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Dislocation dynamics in a dodecagonal quasiperiodic structure

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We have developed a set of numerical tools for the quantitative analysis of defect dynamics in quasiperiodic structures. We have applied these tools to study dislocation motion in the dynamical equation given by Lifshitz and Petrich in 1997, the steady-state solutions of which include a quasiperiodic structure with dodecagonal symmetry. Arbitrary dislocations, parameterized by the homotopy group of the D-torus, are injected as initial conditions and quantitatively followed as the equation evolves in real time. We show that for strong diffusion the results for dislocation climb velocity are similar for the dodecagonal and the hexagonal patterns, but that for weak diffusion the dodecagonal pattern exhibits a unique pinning of the dislocation reflecting its quasiperiodic structure.

1. Introduction

It was realized long ago that dislocations play an important role in determining the mechanical properties of a crystal—whether periodic or not. As a consequence, ever since the discovery of quasicrystals much effort has been invested in the experimental and the theoretical study of their dislocations [1–3], leading to interesting observations such as the special role played by phasons in the motion of dislocations.

Here we study the behaviour of dislocations in a model system based on the dynamical equation of Lifshitz and Petrich (LP) [4], which is modification of the well-known Swift–Hohenberg (SH) equation [5]. The dynamics of the LP equation is relaxational, $\partial_t \rho = -\delta\mathcal{F}/\delta\rho$, driving a continuous two-dimensional density field $\rho(x, y, t)$ towards a minimum of a Lyapunov functional, or 'effective free energy',

$$\mathcal{F}\{\rho\} = \int dx\, dy \left(-\frac{\varepsilon}{2}\rho^2 + \frac{c}{2}\left[(\nabla^2+1)(\nabla^2+q^2)\rho\right]^2 - \frac{1}{3}\rho^3 + \frac{1}{4}\rho^4 \right), \tag{1}$$

yielding a dynamical equation of the form

$$\partial_t \rho = \varepsilon\rho - c(\nabla^2+1)^2(\nabla^2+q^2)^2\rho + \rho^2 - \rho^3. \tag{2}$$

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Among their results, LP showed that, if $q=2\cos(\pi/4)$, $q=2\cos(\pi/6)$, or $q=2\cos(\pi/12)$ and ε is sufficiently small, stable steady-state patterns are obtained (from random initial conditions) with long-range order and square, hexagonal or dodecagonal symmetry respectively. Although the LP equation cannot describe the dynamics of real solid-state quasicrystals and is probably more appropriate for soft matter or fluid phenomena such as Faraday waves, it offers a unique opportunity for the quantitative study of dislocations in a system (exhibiting both periodic and quasiperiodic long-range order) whose dynamics is exactly known.

2. Injection and tracking of dislocations

The Lyapunov functional $\mathcal{F}$ in equation (1) is clearly invariant under any translation or rotation of space. The steady-state solutions that are obtained are symmetry-broken ground states of $\mathcal{F}$, whose Fourier transform has the form

$$\rho(\boldsymbol{r}) = \sum_{\boldsymbol{k}\in L} \rho(\boldsymbol{k})\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{3}$$

where the (reciprocal) lattice L is a finitely generated $\mathbb{Z}$ module; that is, it can be expressed as the set of all integral linear combination of a finite number D of d-dimensional wave vectors. In the special case where D, called the rank of the structure, is equal to the physical dimension d, the structure is periodic.

Any particular ground state $\rho(\mathbf{r})$ of $\mathcal{F}$ is *indistinguishable* from a whole set of ground states that are related by so-called gauge transformations

$$\forall \boldsymbol{k} \in L: \quad \rho'(\boldsymbol{k}) = \mathrm{e}^{2\pi\mathrm{i}\chi(\boldsymbol{k})}\rho(\boldsymbol{k}), \tag{4}$$

where $\chi(\boldsymbol{k})$, called a *gauge function*, has the property that $\chi(\boldsymbol{k}_1+\boldsymbol{k}_2)=\chi(\boldsymbol{k}_1)+\chi(\boldsymbol{k}_2)$, possibly to within an additive integer, whenever $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ are in L. As described in detail by Dräger and Mermin [6], gauge functions form a vector space V^* of all real-valued linear functions on the lattice L. Because L has rank D, any linear function is completely specified by giving its values on D integrally independent lattice vectors. The space V^* is therefore a D-dimensional vector space over the real numbers. The space V^* contains, as a subset, all the integral-valued linear functions on L, denoted by L^*. Gauge functions in L^* leave the ground-state density invariant. Gauge functions that belong to the quotient space V^*/L^* take the ground stage described by ρ into a different and yet indistinguishable ground state described by some other density function ρ'. Thus, one can parameterize all the related ground states of $\mathcal{F}$ on a simple D-torus, namely the order parameter space V^*/L^*.

With this in mind we can easily construct a general dislocation in a two-dimensional periodic or quasiperiodic density. As we traverse in a loop around the position of the dislocation, say the origin, we locally change the ground state $\rho(\boldsymbol{r})$ by a gradually varying gauge function which winds around the ith direction of the D-torus n_i times and returns back to the original point. This is most readily accomplished by using an angle-dependent local gauge function $\chi_\theta(\boldsymbol{k})$ that assigns to the ith basis vector $\boldsymbol{b}^{(i)}$ of L the value $n_i\theta$. Thus, the most general dislocation is characterized by a set of D integers $(n_1,\ldots,n_D)$, which for a periodic crystal reduces

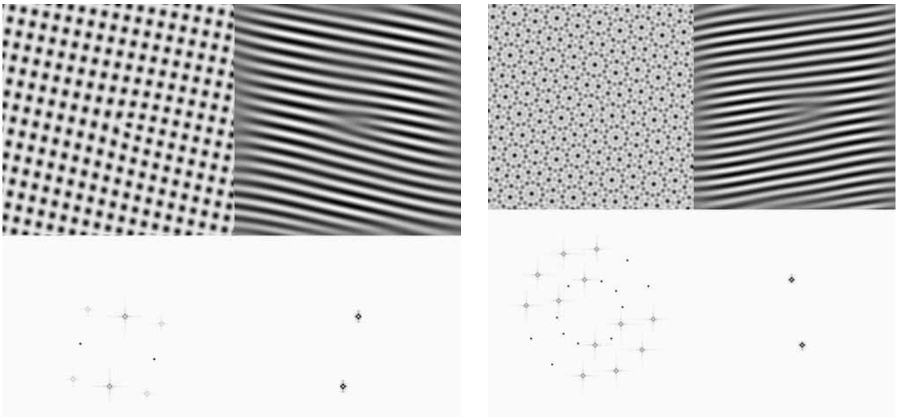

Figure 1. Top left (in both figures), snapshot of the numerical solution of the LP equation (2) showing a square and a dodecagonal pattern, a short time after a dislocation has been injected; bottom left, Fourier transform of the pattern (note the fuzzy Fourier coefficients, containing the information of the angle-dependent local gauge transformation); bottom right, a pair of filtered fuzzy Bragg peaks; top right, inverse Fourier transform of the filtered peaks showing the dislocation.

to the familiar d-dimensional Burgers vector. Not surprisingly, the set of all dislocations forms a rank-D $\mathbb{Z}$ module, the so-called homotopy group of the D-torus [7]. Examples of dislocations (injected in this manner into the square and dodecagonal ground states of the LP equation (2)) are shown in figure 1 after a short relaxation time.

Once injected into the structure, the positions of dislocations are tracked numerically, as demonstrated in figure 1, by filtering individual pairs of Bragg peaks in the Fourier transform and then performing an inverse Fourier transform to visualize the dislocations present in each individual density wave. This allows us to follow the positions of the dislocations in real time and to obtain quantitative measurements of their velocities as described below.

3. Dislocation dynamics under stress

We apply external stress on a structure containing a single dislocation by squeezing it in a particular direction and then allowing it to evolve under the dynamics of the LP equation. We quantify the amount of stress by the change δq in the wavenumber of the fundamental density wave in the direction of the applied stress, relative to its wavenumber in the relaxed steady-state density. We have calculated elsewhere [8], using the approaches of Siggia and Zippelius [9] and of Tesauro and Cross [10], that under such circumstances with the parameters used in our simulation the dislocation should climb with a velocity which is linear in the stress δq and is proportional to the parameter c, playing the role of a generalized diffusion coefficient. This should be contrasted with the fact that for dynamics governed by the SH equation [5] the climb velocity is proportional to $\delta q^{3/2}$.

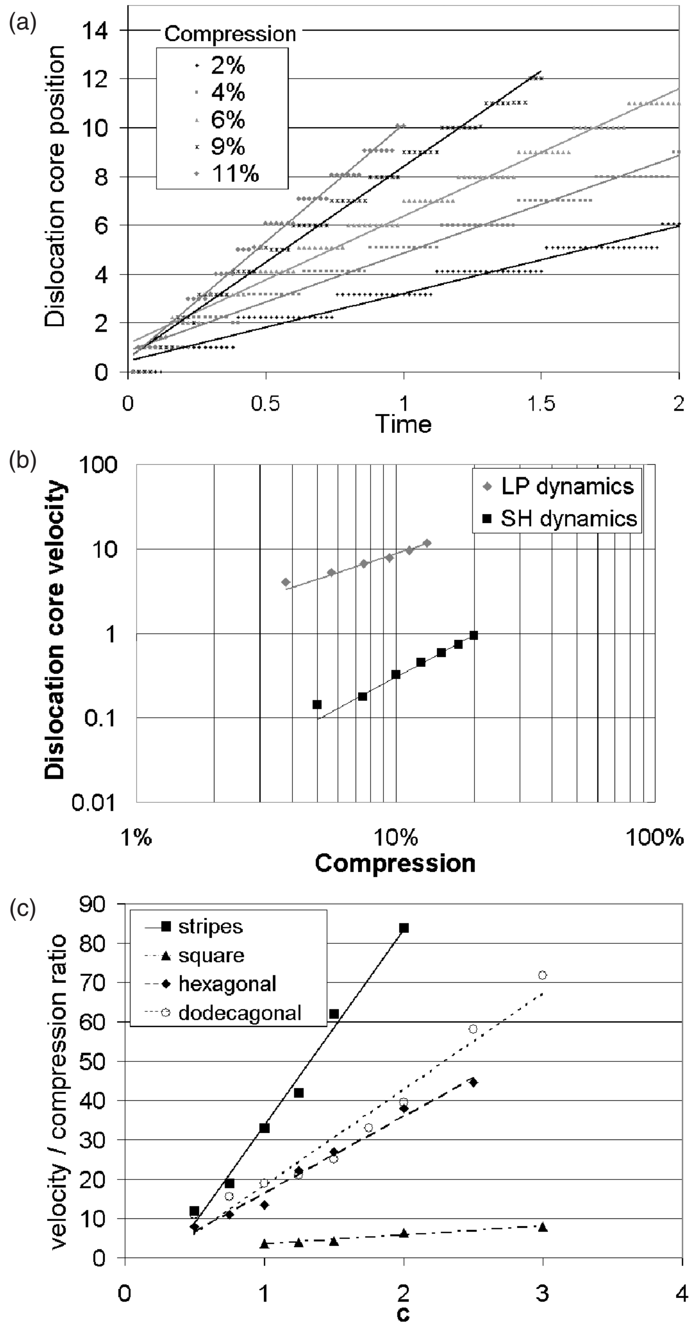

Figure 2. Measurement of dislocation climb velocity under stress for large values of the diffusion constant c. (a) Position of a dislocation core in a dodecagonal pattern as a function of time under LP dynamics; (b) Dependence of dislocation climb velocity on the applied stress, where $v \propto \delta q^{3/2}$ for SH dynamics, and $v \propto \delta q$ for LP dynamics; (c) Dependence of the dislocation climb velocity on the diffusion constant c under LP dynamics for different patterns.

Figure 2 summarizes our measurements of dislocation velocities obtained using the automatic numerical procedure for tracking the dislocation, described above. Figure 2(a) shows the position of a dislocation as a function of time for different values of stress δq, as measured under the dynamics of the LP equation for a dodecagonal pattern. For sufficiently large values of the diffusion constant c the dislocation climbs at a relatively constant speed, which indeed varies linearly with the applied stress, as shown in figure 2(b).

Figure 2(c) compares the measurements for different steady-state solutions of the LP equation. We find that the stripe pattern is the easiest for dislocation climb, with the climb velocity $v \approx 45c\,\delta q$, and that the square pattern is the most resistant, with $v \approx 3c\,\delta q$. Interestingly, the proportionality constants for the hexagonal and the dodecagonal patterns are very similar, with $v \approx 25c\,\delta q$. A possible explanation might be that the two triplets of wave vectors making up the dodecagonal pattern act independently as two hexagonal patterns during the climb process.

4. Dislocation dynamics under stress in the limit of weak diffusion

As the value of the diffusion constant c decreases, the local features of the pattern become important and the dislocation no longer climbs at a constant rate. In a periodic pattern, such as the square or the hexagonal densities, the motion of the dislocation nearly comes to a stop at regularly spaced positions, or pinning sites, as shown by the lower curve of figure 3. These sites correspond to positions where peaks in the density must first be annihilated before the dislocation can continue in its climb. In the quasiperiodic dodecagonal pattern a qualitatively different behaviour occurs in which the dislocation is pinned at irregular intervals, as shown by the upper curves of figure 3. It seems likely that, because the quasiperiodic pattern

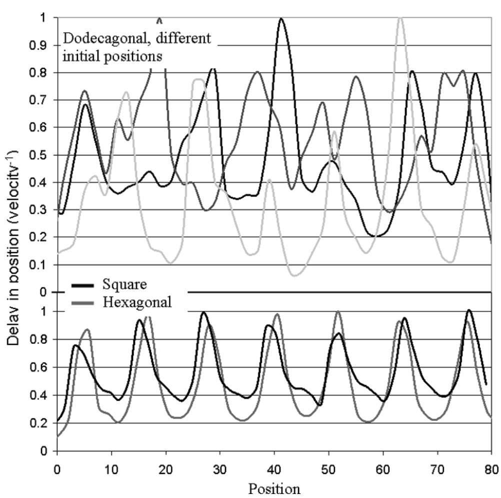

Figure 3. Periodic pinning of a dislocation in a square and a hexagonal pattern for a small value of the diffusion constant c (lower curve) and irregular pinning of a dislocation in a dodecagonal pattern due to the lack of periodicity (upper curves).

contains different local environments, the dislocation is more strongly pinned at certain sites than others, and these sites never quite repeat. This phenomenon has been observed in other models of dislocation motion by Mikulla *et al*. [11] and Fradkin [12].

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