One-harmonic structures in the two-dimensional incommensurate solids

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(Received 13 July 1981)

We compare the one-harmonic incommensurate configuration derived from the many-wall solution of the sine-Gordon equation with that found within the discrete model in the weak-pinning limit. We show explicitly that they coincide in the long-wavelength regime where there is no pinning and discuss the stability of the pinned short-wavelength deformations. General structure of the ground state and the experimental evidence of weak and strong pinning in periodically modulated superconductors are also discussed.

Experimental investigations of two-dimensionally (2D) modulated systems reveal a great variety of structures. Commensurate (C) and incommensurate (IC) phases have been observed in monolayers adsorbed on a crystal substrate[1] and in periodically modulated superconductors.[2,3] In the present paper we study the long period structures of the 2D solids on an anisotropic substrate at zero temperature. Let N particles be at the positions $\vec{r}_i$, weakly coupled to the substrate, which creates the periodic potential

$$U=\tilde{\epsilon}\sum_{i=1}^{N}\cos\vec{q}\cdot(\vec{r}_i-\vec{r}_0) \ , \tag{1}$$

where $\vec{q}$ is the modulation vector of the amplitude $q=2\pi/L$, $\vec{q}\cdot\vec{r}_0$ defines the phase with respect to modulation, and $\tilde{\epsilon}$ is the pinning energy per particle. We assume that the interaction $V(\vec{r}_j-\vec{r}_i)$ between the particles on a smooth substrate produces a hexagonal lattice. This "natural" lattice is not stationary on the anisotropic substrate except when they are commensurate, i.e., when $\vec{q}=\vec{g}$ (matching configurations), $2\vec{q}=\vec{g}$,. . . etc., where $\vec{g}$ is one of the reciprocal-lattice vectors.[4,5] However, the particle configuration may accommodate to the pinning potential by forming in the vicinity of each matching a C phase which is stationary for any value of the misfit $\vec{p}=\vec{q}-\vec{g}$.[4,6] For the simple commensurability this is a lattice of isoscelles triangles of height L; otherwise, it consists of rows of particles along each two, three, . . . , etc., potential minima lines. The domain of stability $p\leq p_c$ of the C phases is calculated in the weak-pinning (WP) limit by Pokrovsky and Talapov.[7]

Our aim is to study the IC phase which appears when $p>p_c$, comparing that found in the *continuum* model[7] with the one-harmonic solution of the *discrete* stationarity equations.[4,5] We show that these configurations coincide exactly when $p\gtrsim p_c$, except if p is very close to p_c. When p increases, the one-harmonic structure may persist as the ground-state configuration even in the short-wavelength regime $p\sim q$.

In the discrete model[4,5] the displacement $\Delta\vec{r}_i=\vec{r}_i-\vec{r}_i^{\,0}$ of each particle with respect to its original position $\vec{r}_i^{\,0}$ is approximated by a single harmonic

$$\Delta\vec{r}_i=\vec{u}\sin\vec{q}\cdot(\vec{r}_i^{\,0}-\vec{r}_0) \ , \tag{2}$$

where the amplitude $|\vec{u}|$ is assumed to be small compared to the substrate periodicity L. Physically, this means that the above approximation applies only when the pinning forces are much smaller than the restoring forces. The displacement field $\Delta\vec{r}_i$ is then determined by the linearized stationarity equations[4,5]

$$(\hat{D}\vec{u}-\tilde{\epsilon}\vec{q})\sin\vec{q}\cdot(\vec{r}_i^{\,0}-\vec{r}_0)=0 \ , \tag{3}$$

where $\hat{D}$ is the dynamical matrix with components

$$D_{\alpha\beta}=\sum_{i=1}^{N}\frac{\partial^2 V}{\partial X_i^{\alpha}\partial X_i^{\beta}}(1-\cos\vec{q}\cdot\vec{r}_i^{\,0}) \ . \tag{4}$$

X^{α}, $X^{\beta}(\alpha,\beta=1,2)$ denote the Cartesian coordinates in the system of the lattice (Fig. 1).

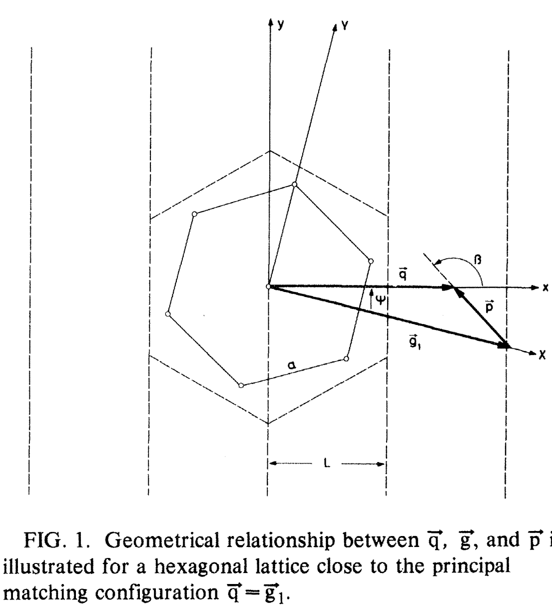

FIG. 1. Geometrical relationship between $\vec{q}$, $\vec{g}$, and $\vec{p}$ is illustrated for a hexagonal lattice close to the principal matching configuration $\vec{q}=\vec{g}_1$.

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The configuration obtained with (2) is stationary whenever $\sin\vec{q}\cdot(\vec{r}_i^{\,0}-\vec{r}_0)\neq 0$.[4] The gain of the potential energy (per unit area) associated with the harmonic distortion is[5]

$$\Delta E=-n\vec{u}\hat{D}\vec{u}(1-\delta_{2\vec{q},\vec{g}}\cos\vec{q}\cdot\vec{r}_0) \ , \qquad (5)$$

where n is the particle density.

In the above approximation the only pinned harmonic configurations are the so-called Bragg configurations,[5] obtained by distortion of the hexagonal lattice with $\vec{g}=2\vec{q}$. We do not go beyond this approximation since the pinning of a general C state drops rapidly with the order of commensurability.[7,8]

Let us now examine the behavior of the above solution in the vicinity of a given matching, taking as an example $\vec{q}=\vec{g}_1$. Assuming that p is small, $p/q\sim p/g<<1$, we explicitly calculate the components of $\hat{D}$ and $\vec{u}$ in the XOY system (Fig. 1). In this long-wavelength regime the dynamical matrix $D_{\alpha\beta}$ is related to the elastic deformation of the "natural" lattice. Using its periodicity in the reciprocal space

$$D_{\alpha\beta}(\vec{q}+\vec{g})=D_{\alpha\beta}(\vec{q})=D_{\alpha\beta}(\vec{p})$$

it is easy to show that for $p/g<<1$

$$D_{11}=D_{22}\approx\frac{1}{2n}(\lambda+3\mu)p^2 \ ,$$
$$D_{12}=D_{21}\approx-\frac{1}{2n}(\lambda+\mu)p^2 \ , \qquad (6)$$

where λ and μ are the usual Lammé coefficients of the hexagonal lattice in two dimensions.

The deformation amplitude components, given by Eq. (3), then become

$$u_X=\tilde{\epsilon}q\frac{D_{22}\cos\psi-D_{12}\sin\psi}{\det\hat{D}}\approx\frac{1}{2}\frac{q}{p^2}\frac{\epsilon}{\mu} \ ,$$
$$u_Y\approx u_X \ , \qquad (7)$$

where $\epsilon=n\tilde{\epsilon}$ and ψ is the rotation angle of the natural lattice with respect to the $\vec{q}$ axis (Fig. 1). The corresponding energy gain is

$$\Delta E=-\frac{n}{4}q^2\tilde{\epsilon}^2\frac{D_{11}\sin^2\psi-D_{12}\sin2\psi+D_{22}\cos^2\psi}{\det\hat{D}}$$
$$\approx-\frac{1}{8}\frac{q^2}{p^2}\frac{\epsilon^2}{\mu} \ . \qquad (8)$$

The divergence occurring in (7) and (8) when $p\to 0$ does not bother us, since we expect our IC phase to make sense only for p greater than $p_c\approx q(\epsilon/2\mu)^{1/2}$ as otherwise u_X would be greater than q^{-1}. Consequently, small p in the IC phase implies $(\epsilon/\mu)^{1/2}<<1$.

For p small, the rotation ψ is small as well, and in the minimum energy configuration[5]

$$\sin\psi\approx-\frac{p_X}{q}, \quad \cos\psi\approx 1 \qquad (9)$$

whereas the angle β between $\vec{q}$ and $\vec{p}$ vectors (cf. Fig. 1) is practically equal to $3\pi/4(g_1>q)$ or $7\pi/4(g_1<q)$, since

$$\sin^2\beta=\frac{1}{1+(q/g)^2}\approx\frac{1}{2} \ . \qquad (10)$$

With the same accuracy we find

$$p_X=p\cos(\beta+\psi)\approx\mp\frac{p}{\sqrt{2}} \ ,$$
$$p_Y=p\sin(\beta+\psi)\approx\pm\frac{p}{\sqrt{2}} \ . \qquad (11)$$

Thus the positions of the particles are

$$\vec{r}_i\approx\vec{r}_i^{\,0}\pm\vec{u}\sin\frac{p}{\sqrt{2}}(-X_i^0+Y_i^0) \ , \qquad (12)$$

where

$$\vec{r}_i^{\,0}=\{X_i^0,Y_i^0\}=\frac{a}{2}\{n_i\sqrt{3},m_i\}$$

and $\vec{u}$ is given by (7).

Until this point we have discussed the results of the discrete approach. One important difference between the discrete and continuum cases is that in the latter there is no rotation ($\psi=0$). Since $\vec{p}$ is taken to be collinear with $\vec{g}$, one in fact works in the coordinate system related to $\vec{q}=\vec{g}+\vec{p}$. In order to compare the results of the continuum model[7] with the above one-harmonic approximation, we write Eqs. (12) in coordinate system xOy, with Ox axis along $\vec{q}$

$$x_i\approx X_i^0-\frac{p_X}{q}Y_i^0\mp\frac{1}{2}\frac{q}{p^2}\frac{\epsilon}{\mu}\sin\frac{p}{\sqrt{2}}(X_i^0-Y_i^0) \ ,$$
$$y_i\approx Y_i^0+\frac{p_X}{q}X_i^0\mp\frac{1}{2}\frac{q}{p^2}\frac{\epsilon}{\mu}\sin\frac{p}{\sqrt{2}}(X_i^0-Y_i^0) \ . \qquad (13)$$

We now turn to the results of the continuum limit where the discrete lattice is treated as an elastic continuum with the Lammé coefficients λ and μ, whereas the pinning potential is taken as local.[7] When $\lambda>>\mu$, the IC phase consists of nearly registered regions, separated by the walls inclined at the angle $\theta\approx\pi/4$ with respect to the modulation axis. Using the nome expansion of the elliptic integral occurring in the phase of the displacement field[8,9] it can be shown that the particles are situated at[7,8]

$$x = x^0\left(1 - \frac{p_x}{q}\right) + \frac{2\pi}{\mathcal{P}}x' + \frac{4}{q}\sum_{s=1}^{\infty}\frac{Q^s}{s(1+Q^{2s})}\sin\frac{2\pi q x' s}{\mathcal{P}} ,$$

$$y = y^0\left(1 + \frac{p_x}{q}\right) + \frac{2\pi}{\mathcal{P}}x' + \frac{4}{q}\sum_{s=1}^{\infty}\frac{Q^s}{s(1+Q^{2s})}\sin\frac{2\pi q x' s}{\mathcal{P}} , \tag{14}$$

where

$$x' = -x^0\sin\theta + y^0\cos\theta \approx \frac{1}{\sqrt{2}}(-x^0 + y^0)$$

and the coordinates x^0 and y^0 correspond in the discrete picture to $x_i^0 = (a\sqrt{3}/2)n_i$, $y_i^0 = (a/2)m_i$, respectively. The nome $Q = \exp[-K'(k)/K(k)]$ and the wall density $|1/\mathcal{P}| = \pi/2l_0kK(k)$ are expressed[8,9] via the elliptic integrals $K'(k)$ and $K(k)$, where k runs from 1 (its value at the C-IC transition) to 0 and $l_0 = \pi\sqrt{2\mu/\epsilon}$. When $\lambda >> \mu$, k is related to p_x by the equation[7]

$$p_x = p_{xc}\frac{E(k)}{k} , \tag{15}$$

where

$$|p_{xc}| = |p_x(k=1)| \approx \frac{2}{\pi}\left(\frac{\epsilon}{\mu}\right)^{1/2} q . \tag{16}$$

Physically, one expects that the IC phase can be described by a single harmonic distortion when the distance between walls $|\mathcal{P}|$ is comparable to the wall width kl_0.[8] This occurs for small k, when $p_x \gtrsim p_{xc}$ and the nome Q is small (cf. Fig. 2). Using the asymptotic formula[9] for the elliptic integrals $E(k)$ and $K(k)$ valid for small k, we find

$$\frac{2\pi}{\mathcal{P}} \approx -\sqrt{2}\frac{p_x}{q} \tag{17}$$

$$Q \approx \frac{\pi^2}{64}\left(\frac{p_{xc}}{p_x}\right)^2 \tag{18}$$

$$x \approx x^0 - \frac{p_x}{q}y^0 + \frac{1}{4}\frac{\epsilon}{\mu}\frac{q}{p_x^2}\sin p_x(x^0 - y^0)$$

$$y \approx y^0 + \frac{p_x}{q}x^0 + \frac{1}{4}\frac{\epsilon}{\mu}\frac{q}{p_x^2}\sin p_x(x^0 - y^0) . \tag{19}$$

In the same limit the energy gain is

$$\Delta E \approx -\frac{1}{16}\frac{\epsilon^2}{\mu}\frac{q^2}{p_x^2} , \tag{20}$$

whereas the general result of the Ref. 7 in our notation is given by

$$\Delta E = \epsilon\left(1 - \frac{2}{k^2} + \frac{8}{\pi^2}\frac{E^2(k)}{k^2}\right) . \tag{21}$$

The comparison between (20) and (21) (see Fig. 2) shows a fairly good agreement when $p_x/p_{xc} \gtrsim 1.5$. Since $|p_{xc}|$ itself is assumed to be small, $|p_{xc}|/q \sim (\epsilon/\mu)^{1/2} << 1$, the one-harmonic IC configuration derived from the many-wall solution of the sine-Gordon equation may be compared to that found in the discrete case for p small. Comparing Eqs. (13) to (19) and (8) to (20) we see that they are identical if we take $p_x = \mp p/\sqrt{2}$ [cf. Eq. (11)]. A similar result is obtained in the 1D case in the WP limit.[8] One important difference is that in the 2D case there is a rotation of the whole ground-state configuration with respect to the modulation axis. This rotation is taken into account explicitly in the discrete case [via the terms linear in p_x/q in Eqs. (13)], whereas the continuum model it enters via the angle θ between the wall direction and $\vec{q}$ axis.

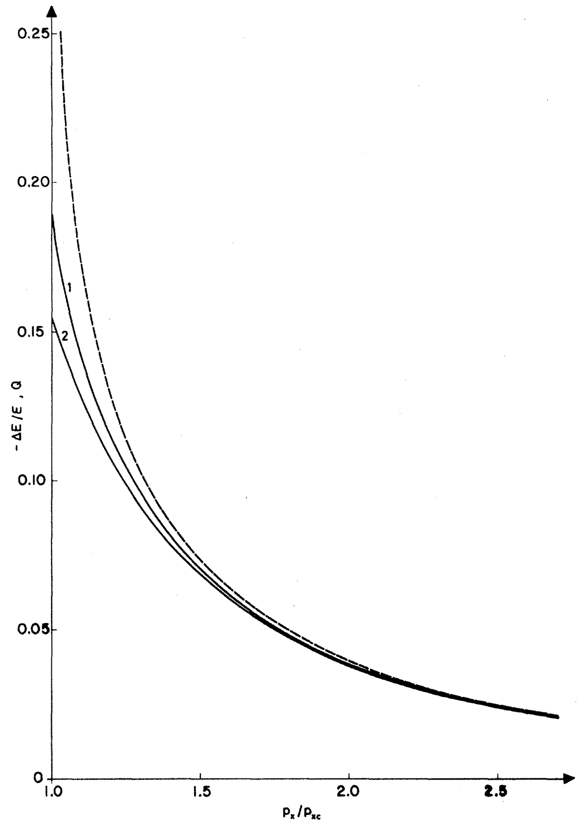

FIG. 2. The nome Q (dashed line) and the relative energy gain $-\Delta E/\epsilon$ (full lines) are plotted as functions of p_x/p_{xc}. Line 1 gives $-\Delta E/\epsilon$ according to Pokrovsky-Talapov theory, and line 2 shows the corresponding result of the single-harmonic approximation [Eq. (20)].

In the above calculation we obtained the one-harmonic approximation analytically when $p_x \gtrsim 1.5p_{xc}$. Actually, it can be used even much closer to p_{xc} since Q is considerably smaller than one when $p_x \gtrsim 1.1p_{xc}$ (cf. Fig. 2). This makes the whole picture of the ground state in the WP limit very simple. The strong nonlinearity of the problem causes the divergence of the linear solutions near the transition to the C phase but this nonlinear region is very narrow and the equilibrium configuration can be approximated reasonably well by the one-harmonic solution even close to p_c. In the short-wavelength region ($p \sim q$) some harmonic configurations (e.g., Bragg configurations) are pinned as we have seen. This is a consequence of the discrete nature of the lattice: in the simple version of the continuum theory[7] the walls separating the nearly commensurate regions do not "see" the substrate potential.[10] It is necessary to include the interaction between the fluctuating walls as well as their interaction with the substrate in order to reach the pinning transition.[10] The pinning of the Bragg configurations $2\vec{q} = \vec{g}$ (and of higher-order commensurabilities) may be seen experimentally in the WP case only, i.e., for ϵ/μ small. The domains of stability of the first-order commensurate phases are then narrow and do not cover the higher-order commensurabilities. Moreover, the stable Bragg configurations are only those with small distortion amplitude, $u < q^{-1}$. This condition, resulting from the force balance [Eq. (3)], is in fact very similar to the analycity-breaking criterion used by Aubry in his study of the 1D epitaxial problem.[11] If the pinning is strong enough, this requirement cannot be satisfied even far from the matching configurations, as can be seen from (3).

The above conclusions appear to be in accordance with recent numerical results by Bak,[12] for a similar model in one dimension, except for the absence of a chaotic phase between C and IC configurations. These chaotic regions, which become narrower as the pinning weakens, cannot be reached by the above analytic approach. However, they certainly may exist in the two-dimensional case, too. For the latter we expect that in the WP limit they are also narrow. Outside the first-order C phases and the adjacent chaotic phases, the equilibrium configuration can be obtained by rotation, translation, and harmonic distortion (including higher harmonics when necessary) of the original lattice.

Experimentally, both weak and strong pinning have been observed in periodically inhomogeneous superconductors,[2,3] where the shape of the critical current density curve as a function of magnetic field $j_c(H)$ reflects the nature of the pinned flux lines configurations. On the ground of a previous calculation[13] we find that in the experiments by Martinoli *et al.*[3] on thin superconducting films of modulated thickness ϵ/μ is very small. For the relevant parameter values in the experiment[3] and using the corresponding bulk value[14] for the shear moduls μ, we obtain $\epsilon/\mu \approx 0.01$. This is consistent with the experimentally observed weak pinning with narrow principal peaks and a broader Bragg peak.[3]

In the experiments by Raffy *et al.*[2] on superconducting alloys with modulated impurity concentration, high and broad principal peaks indicate the existence of strongly pinned C phases.[15] This is in accordance with our estimate of $\epsilon/\mu \sim 1$ in the relevant range of parameters,[2] in particular for the average Ginzburg-Landau parameter $\bar{\kappa}$ between 2 and 3. However, since ϵ is proportional to the free-energy density of flux lines[15] it decreases rapidly with the increasing $\bar{\kappa}$. Thus, we expect that the pinning in a modulated alloy with $\bar{\kappa} \sim 10$ would be similar to that observed by Martinoli *et al.*,[3] with Bragg structures more pronounced than in small $\bar{\kappa}$ alloys.

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