice have different dimensions and are, thus, completely inequivalent.

The Burgers-vector lattice just constructed contains no vector that lies either in the $\mathbf{u}=0$ or the $\mathbf{v}=0$ planes. The simplest physical consequence of this fact is that a dislocation does not correspond to the insertion (or removal) of a layer of atoms. In addition, a vector in the $\mathbf{u}=0$ subspace outside the Wigner-Seitz cell in B^4 can be reduced to a vector with a nonzero component in the $\mathbf{v}=0$ subspace via a translation by a Burgers vector. For example, a translation of the form $\mathbf{v}=(0,R)$ [i.e., $\tilde{\mathbf{u}}=(0,0,0,R)$] is equivalent to a translation in $\mathbf{u}$ of $(0,-R)$ because $\tilde{\mathbf{R}}_0=(0,-R,0,-R)$ is a Burgers vector (see Fig. 1). These properties are to be contrasted with those of conventional crystals and incommensurate lattices. In the former case, the Burgers-vector lattice is equivalent to the lattice of atomic positions, and a dislocation does correspond to an insertion of a layer of atoms. In the latter case, the Burgers-vector lattice is a direct sum of lattice displacements of the incommensurate sublattices comprising the crystal. Dislocations with elementary Burgers vectors can, therefore, be interpreted as an insertion of layer of atoms in one of the sublattices.

We have found it useful to study real-space patterns with tenfold symmetry and the effect on such patterns of translations and distortions in $\tilde{\mathbf{u}}$. The function

$$\rho(\mathbf{r}) = \sum_n \cos(\mathbf{G}_n \cdot \mathbf{r} + \mathbf{G}\cdot\mathbf{u} + a\mathbf{G}_{\langle 3n\rangle_5}\cdot\mathbf{v}), \qquad (7)$$

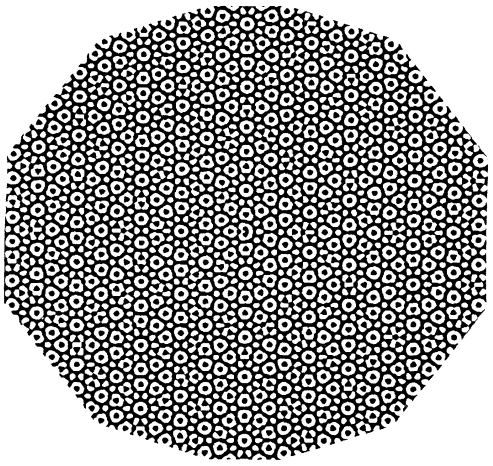

FIG. 2. A single dislocation with Burgers vector $\tilde{\mathbf{R}}_0+\tilde{\mathbf{R}}_2+\tilde{\mathbf{R}}_3$ has been inserted at the center of the figure. It is most easily seen by viewing the figure at grazing angle.

with a corresponding to $b=1$, was calculated on a grid of points $\mathbf{r}$. Pictures (Fig. 1) were then generated on a dot-matrix printer by printing a black dot at $\mathbf{r}$ if $\rho(\mathbf{r})>0$ and a white dot (unshaded) if $\rho(\mathbf{r})\leq 0$. For $v_y=R$, tenfold symmetry reappears at a new center translated by $\mathbf{r}=(0,-R)$ relative to the first, in agreement with the statements of the previous paragraph. In Fig. 2, we show a dislocation centered at the origin (center of the figure) with Burgers vector $\tilde{\mathbf{R}}_0+\tilde{\mathbf{R}}_2+\tilde{\mathbf{R}}_3$. This figure was generated by setting $\phi_0=0$ and $\phi_2=\phi_4=-\phi_1=-\phi_3=\tan^{-1}(y/x)$.

Constant $\mathbf{u}$ and $\mathbf{v}$ leave the energy of the system unchanged. One would, therefore, expect[4] the energy associated with nonuniform $\mathbf{u}$ and $\mathbf{v}$ to be described by an elastic free-energy quadratic in the first spatial derivatives of $\mathbf{u}$ and $\mathbf{v}$. From the known behavior of $\mathbf{u}$ and $\mathbf{v}$ under the discrete operations of the tenfold symmetry group, it is straightforward, with use of group theory, to construct all quadratic invariants involving $\partial_i v_j$ and $u_{ij}=\frac{1}{2}(\partial_i u_j+\partial_j u_i)$. In this way, we find an elastic energy density of the form

$$\begin{aligned} f_{\rm el} = {} & \tfrac{1}{2}\lambda u_{ll}u_{ii} + \mu u_{ij}u_{ij} + \tfrac{1}{2}K_1(\partial_i v_j)(\partial_i v_j) + K_2[(\partial_x v_x)(\partial_y v_y) - (\partial_y v_x)(\partial_x v_y)] \\ & + K_3[(u_{xx}-u_{yy})(\partial_x v_x + \partial_y v_y) + 2u_{xy}(\partial_x v_y - \partial_y v_x)] \\ & + K_4[2u_{xy}(\partial_x v_x + \partial_y v_y) - (u_{xx}-u_{yy})(\partial_x v_y - \partial_y v_x)], \end{aligned} \qquad (8)$$

where summation on repeated indices i and j is understood. Note that in the absence of dislocations, the term following K_2 reduces to zero after integration by parts leaving a totally isotropic $\mathbf{v}$-$\mathbf{v}$ elastic energy. In this case, stability requires $\mu>0$, $\lambda+\mu>0$, $K_1>0$, and $\mu K_1 > 2(K_3^2+K_4^2)$. The effective elastic energy that determines the mechanical properties of the system is a function only of the strains u_{ij} and is obtained by integrating out the $\mathbf{v}$ degrees of freedom. Isotropy of the $\mathbf{v}$-$\mathbf{v}$ elastic energy is essential if this effective elastic energy is to be isotropic (i.e., contain only two independent elastic constants).

The preceding treatment of tenfold symmetry in two dimensions is easily generalized to icosahedral symmetry in three dimensions. Here there are the six vectors pointing to the six vertices of an icosahedron in the upper half

plane. They can be written as follows

$$\mathbf{G}_1 = G(0,0,1); \quad \mathbf{G}_n = G[\sin\beta\cos(n-2)\theta,\ \sin\beta\sin(n-2)\theta, \cos\beta], \quad n=2,\ldots,6, \tag{9}$$

where $\theta = 2\pi/5$ and $\cos\beta = 5^{-1/2}$. There are six independent phases ($n_i = 2$, $N_R = 2d = 6$)ϕ_n which can be parametrized by two three-component fields $\mathbf{u}$ and $\mathbf{v}$ which can be normalized so that

$$\phi_n = \mathbf{G}_n \cdot \mathbf{u} + \mathbf{H}_n \cdot \mathbf{v}, \tag{10}$$

where

$$\mathbf{H}_1 = G(0,0,-1); \quad \mathbf{H}_n = G[\sin\beta\cos3(n-2)\theta,\ \sin\beta\sin3(n-2)\theta,\ \cos\beta], \quad n=2,\ldots,6. \tag{11}$$

A six-dimensional lattice can now be constructed from the direct sum of $\mathbf{G}_n$ and $\mathbf{H}_n$, the vectors $\tilde{\mathbf{G}}_n = \mathbf{G}_n \oplus \mathbf{H}_n$ with components $\tilde{\mathbf{G}}_{n\alpha}$, $\alpha = 1,\ldots,6$. Since there is no constraint on $\sum\phi_n$, Burgers vectors $\tilde{\mathbf{R}}_n$ in a six-dimensional Burgers-vector space B^6 can now be constructed by requiring $\phi_n = 2\pi$ and all other $\phi_k = 0$. We obtain

$$\tilde{\mathbf{R}}_{n\alpha} = \pi\tilde{\mathbf{G}}_{n\alpha}/G^2, \quad \tilde{\mathbf{R}}_n \cdot \tilde{\mathbf{R}}_m = (2\pi^2/G^2)\delta_{nm}. \tag{12}$$

Thus, the vectors $\tilde{\mathbf{R}}_n$ point to the vertices of a six-dimensional hypercube. Again no Burgers vector lies in the $\mathbf{v}=0$ or $\mathbf{u}=0$ subspaces. Thus, as before, dislocations do not correspond to insertion or removal of an extra layer of atoms, and vectors in the $\mathbf{u}\equiv 0$ plane acquire a nonzero component in the $\mathbf{v}=0$ subspace after translation into the Wigner-Seitz cell by a Burgers vector.

The elastic energy can be calculated by use of the known transformation properties of $\mathbf{u}$ and $\mathbf{v}$. There are two elastic constants coupling $\mathbf{u}$ to $\mathbf{u}$, two coupling $\mathbf{v}$ to $\mathbf{v}$, but only one coupling $\mathbf{u}$ to $\mathbf{v}$. We find

$$\begin{aligned} f_{\rm el} = {} & \tfrac{1}{2}\lambda u_{ii}u_{ii} + \mu u_{ij}u_{ij} + \tfrac{1}{2}K_1(\partial_i v_j)(\partial_i v_j) \\ & + \tfrac{1}{2}K_2[(\partial_z v_z)^2 - (\partial_x v_z)^2 - (\partial_y v_z)^2 - (\partial_z v_x)^2 - (\partial_z v_y)^2 \\ & \quad + 2(\partial_x v_x)(\partial_x v_z + \partial_z v_x) - 2(\partial_y v_y)(\partial_x v_z - \partial_z v_x) \\ & \quad - 2(\partial_x v_y)(\partial_y v_z + \partial_z v_y) - 2(\partial_y v_x)(\partial_y v_z - \partial_z v_y)] \\ & + K_3[(u_{xx} + u_{yy} - 2u_{zz})(\partial_z v_z) + (u_{xx} - u_{yy})(\partial_x v_x + \partial_y v_y + \partial_z v_x) \\ & \quad + 2u_{xy}(\partial_x v_y - \partial_y v_x - \partial_z v_y) + 2u_{xz}(\partial_x v_x + \partial_x v_z - \partial_y v_y) + 2u_{yz}(\partial_y v_z - \partial_x v_y - \partial_y v_x)]. \end{aligned} \tag{13}$$

Stability requires $\mu > 0$, $\lambda + 2\mu/3 > 0$, $K_1 - 2K_2 > 0$, $K_1 + K_2 > 0$, and $(K_1 + K_2)\mu > 3K_3^2$.

The elastic energies of Eqs. (8) and (13) are quadratic in the gradient operators and the fields $\mathbf{u}$ and $\mathbf{v}$. It follows from the equipartition theorem that $\langle \tilde{\mathbf{u}}_\alpha(\mathbf{q})\tilde{\mathbf{u}}_\beta(-\mathbf{q})\rangle \sim q^{-2}$, where $\langle\cdots\rangle$ signifies a thermodynamic average and $\mathbf{q}$ is a wave number. Thus, the Debye-Waller factor $\exp[-\tilde{\mathbf{G}}_\alpha\tilde{\mathbf{G}}_\beta\langle\tilde{\mathbf{u}}_\alpha(\mathbf{r})\tilde{\mathbf{u}}_\beta(\mathbf{r})\rangle/2]$ is nonzero in three dimensions and tends to zero as a power of the size of the sample in two dimensions as is the case in conventional crystals. Using the elasticity and dislocation theories presented here, it is straightforward to calculate the energies of isolated dislocations and the energies of interactions among dislocations. These energies are qualitatively similar to those of conventional crystals indicating that the quasicrystalline state is stable against the formation of dislocations. We have derived the equations governing the hydrodynamics of quasicrystals and find that there are d diffusive modes associated with $\mathbf{v}$ in addition to the modes found in conventional crystals.

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[4]In strongly coupled systems in one dimension, it is possible for the variable associated with relative motion of two incommensurate sublattices to become pinned and thus lose its hydrodynamic character [M. Peyrard and S. Aubry, J. Phys. C. **16**, 1593 (1983)]. We do not know if such pinning can occur in the quasicrystals discussed here.