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LETTER TO THE EDITOR

Continual dynamics of defects in thermal convection

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Abstract. Defect-phase dynamics is incorporated to obtain a coupled set of equations of motion for many topological defects (edge-type dislocations) in a Rayleigh-Bénard roll structure. An illustrative application of the theory is presented.

Rayleigh-Bénard instability provides a canonical example of a transition driven by a spatially homogeneous forcing in non-equilibrium systems: a spatially uniform conducting state becomes unstable at the threshold to a convective state with spatially periodic roll structure. In the idealised laterally infinite system, the overall position of the rolls and their orientation may be arbitrary. Therefore, the dynamics driven by spatial inhomogeneities above onset naturally involves the slowly varying variable, i.e. the phase variable (Pomeau and Manneville 1979), describing the position and orientation of the local roll structure. At the same time, the motion of topological defects, such as dislocations, disclinations and grain boundaries, is a prominent feature in the actual large-aspect-ratio system and seems to be playing an important role in the pattern evolution (Heutmaker *et al* 1985, Ahlers *et al* 1985, Pocheau *et al* 1985 and references therein). A method, the so-called defect-phase dynamics, to describe the combined dynamics of slow deformations of roll pattern and an isolated defect (or a small number thereof) in this pattern has recently been proposed and developed by us (Brand and Kawasaki 1984, Kawasaki 1984a, b, Shiwa and Kawasaki 1986). In this letter, this method is presented further to deal with the situation where a great number of defects† are present, where we also incorporate the method of Zippelius *et al* (1980).

We assume that there exists the phase variable, $\phi(\boldsymbol{r}, t)$, which is a slowly varying function of the horizontal coordinates, $\boldsymbol{r} \equiv (x, y)$, and time, t. Consider a set of N dislocations at a discrete set of points $\{\boldsymbol{R}^{(\nu)}\}$, $\nu = 1, 2, \ldots, N$, with 'charge' $\kappa^{(\nu)}$. The variable ϕ is multivalued in the presence of defects

$$\oint_{C^{(\nu)}} \nabla\phi \cdot \mathrm{d}\boldsymbol{l} = 2\pi\kappa^{(\nu)} \qquad \kappa^{(\nu)} = \pm 1 \tag{1}$$

where the integration is over a contour $C^{(\nu)}$ encircling the νth defect, and $\nabla = (\partial x, \partial y)$ throughout the letter.

In order to construct dynamic equations in the presence of moving dislocations, we first define a dislocation charge density,

$$\mathscr{B}(\boldsymbol{r}) = 2\pi \sum_{\nu} \kappa^{(\nu)} \delta(\boldsymbol{r} - \boldsymbol{R}^{(\nu)}).$$

† Here we consider only the edge-type dislocations.

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Hence,

$$\mathscr{B} = \hat{z} \cdot (\nabla \times \boldsymbol{Q}) \qquad \boldsymbol{Q} \equiv \nabla \phi$$

due to equation (1), $\hat{z}$ being the unit vector along the vertical z direction. Because dislocations can be created and/or destroyed only in pairs of opposite charge (sign) or at boundaries, we have a continuity equation

$$\partial_t \mathscr{B} = -\nabla \cdot \boldsymbol{J}$$

with a dislocation current, $\boldsymbol{J}$

$$\boldsymbol{J} = 2\pi \sum_{\nu} \kappa^{(\nu)} \dot{\boldsymbol{R}}^{(\nu)} \delta(\boldsymbol{r} - \boldsymbol{R}^{(\nu)})$$

where a dot denotes the time derivative. It then follows that

$$\partial_t \boldsymbol{Q} - \boldsymbol{J} \times \hat{z} = -\nabla \Xi.$$

Here $\Xi(\boldsymbol{r})$ is a single-valued function of position and is to be identified from the knowledge of phase dynamics in the absence of defects when $\boldsymbol{J} = 0$ (Zippelius *et al* 1980, Kawasaki 1984a). Thus, when the phase dynamic equation takes the form

$$\partial_t \phi = -\nabla \cdot \tilde{\boldsymbol{w}}$$

it gives the identification

$$\Xi = -\nabla \cdot \tilde{\boldsymbol{w}}.$$

To model the dislocation motion producing the current density $\boldsymbol{J}$, we consider a collection of N dislocations moving under a Peach–Koehler-type force (Kawasaki 1984a), $\boldsymbol{X}_l^{(\alpha)}(\boldsymbol{R}^{(\nu)}, t)$:

$$\dot{\boldsymbol{R}}^{(\nu)}(t) = \boldsymbol{\zeta}^{(\alpha)} \cdot \boldsymbol{X}_l^{(\alpha)}(\boldsymbol{R}^{(\nu)}) + \boldsymbol{\eta}^{(\nu)}(t). \tag{2}$$

Here, the superscript α distinguishes the sign of charge ($\alpha = \pm$) of the νth dislocation and a fluctuating noise source $\boldsymbol{\eta}$ is assumed to be Gaussian and white:

$$\langle \boldsymbol{\eta}^{(\nu)}(t) \boldsymbol{\eta}^{(\mu)}(t') \rangle = 2 k_B T \boldsymbol{\zeta}^{(\alpha)} \delta_{\mu\nu} \delta(t - t')$$

$\boldsymbol{\zeta}^{(\alpha)}$ being the defect mobility tensor, T the temperature and k_B the Boltzmann constant.

Now we may define the macroscopic dislocation charge density, $b(\boldsymbol{r}, t) \equiv \langle \mathscr{B} \rangle$, as the average of $\mathscr{B}$ over the microscopic random force $\boldsymbol{\eta}$, and it can be written as the difference of number densities of the dislocations, $\Gamma^{(\pm)}(\boldsymbol{r}, t)$, with opposite charges

$$b(\boldsymbol{r}, t) = 2\pi[\Gamma^{(+)}(\boldsymbol{r}, t) - \Gamma^{(-)}(\boldsymbol{r}, t)].$$

The defect dynamics (2) gives the Fokker–Planck-type equation obeyed by $\Gamma^{(\alpha)}$, $\alpha = \pm$, which is of the form

$$\partial_t \Gamma^{(\alpha)} = -\nabla \cdot \boldsymbol{j}^{(\alpha)} + P^{(\alpha)}$$

$$\boldsymbol{j}^{(\alpha)}(\boldsymbol{r}, t) = -\boldsymbol{\Delta}^{(\alpha)} \cdot [\nabla - (k_B T)^{-1} \boldsymbol{X}_l^{(\alpha)}(\boldsymbol{r}, t)] \Gamma^{(\alpha)}(\boldsymbol{r}, t). \tag{3}$$

Here $\boldsymbol{\Delta}^{(\alpha)} \equiv k_B T \boldsymbol{\zeta}^{(\alpha)}$ is a diffusion tensor of defects (the Einstein relation) and the second term on the right-hand side of (3) represents the drift of defects due to the local force exerted upon them; $P^{(\alpha)}$ is the production rate of α-type dislocations upon which conservation of b imposes the constraint

$$P^{(+)} = P^{(-)}.$$

Symmetry properties

$$\boldsymbol{X}_l^{(+)} = -\boldsymbol{X}_l^{(-)} \equiv \boldsymbol{X}_l$$

$$\boldsymbol{\zeta}^{(+)} = \boldsymbol{\zeta}^{(-)} \equiv \boldsymbol{\zeta} \qquad \boldsymbol{\Delta}^{(+)} = \boldsymbol{\Delta}^{(-)} \equiv \boldsymbol{\Delta}$$

then express $\boldsymbol{j} \equiv \langle \boldsymbol{J} \rangle = 2\pi(\boldsymbol{j}^{(+)} - \boldsymbol{j}^{(-)})$ as a function of b:

$$\boldsymbol{j} = 2\pi\rho_{\mathrm{D}}\boldsymbol{\zeta} \cdot \boldsymbol{X}_l - \boldsymbol{\Delta} \cdot \nabla b \tag{4}$$

where we have introduced the total dislocation density ρ_{D}

$$\rho_{\mathrm{D}}(\boldsymbol{r}, t) = \Gamma^{(+)}(\boldsymbol{r}, t) + \Gamma^{(-)}(\boldsymbol{r}, t).$$

Once supplemented with an equation of motion for ρ_{D}, the set of equations

$$\partial_t b + \nabla \cdot \boldsymbol{j} = 0$$

$$\partial_t Q = \boldsymbol{j} \times \hat{\boldsymbol{z}} + \nabla(\nabla \cdot \tilde{\boldsymbol{w}}) \tag{5}$$

and (4) constitutes a closed system of equations for macroscopic hydrodynamics in the presence of defects. In the following we illustrate its use by restricting ourselves to the simplest possible case.

We shall take up a canonical phase equation of Cross and Newell (1984):

$$\tau(Q)\partial_t\phi = -\nabla \cdot [\boldsymbol{Q}B(Q)] \tag{6}$$

where τ and B are known functions of Q. Equation (6) can be cast into a potential form when linearised in $\nabla\tilde{\phi}(\boldsymbol{r}) \equiv \boldsymbol{Q}(\boldsymbol{r}) - \boldsymbol{q}(\boldsymbol{r})$, where $\boldsymbol{q}$ is the local wavevector of the underlying periodic structure which may vary slowly in space, to yield

$$\tilde{\boldsymbol{w}} = D(\boldsymbol{q}) \cdot \nabla\tilde{\phi}.$$

Here the phase diffusion tensor $\boldsymbol{D}$ is obtained as

$$\boldsymbol{D}(q) = \tau(q)[D_\parallel(q)\hat{\boldsymbol{q}}\hat{\boldsymbol{q}} + D_\perp(q)(\boldsymbol{1} - \hat{\boldsymbol{q}}\hat{\boldsymbol{q}})] \qquad \hat{\boldsymbol{q}} \equiv \boldsymbol{q}/|\boldsymbol{q}|$$

$$D_\parallel(q) = -\mathrm{d}[qB(q)]/\mathrm{d}q\tau(q) \qquad D_\perp(q) = -B(q)/\tau(q).$$

Then, the local force is given by (Kawasaki 1984b)

$$\boldsymbol{X}_l = 2\pi\tilde{\boldsymbol{w}} \times \hat{\boldsymbol{z}}.$$

If we take the long-wavelength limit of (5), we find that

$$\partial_t\nabla\tilde{\phi} = -4\pi^2\rho_{\mathrm{D}}\hat{\boldsymbol{z}} \times \boldsymbol{\zeta} \cdot (\boldsymbol{D} \cdot \nabla\tilde{\phi} \times \hat{\boldsymbol{z}}).$$

Let us now assume that the defect motion is so slow that ρ_{D} can be taken to be conserved, and also we assume that defects are uniformly distributed over the sample. Then we may set $\rho_{\mathrm{D}}(\boldsymbol{r}, t) = \text{constant}$. Furthermore, we put $\hat{\boldsymbol{q}} = \hat{\boldsymbol{x}}$† so that $\boldsymbol{\zeta} = \zeta_\parallel\hat{\boldsymbol{x}}\hat{\boldsymbol{x}} + \zeta_\perp\hat{\boldsymbol{y}}\hat{\boldsymbol{y}}$. Consequently, we obtain

$$\partial_t\nabla^2\tilde{\phi} = -4\pi^2\rho_{\mathrm{D}}(\zeta_\perp D_\parallel\partial_x^2 + \zeta_\parallel D_\perp\partial_y^2)\tilde{\phi}$$

† This situation can be easily realised by using the thermal printing technique of Chen and Whitehead (1968). Alternatively, one may use a wedged sample (Prost *et al* 1984).

which yields the eigenfrequency of the mode with wavevector $\boldsymbol{k}$ ($\hat{k}_x \equiv k_x/k$, etc):

$$\omega = -\mathrm{i}4\pi^2\rho_{\mathrm{D}}(\zeta_\perp D_\parallel \hat{k}_x^2 + \zeta_\parallel D_\perp \hat{k}_y^2) \qquad 4\pi^2\rho_{\mathrm{D}} \gg k^2. \tag{7}†$$

This defect (phase) relaxation mode exhibits a 'critical slowing down' near either zigzag instability (when $\boldsymbol{k}\|\hat{\boldsymbol{y}}$) or Eckhaus instability ($\boldsymbol{k}\|\hat{\boldsymbol{x}}$). Of course, when there exists no defect, $\rho_{\mathrm{D}} = 0$, we recover the phase diffusion mode (Pomeau and Manneville 1979, Wesfreid and Croquette 1980, Croquette and Schosseler 1982),

$$\omega = -\mathrm{i}(D_\parallel k_x^2 + D_\perp k_y^2).$$

It might be worth pointing out a close analogy of the dispersion of (7) to that of a relaxation mode of free dislocations above the dislocation unbinding transition in two-dimensional melting (Zippelius *et al* 1980).

The generalisation of (7) to a more complicated configuration of dislocations would be very difficult: nothing has been assumed about the way dislocations are created and annihilated; moreover, for more general cases, the local nature of roll axis, $\boldsymbol{q}(\boldsymbol{r})$, cannot be neglected. Since the proposed set of coupled equations is able to treat such general features, we hope that efforts along this line will clarify the intriguing behaviour of defects in thermoconvective structures.

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† The quasistatic approximation we used for the dislocation motion is justified for $|\omega|^{-1}u \ll \rho_{\mathrm{D}}^{-1/2}$ where u is the average dislocation velocity, provided the creation of dislocations occurs on a time scale of comparable magnitude to one of annihilation, $\rho_{\mathrm{D}}^{-1/2}/u$. Replacing u by the climb velocity of an isolated dislocation, we estimate it as $u \sim (\tau_0^{1/2} q_0/\xi_0) D_\perp^{3/2}$ (Siggia and Zippelius 1981, Shiwa and Kawasaki 1986), $|\omega| \sim 4\pi^2\rho_{\mathrm{D}}\zeta_\parallel D_\perp$ with $D_\perp = (\xi_0^2/\tau_0)\ (\delta q/q_0)$ (see, e.g., Cross 1983). Here ξ_0 and τ_0 are coherence length and characteristic time of the convective layer without defects, and $\delta q = q - q_0$, q_0 being the critical wavenumber at the threshold. Then the above condition is rewritten as $(q_0/4\pi^2\zeta_\parallel)(\delta q/q_0)^{1/2} \ll \rho_{\mathrm{D}}^{1/2}$, which is expected to be well borne out near the convective threshold.