Dislocation motion in cellular structures

Y. Pomeau* and S. Zaleski

Groupe de Physique du Solide, Ecole Normale Supérieure, 24 Rue Lhomond, 75231 Paris, France

P. Manneville

DPh.G./PSRM, Centre d'Etudes Nucléaires Saclay, 91191 Gif-sur-Yvette, France (Received 10 March 1982)

The slow motions of cellular structures of parallel rolls are described by the amplitude equation in the weakly nonlinear domain. As this equation has a variational structure, the Peach-Köhler force exerted on a dislocation can be computed in the same way as for usual crystals. When the cellular structure is really described by variational equations, this force keeps its variational origin (it is the gradient of some energy) and vanishes for some optimal wave number. In thermoconvection in porous layers, this variational structure of the dynamics is lost at perturbative order beyond the one giving the usual amplitude equation. Therefore, the notion of an optimal wave number loses its meaning, and the quantity equivalent to the Peach-Köhler force does not vanish anymore at the wave number of marginal stability for perpendicular diffusion, contrary to what happens in variational systems where this condition defines the optimal structure. Another consequence of this nonvariational dynamics is the occurrence of gliding motion of dislocations in uniformly curved rolls, a situation where no Peach-Köhler force exists in variational systems.

I. INTRODUCTION

In crystals, the Peach-Köhler force¹ is one of the forces acting on dislocations. In two-dimensional layered structures under compression (positive pressure), this force tends to eliminate the supplementary layer ending at the dislocation. On the other hand, if the pressure is negative, the half infinite supplementary layer tends to grow under the Peach-Köhler force. Owing to this force (whatever its sense is) the dislocation gets a climb motion. The corresponding climb velocity is obtained by the balance between this force and various dissipative phenomena. This velocity has been computed by Siggia and Zippelius² within the framework of the amplitude equation.³ This amplitude equation describes parallel or nearly parallel rolls near the onset of Rayleigh-Bénard convection. As it has a variational structure, one may derive from it an energy per unit volume, a pressure, and finally an expression of the Peach-Köhler force. And, owing to this peculiar structure, this Peach-Köhler force and the perpendicular phase diffusion coefficient⁴ vanish at the same wave number of the underlying pattern. As noticed before,⁴ this vanishing of the perpendicular phase diffusion coefficient is associated with the "optimal wave number," that is precisely the one corresponding to the absence of external pressure. Of course, this "pressure" is a formal device and has no direct connection with the usual hydrostatic pressure. Its general formal expression is derived in Appendix A.

However, the existence of this variational structure is rather exceptional in the nonlinear dynamics of nonequilibrium phenomena, and one may expect that this picture deduced from the lowest-order amplitude equation changes when higher-order (and presumably nonvariational) corrections to this amplitude equation are considered. The origin of these corrections can be described as follows: Let ϵ be the control parameter. This is, for instance, the difference between the actual value of the Rayleigh number and its critical value for the onset of convection in an infinite layer heated from below. At $\epsilon = 0$, parallel rolls with wave number q_0 become marginally stable. In the supercritical domain ($\epsilon > 0$), a whole band of width of order $\epsilon^{1/2}$ becomes linearly unstable around q_0 . The amplitude equation is valid for wave numbers $q_0 + O(\epsilon^{1/2})$ whenever $0 < \epsilon \ll 1$. But various mechanisms of wave number selection limit^{5,6} the wave number of steady patterns to the range $q_0 + O(\epsilon)$ in slightly supercritical conditions. In this domain, supplementary terms must be accounted for in the amplitude theory and, in general, these new terms break the variational structure of the amplitude equation existing at its

27

This nonvariational structure of the amplitude equations (for free slip and rigid boundaries) was given by Siggia and Zippelius.⁷ These authors pointed out the importance of correction arising from the generation of vertical vorticity in Rayleigh-Bénard convection at finite Prandtl number. This vertical vorticity generates a long-wavelength horizontal flow. In slowly modulated rolls, the Reynolds stress tensor has a slowly modulated part, too, and this can be compensated by large-scale horizontal flows only.⁸ As this stress tensor is absent at infinite Prandtl number and for porous flows, this sort of phenomenon is absent in these situations.

In the present article, we consider the effect of these new terms on the motion of dislocations in two models of cellular structure. In Sec. II, we study a model proposed by Sivashinsky,⁹ with a "built-in" variational structure. We show by various arguments (perturbative and nonperturbative) that the Peach-Köhler force and the perpendicular diffusion coefficient vanish exactly at the same wave number for steady parallel rolls. In Sec. III, we study the climb of dislocations in rolls generated by thermoconvection in a porous layer of fluid. This model allows simple calculations near the onset of convection and corresponds to physically realizable experiments.¹⁰ Since it has no variational structure, vanishing of the Peach-Köhler force and of the perpendicular diffusion coefficients give uncorrelated conditions. Strictly speaking, no force exists in a nonvariational system since no energy is present. Nevertheless, in this model the absence of climb motion for a dislocation is equivalent to the vanishing of a quantity giving formally the Peach-Köhler force in the variational case, whence it makes sense to speak of Peach-Köhler force in this extended meaning.

Finally, we show in Sec. IV the existence of a gliding motion (perpendicular to the rolls) in nonvariational systems. If rolls are curved with a uniform radius of curvature, no Peach-Köhler force produces gliding in a variational system, as displacement perpendicular to the rolls does not change the energy. But such a motion exists in nonvariational systems, and one may even expect that gliding velocity may be substantially larger than the climb velocity in some situation.

II. DISLOCATION MOTION IN A VARIATIONAL MODEL

Sivashinsky⁹ has proposed a variational model for describing the slow fluctuations of a thermoconvective structure in a layer between two poorly conducting horizontal plates. The equation of this model is in a dimensionless form

$$A_t = -\frac{\delta \underline{V}}{\delta A} , \qquad (2.1a)$$

where $A_n \equiv (\partial A / \partial n)$ (n = x, y, t), A being a scalar function of time and horizontal position, and where $\partial V / \partial A$ is the Fréchet derivative of

$$\underline{V}[A] \equiv -\int dx \, dy \left[\frac{(\epsilon - q_0^4)}{2} A^2 + q_0^2 (\vec{\nabla} A)^2 - \frac{1}{2} (\Delta A)^2 - \frac{1}{4} (\vec{\nabla} A)^4 \right].$$

The explicit form of Eq. (2.1) is the nonlinear partial differential equation

$$A_{t} = [\epsilon - (\Delta + q_{0}^{2})^{2}]A + (A_{x}^{3})_{x} + (A_{y}^{3})_{y} + A_{xx}A_{y}^{2} + A_{yy}A_{x}^{2} + 4A_{xy}A_{x}A_{y} . \qquad (2.1b)$$

Any steady solution of (2.1b) makes the functional V[A] stationary. We do not worry hereafter in this work about "lateral" boundary conditions since we shall consider dislocations isolated in an (a priori) infinite structure (this may well be rather difficult to approach in real life experiments). In Appendix A, we derive some properties of this model, depending specifically on its variational formulation. In particular, this formulation allows one to derive shortly the Peach-Köhler force. This force moves a dislocation parallel to the roll in a structure of parallel rolls ("climbing motion"). If qis the wave number of this steady roll structure, then the Peach-Köhler force is proportional to $dV_{\rm per}/dq$, where $V_{\rm per}$ is the potential per unit length for a periodic solution.

In what follows, we give a "microscopic" derivation of the Peach-Köhler force; that is, we start from (2.1b) without utilizing explicitly the variational formulation. This is done with the goal of showing, in Sec. III, some new effects occurring in a nonvariational model, the difference being clearer at the level of the microscopic calculation. We want to study dislocations in a structure with a wave number close to the optimal one, making $\underline{V}[A]$ lower. If the wave number takes this optimal value, say q_{opt} , then the Peach-Köhler force vanishes and the dislocation stays at rest (in usual elasticity theory, this is indeed equivalent to the vanishing of the pressure or torsion exerted on the crystal structure). Near $\epsilon = 0_+$ and $q = q_{opt}$, we derive the climb velocity by expansion in ϵ and $\delta (\equiv q - q_{opt})$. It appears as a solvability condition for the equation of the complex amplitude. Near the onset of instability ($\epsilon \sim 0_+$), the rest state A=0 is linearly unstable against periodic perturbations A(x) with a wave number close to q_0 . As the bifurcation is normal or supercritical, a periodic steady state is reached such that

$$A = \frac{1}{2} (\chi e^{iq_0 x} + \chi^* e^{-iq_0 x}) + O(\epsilon^{3/2}) , \qquad (2.2)$$

where $\chi(\sim \epsilon^{1/2})$ is the complex amplitude, and the asterisk denotes the complex conjugation (we shall also denote the complex conjugation of the preceding expression by c.c.). Near $\epsilon = 0$, one gets by standard methods³ the amplitude equation for the slow variations of χ at order $\epsilon^{3/2}$.

It is enough to replace A in (2.1b) by its expansion (2.2) at first order, and then to retain terms as $e^{iq_0x}O(\epsilon^{3/2})$. One needs, at this order, the lowest-order term on the right-hand side of Eq. (2.2). The amplitude equation at next order, i.e., ϵ^2 , is derived in a similar way, still by using the lowest-order term in the right-hand side of Eq. (2.2):

$$\chi_t = \Lambda_1[\chi] \tag{2.3a}$$

with

$$\Lambda_{1}[\chi] \equiv \epsilon \chi + (2q_{0}\partial_{x} - i\partial_{y^{2}}^{2})^{2}\chi - \frac{3}{4}q_{0}^{4} |\chi|^{2}\chi .$$
(2.3b)

This is obtained by taking the order-of-magnitude estimates

$$\chi \sim \partial_x \sim \partial_{y^2}^2 \sim \epsilon^{1/2}$$

and $\partial_t \sim \epsilon$. In this way all terms in (2.3b) are of order $\epsilon^{3/2}$.

Equation (2.3a) has steady solutions in the form

$$\chi = a e^{i \delta x} \tag{2.4}$$

with

$$a(\delta) = \left[\frac{4}{3q_0^4}(\epsilon - 4q_0^2\delta^2)\right]^{1/2}.$$

Moreover, Eq. (2.3) has a variational structure, since

$$\chi_t = -\frac{\delta U_1}{\delta \chi^*}$$
 and

$$\chi_t^* = -\frac{\delta U_1}{\delta \chi}$$

with

$$U_1 = -\frac{1}{2} \int \left[\epsilon |\chi|^2 - |(2q_0\partial_x - i\partial_{y^2}^2)\chi|^2 - \frac{3}{8}q_0^4|\chi|^4 \right] dx \, dy \, .$$

From the equation of motion, U_1 , a real quantity, must necessarily decrease as

$$U_{1,t} = U_{1,\chi} \chi_t = -U_{1,\chi} U_{1,\chi}^*$$
.

In the absence of lateral boundaries, the minimum of U_1 is reached for $\delta = 0$, among all solutions (2.4) with $|\delta| \le (\epsilon/4q_0^2)^{1/2}$. Hence, as climb of dislocation amounts to replace a region with *n* rolls by a region with (n + 1) rolls, it changes the wave number. Thus, a stationary solution of (2.3) with a dislocation is possible if it is connected at infinity with a structure minimizing the potential U_1 with respect to the wave number variation.

Let χ_0 be the steady solution of (2.3) with a dislocation; that is, it verifies

$$\Lambda_1[\chi_0] = 0 \tag{2.5a}$$

with the (external) boundary conditions

$$\chi_0 \xrightarrow[(\mathbf{x},\mathbf{y}) \to \infty]{} a_0 e^{i\varphi(\mathbf{x},\mathbf{y})} .$$
 (2.5b)

 $a_0 \equiv a(\delta = 0), \varphi$ being such that

$$\oint_C d\vec{s} \cdot \vec{\nabla} \varphi = 2\pi , \qquad (2.5c)$$

where C is a closed curve encircling the dislocation.

Now, we shall find first the wave number δ such that the dislocation is still steady when higher-order terms are accounted for in the amplitude equation. This next-order amplitude equation reads, for steady states,

$$\Lambda_1[\mathcal{X}] + \Lambda_2[\mathcal{X}] = 0 , \qquad (2.6a)$$

where Λ_1 has been already defined in (2.3b), while

$$\Lambda_{2}[\chi] \equiv -4iq_{0}\chi_{x^{3}} - 2\chi_{y^{2}x^{2}} + 3iq_{0}^{3} |\chi|^{2}\chi_{x} - \frac{1}{2}q_{0}^{2} |\chi_{y}|^{2}\chi + \frac{3}{4}q_{0}^{2}\chi_{y}^{2}\chi^{*} - \frac{1}{4}q_{0}^{2}\chi_{yy}^{*}\chi^{2} + \frac{1}{2}q_{0}^{2}\chi_{yy} |\chi|^{2} + O(\epsilon^{5/2}).$$
(2.6b)

It can be verified that, if $\partial_x \sim \epsilon^{1/2} \sim \chi \sim \partial_{y^2}^2$, all terms in $\Lambda_2[\chi]$ are of order ϵ^2 . This form of $\Lambda_2[\chi]$ is obtained from the original equation (2.1b) by any standard method of derivation of the amplitude

equation carried up to next order. A particularly noticeable feature of Eq. (2.6a) is that it is still the Euler-Lagrange equation making stationary a functional U_2 (U_2 is given explicitly in Appendix A).

Since $\Lambda_2[\chi]$ is, in some sense, a perturbation of $\Lambda_1[\chi]$, it is quite natural to seek for a dislocation solution perturbatively starting with the solution of (2.5) at lowest order.

We know that $\Lambda_2[\chi]$ is formally of order ϵ^2 , although $\Lambda_1[\chi]$ is of order $\epsilon^{3/2}$. But if we consider, instead of χ_0 , a solution $\chi_0 e^{i\delta x}$ with $\delta \sim \epsilon$, it is easy to see that terms of order δ that appear then in $\Lambda_1[\chi_0 e^{i\delta x}]$ are of order ϵ^2 , as $\Lambda_2[\chi_0]$ itself. Hence, it is natural to consider, at order ϵ^2 , both $\Lambda_2[\chi_0]$ and terms of order δ in $\Lambda_1[\chi_0 e^{i\delta x}]$. Accordingly, we seek a dislocation solution of (2.6a) in the form

$$\chi = \chi_0 e^{i \delta x} + \chi_1 + \cdots ,$$

where $\chi_0 \sim \epsilon^{1/2}$ is the solution of (2.5), $\delta \sim \epsilon$, and $\chi_1 \sim \epsilon$. Thus χ_1 is the solution of

$$\frac{D\Lambda_{1}}{D\chi}\Big|_{\chi=\chi_{0}}\chi_{1}=8iq_{0}^{2}\chi_{0,x}\delta+3iq_{0}^{3}|\chi_{0}|^{2}\chi_{0,x}$$
$$+M_{NL}+O(\epsilon^{5/2}), \qquad (2.7)$$

where $(D\Lambda_1/D\chi)|_{\chi=\chi_0}$ is Λ_1 linearized around χ_0 . The terms M_{NL} , which are not written explicitly on the right-hand side of Eq. (2.7) and are of order ϵ^2 as the first two, are omitted as they do not contribute finally to the sought expression.

Equation (2.7), as so many equations in the analytic theory of cellular structures, bears a solvability condition. Actually Λ_1 is autonomous with respect to x and y, so that $\chi_{0,x}$ and $\chi_{0,y}$ are eigenfunctions of $(D\Lambda_1/D\chi)|_{\chi_0}$ with the eigenvalue zero. So that Eq. (2.7) can be solved (with respect to χ_1) if its right-hand side is orthogonal (with a convenient scalar product) to the adjoint kernel of $(D\Lambda_1/D\chi)|_{\chi_0}$.

With the Hermitian product

$$(\chi^{\alpha},\chi^{\beta}) \equiv \int dx \, dy \, \chi^{\alpha}(x,y) \chi^{\beta*}(x,y) ,$$

one verifies that $(D\Lambda_1/D\chi)|_{\chi_0}$ is Hermitic with this product, so that the solvability condition for (2.7) is $F_{\rm PK} = 0$, with

$$F_{\rm PK} \equiv 8iq_0^2 \delta(\chi_{0,x}, \chi_{0,y}) + 3iq_0^3 (|\chi_0|^2 \chi_{0,x}, \chi_{0,y}).$$
(2.8)

The quantity $F_{\rm PK}$ that appears in Eq. (2.8) may be interpreted as the Peach-Köhler force exerted upon the dislocation. As the Peach-Köhler force, it is proportional to the Burgers vector of the dislocation (equal to the phase rotation around the dislocation) and to the pressure exerted on the structure $(\sim \delta, \text{ as shown in Appendix B}).$

The solvability condition arising from the infinitesimal x translation is always fulfilled, and $(M_{NL}, \chi_{0,y}) = 0$, so that (2.8) is the unique solvability condition. It determines δ , and thus the wave number of the structure, such that a dislocation stays at rest.

Now we want to show that the wave number $q_0 + \delta, \delta$ being defined by $F_{\rm PK} = 0$ is the optimal wave number near $\epsilon = 0$. For this, let us write χ_0 as $ae^{i\varphi}, a, \varphi \in R$. The real part of the solvability condition involves first

$$\operatorname{Re}[i(\chi_{0,x},\chi_{0,y})] \equiv \frac{1}{2} \int dx \, dy (\chi_{0,y}^*\chi_{0,x} - \chi_{0,y}\chi_{0,x}^*)$$
$$= \frac{1}{2} \int dx \, dy \left[\hat{e}_z, \vec{\nabla}, \begin{bmatrix} a^2 \varphi_x \\ a^2 \varphi_y \\ 0 \end{bmatrix} \right],$$

where $(\vec{v}_1, \vec{v}_2, \vec{v}_3)$ is the 3×3 determinant made of the Cartesian coordinates of the three 3d vectors \vec{v}_1 , \vec{v}_2 , and \vec{v}_3 , \hat{e}_z is the unit vector perpendicular to the (x,y) plane, and $(a^2\varphi_x, a^2\varphi_y, 0)$ are the three components of the vector $a^2 \vec{\nabla}_{x}$.

By the Stokes formula, and as the amplitude modulus a tends to a constant at large distances from the dislocation core,

$$\operatorname{Re}[i(\chi_{0,x},\chi_{0,y})] = \frac{1}{2}a^2 \oint_c d\vec{s} \cdot \vec{\nabla}\varphi$$
$$= \pi a^2 ,$$

where we have used the external boundary condition (2.5c). The scalar product

$$\operatorname{Re}[i(|\chi_0|^2\chi_{0,x},\chi_{0,y})]$$

is computed in the same way and the solvability condition becomes

$$16a^{2}q_{0}^{2}\delta + 3q_{0}^{3}a^{4} = 0 .$$

As $a^{2} = 4/3q_{0}^{4}$, we have
 $\delta = -\frac{\epsilon}{4q_{0}^{3}} .$ (2.9)

This $|q_0+\delta|$ is the optimal wave number near $\epsilon=0$ for periodic steady solution.⁶ This is also⁶ the unique wave number making possible a steady bending of the rolls. It has been shown elsewhere⁴ that the perpendicular diffusion coefficient D_1 vanishes at this optimal wave number. Nevertheless, we shall show in Sec. III that this is an accident; for nonvariational model, in general, $F_{\rm PK}$ and D do not vanish simultaneously, as a function of the roll structure.

If δ does not satisfy Eq. (2.9) near $\epsilon = 0$, the solvability condition for Eq. (2.7) is no more fulfilled. To satisfy this condition, one has to add one more free parameter, i.e., the velocity of the dislocation. We start now from a solution $\chi_0(x, y - vt)$, v being the dislocation velocity, and perturb it. The time dependence of the unperturbed solution adds $-v\chi_{0,y}$ on the right-hand side of (2.7), and the solvability condition becomes

$$F_D = F_{\rm PK} , \qquad (2.10)$$

where F_{PK} has the same expression as in (2.8b), although the drag F_D is formally

$$F_D = v \int |\chi_{0,y}|^2 dx \, dy \, .$$

Siggia and Zippelius² have shown that F_D diverges as it stands, owing to the large distance behavior of the phase around the dislocation.

Far from the dislocation core the phase φ obeys

$$\frac{\partial \varphi}{\partial t} = -v\varphi_{y}$$
$$= D_{\perp}\varphi_{yy} + D_{\parallel}\varphi_{xx} - \varphi_{y^{4}} - 2\pi D_{\parallel}\delta_{0}'\Theta(y) , \qquad (2.11)$$

where v is again the dislocation velocity along y, D_{\perp} and D_{\parallel} are the phase diffusion coefficients given near $\epsilon = 0_+, \delta \sim \epsilon$ by

$$D_{\parallel} = 4q_0^2 + O(\epsilon) ,$$

$$D_{\perp} = 4q_0(\delta - \delta_{\text{opt}}) + O(\epsilon^2)$$

and δ_{opt} being given by (2.9) near $\epsilon = 0_+$. Furthermore, $\delta'_0(x)$ is the derivative of the Dirac function (no confusion is to be made with the small variations of the wave number around q_0 , also denoted as δ) and Θ the step function. Near $\delta = \delta_{opt} F_D$ is dominated by the large distance contribution that reads²

$$F_{D} = 2va^{2}D_{||}^{2} \int \int \frac{k^{2}dk \, dq}{(D_{||}k^{2} + D_{\perp}q^{2} + q^{4})^{2} + q^{2}v^{2}}$$
$$= \pi a^{2}v \left[\frac{2D_{||}}{D_{\perp}}\right]^{1/2} \Gamma \left[\frac{v^{2}}{D_{\perp}^{3}}\right], \qquad (2.12)$$

where

$$\Gamma(\alpha) \equiv \int_{-\infty}^{+\infty} dq \{q^2 + \alpha q^4 + [q^2 + (q^2 + \alpha q^4)^2]^{1/2} \}^{-1/2}.$$

One deduces at once from (2.10) and (2.12) that

$$v \simeq \beta' (4q_0)^{3/2} (\delta - \delta_{opt})^{3/2}$$

for $\delta - \delta_{opt} \sim \epsilon$, β' being a numerical constant. This

numerical constant cannot be really calculated, since (2.12) is only an approximate form of F_D . This gives the correct behavior of F_D as far as the power dependence on ϵ , δ , and v is concerned. However, to obtain (2.12), nonlinear terms [as $(\varphi_y)^2 \varphi_{yy}$] have been omitted in Eq. (2.11) that are of the same order of magnitude as the included ones. These nonlinearities make an analytic derivation of β' difficult.

III. CLIMB OF DISLOCATION IN DARCY-RAYLEIGH THERMOCONVECTION

In this section, we consider the climb of dislocation in a system of rolls generated by thermoconvection in a porous medium between two heatconducting horizontal parallel plates (or Darcy-Rayleigh thermoconvection). To make analytic predictions, as much as possible, we shall limit ourselves to the vicinity of the convection threshold. Therein, most properties are accessible to a perturbation analysis, owing to the supercritical—or normal—character of the bifurcation conduction \rightarrow convection.

The interest of this kind of convection is twofold. First, the analysis of the onset of convection is straightforward. Then the experimental realization of this flow is possible, while the classical free-free model of convection of Rayleigh has no immediate applicability to experiments. Furthermore, this Rayleigh model has a Galilean invariance, making it quite different from the usual convection models with rigid horizontal boundaries.

The onset of convection in an infinite porous layer is reached when the value of the dimensionless Darcy-Rayleigh number (R_D) is $4\pi^2$ and the dimensionless horizontal wave number q is π . We shall be concerned with the domain of values of R_D and qsuch that $R_D = 4\pi^2 + \epsilon$, $q = \pi + \delta$, $\delta \sim \epsilon = 0_+$ (our notations are those of Secs. I and II whenever the quantities have the same qualitative meaning, as ϵ or δ). A number or arguments^{5,6} show that the range of selected wave number in experiments is such that $\delta \sim \epsilon$. In this domain, the usual amplitude equation is not strictly true, because one assumes $\partial_x \sim \delta \sim \epsilon^{1/2}$ to derive it. And, as we are interested in the domain $\delta \sim \epsilon$, we need corrections to the amplitude equation of the same nature as the ones occurring in Eq. (2.6b). But, contrary to what happens in Sivashinsky's model, no variational formulation exists at this order in the present model.

In what follows, we shall derive, first, the ampli-

tude equation at the same order as in Eq. (2.6). Then we shall explain how to get the climb velocity from this equation in the domain $\delta \sim \epsilon \simeq 0_+$.

Our starting point is the following dimensionless form of the Darcy-Boussinesq equations^{10,11}:

$$\Delta \psi_t + R_D \Delta_h \psi + \Delta^2 \psi = S[\psi] , \qquad (3.1a)$$

where $S[\psi]$ is quadratic with respect to ψ ,

$$S[\psi] \equiv \psi_{xz} \Delta \psi_x + \psi_{yz} \Delta \psi_y - (\Delta_h \psi) \Delta \psi_z , \quad (3.1b)$$

and where we have used the notations $\Delta_h = \partial_{x^2}^2 + \partial_{y^2}^2$ (x and y are horizontal coordinates), $\Delta = \Delta_h + \partial_{z^2}^2$ (z is a vertical coordinate), and R_D is the Darcy-Rayleigh number. Furthermore, the boundary conditions are $\psi = \psi_{zz} = 0$ at z = 0, 1. The derivation of the "next order" amplitude equation from (3.1) implies a lot of algebra, so that we shall sketch only the main steps.

In the domain $R_D = 4\pi^2 + \epsilon$, $\epsilon = 0_+$ and ψ expands as

$$\boldsymbol{\psi} = \boldsymbol{\psi}^{(1)} + \boldsymbol{\psi}^{(2)} + \cdots$$

where

$$\psi^{(1)} = \frac{1}{2} (\chi e^{i\pi x} + \chi^* e^{-i\pi x}) \sin \pi z (\sim \epsilon^{1/2})$$

 $\psi^{(2)}$ is quadratic with respect to χ , $\psi^{(3)}$ is formally cubic, and so on. Furthermore, χ depends slowly on x, y, and t, so that χ_y, χ_x, χ_t (and any derivative of χ) are small with respect to χ . Now Eq. (3.1) is solved by a double iteration with respect to the amplitude χ and to its (small) derivatives. This kind of adiabatic expansion is straightforward, as far as the principle (not the details) of the calculations are implied, so that we have avoided the recourse to systematic derivations with a complicated formalism and no more rigor than other methods.

Let $S^{(1,1)}$ be the expression obtained by putting $\psi^{(1)}$ into the right-hand side of (3.1b). Retaining quantities with derivatives up to the order χ_x and χ_{y^2} , one finds

$$S^{(1,1)} = \frac{1}{8}\pi^{3} \sin 2\pi z \left[-8\pi^{2} |\chi|^{2} - 12i\pi(\chi\chi_{x}^{*} - \chi^{*}\chi_{x}) - 12 |\chi_{y}|^{2} + 2e^{2i\pi x}(\chi\chi_{yy} - \chi_{y}^{2}) + \text{c.c.} \right].$$
(3.2)

To compute $\psi^{(2)}$ (formally quadratic with respect to χ) up to order $\chi\chi_{yy}$ and $\chi_{x}\chi$, we put $S^{(1,1)}$, as given by (3.2), into the right part of (3.1a). This yields an inhomogeneous equation for $\psi^{(2)}$. As $\psi^{(2)}$ has a finite relaxation time at the onset of convection, we neglect $\Delta\chi_{t}^{(2)}$ so that $\psi^{(2)}$ is the solution of

$$R_D \Delta_h \psi^{(2)} + \Delta^2 \psi^{(2)} = S^{(1,1)} , \qquad (3.3a)$$

where χ is considered as time independent. When one derives $\psi^{(2)}$ from (3.3a), one must take care that χ depends on x and y. In the limit of slow variations of χ ,

$$\psi^{(2)} = \frac{\sin 2\pi z}{16} \left[-\pi \left| \chi \right|^2 - \frac{3i}{2} (\chi \chi_x^* - \chi_x \chi^*) \right] + \frac{\pi^3 \sin 2\pi z}{8} \left[-\frac{3 \left| \chi_y \right|^2}{4\pi^4} + \frac{e^{2i\pi x}}{24\pi^4} (\chi \chi_{yy} - \chi_y^2) + \text{c.c.} \right]$$
(3.3b)

The next step consists of collecting terms cubic in χ in S.

For our purpose, the important terms are the "resonant" ones, i.e., those depending on z and x as $\sin \pi z e^{\pm i\pi x}$ (i.e., as $\psi^{(1)}$ itself). As the computations are rather cumbersome, we have checked our results as much as possible. Some checks having an independent interest are explained in Appendix B. These resonant cubic terms in S are

$$S^{(2,1)} \equiv (\psi_{xz}^{(1)} \Delta \psi_{x}^{(2)} + \psi_{xz}^{(2)} \Delta \psi_{x}^{(1)} + \psi_{yz}^{(1)} \Delta \psi_{y}^{(2)} + \psi_{yz}^{(2)} \Delta \psi_{y}^{(1)} - \Delta_{h} \psi^{(1)} \Delta \psi_{z}^{(2)} - \Delta_{h} \psi^{(2)} \Delta \psi_{z}^{(1)})$$

$$= \frac{\sin \pi z}{8} \pi^{4} [e^{i\pi x} (\frac{5}{4} |\chi|^{2} \chi_{yy} - |\chi_{y}|^{2} \chi + \frac{1}{4} \chi_{yy}^{*} \chi^{2}) + \text{c.c.}]$$

$$+ \frac{\pi^{4} \sin \pi z}{4} \left[-\frac{\pi^{2}}{2} |\chi|^{2} (\chi e^{i\pi x} + \text{c.c.}) + i\pi^{4} |\chi|^{2} (\chi_{x} e^{i\pi x} - \text{c.c.}) - \frac{3i\pi}{4} [e^{i\pi x} (\chi^{2} \chi_{x}^{*} - |\chi|^{2} \chi_{x}) - \text{c.c.}] \right].$$
(3.4)

Collecting, now, all terms with an explicit dependence $e^{i\pi x}\sin\pi z$ in

one gets the amplitude equation at the sought order:

$$-\pi^{2} \left[\epsilon \chi + 4 \left[\partial_{x} - \frac{i \partial_{y^{2}}^{2}}{2\pi} \right]^{2} \chi - \frac{\pi^{4}}{4} |\chi|^{2} \chi - 2\chi_{t} \right]$$

= $-\epsilon \chi_{yy} - i \epsilon \pi \chi_{x} + \frac{\pi^{4}}{4} \left(\frac{5}{4} |\chi|^{2} \chi_{yy} - |\chi_{y}|^{2} \chi + \frac{1}{4} \chi_{yy}^{*} \chi^{2} \right) + \frac{7i \pi^{5}}{8} |\chi|^{2} \chi_{x} - \frac{3i \pi^{5}}{8} \chi^{2} \chi_{x}^{*} .$ (3.5)

This equation will be our basic equation for what follows. On the left-hand side we have written the amplitude equation at the lowest order, although the next order corrections are on the right-hand side. These corrections are necessary if one wants to study the domain of wave number $\pi + \delta$, $\delta \sim \epsilon$. These corrections are of the same order as those occurring in $\Lambda_2[\chi]$ as defined by (2.6b) for the Sivashinsky model.

As in Sec. II, our starting point is the timeindependent dislocation solution of the amplitude equation at the lowest order. That is,

 $\Lambda \chi \equiv \epsilon \chi + 4 \left[\partial_x - \frac{i \partial_{y^2}^2}{2\pi} \right]^2 \chi - \frac{\pi^4}{4} |\chi|^2 \chi$

 $\Lambda \chi_0 = 0$

with

and the external boundary conditions

$$\chi_{0}\underset{(x,y)\to\infty}{\longrightarrow} \left[\frac{4\epsilon}{\pi^4}\right]^{1/2} e^{i\varphi(x,y)}$$

with

$$\oint_c d\vec{s} \cdot \vec{\nabla} \varphi = 2\pi$$

on a large circle.

This describes a dislocation in a roll structure with the horizontal wave number π . Now, as in Sec. II, we seek by perturbation around χ_0 the dislocation solution in a structure with wave number $\pi + \delta$, $\delta \sim \epsilon$. The unperturbed solution is now

$$e^{i\delta x}\chi_0(x,y-vt)$$

At next order, one has to solve the linear equation

$$-\pi^{2} \frac{D\Lambda}{D\chi} \bigg|_{\chi_{0}} = 2\pi^{2} v \chi_{0,y} - \epsilon \chi_{0,y^{2}} - i \epsilon \pi \chi_{0,x} + \frac{\pi^{4}}{4} (\frac{5}{4} |\chi_{0}|^{2} \chi_{0,y^{2}} - |\chi_{0,y}|^{2} \chi_{0} + \frac{1}{4} \chi_{0,y^{2}}^{*} \chi_{0}^{2}) + \frac{i\pi^{5}}{2} |\chi_{0}|^{2} \chi_{0,x} - \frac{3i\pi^{5}}{8} (\chi_{0}^{2} \chi_{0,x}^{*} - |\chi_{0}|^{2} \chi_{0,x}) + 8\pi^{2} i \delta \left[\chi_{0,x} + \frac{i \chi_{0,y^{2}}}{2\pi} \right].$$
(3.6)

One recognizes on the right-hand side of this expression three sorts of terms: $2\pi^2 v \chi_{0,y}$ comes from the $2\pi^2 \chi_t$ in Eq. (3.6), the next terms are nothing but the right-hand side of Eq. (3.6), where χ is replaced by its lowest-order contribution, i.e., χ_0 , and the last term is explicitly proportional to δ and comes from the action of the derivative

$$\left[\partial_x + \frac{i}{2\pi}\partial_{y^2}^2\right]^2$$

on $e^{i\delta x}\chi_0$ at the order δ .

Owing to the autonomous character of Λ with respect to y, one has still to satisfy the following solvability condition:

$$F_D = F_{\rm PK}$$

with

$$F_D = 2\pi^2 v \int |\chi_{0,y}|^2 dx \, dy \,, \qquad (3.7)$$

although F_{PK} is proportional to the scalar product of $\chi^*_{0,v}$ with the terms in the right-hand side of (3.6) that are formally independent of v. Using the same trick as in Sec. II, we obtain

$$F_{\rm PK} = \frac{\epsilon}{\pi} \left[\left[3 - \frac{5\alpha}{16} - \frac{3\alpha'}{16} \right] \frac{\epsilon}{\pi} - 32\delta \right], \quad (3.8)$$

 α and α' being numbers defined by

$$\alpha = \frac{\pi^{6}}{\epsilon^{2}} \int dx \, dy \, |\, \chi_{0,y} \,|^{2} (\,|\, \chi_{0} \,|^{2})_{y}$$

and

$$\alpha' = \frac{\pi^7}{\epsilon^2} \int dx \, dy \, i [\chi_0^2 \chi_{0,x}^* \chi_{0,y}^* - (\chi_0^*)^2 \chi_{0,x} \chi_{0,y}^*)]$$

Both integrals defining α and α' converge, owing to the rapid convergence of the amplitude of χ_0 to its large distance asymptotics. As χ_0 is not known explicitly, we have obtained α and α' by (tedious) numerical computations:

$$\alpha \sim 0.5 \pm 10\%$$
,
 $\alpha' \sim 1.0 \pm 20\%$.

These figures have been found through a direct computer simulation of the evolution equation (2.3) in a closed domain with boundary conditions ensuring a phase dislocation. The integrals were computed on the steady state reached after that the transients have been damped out. To account as much as possible for the boundedness of the geometry in the computer experiment, we have extrapolated our results to an infinite domain through increasingly large geometries (more details about these calculations and figures are given in Appendix C).

This shows, in particular, that F_{PK} does vanish (and that the dislocation stays at rest) for

$$\delta = \delta_+ \equiv \frac{\epsilon}{32\pi} \left| 3 - \frac{5\alpha}{16} - \frac{3\alpha'}{16} \right|$$

This differs from the condition defining the vanishing of D_{\perp} [from Eq. (3.5)]. [This condition can be found to be $\delta \simeq \epsilon + O(\epsilon^2)$, in agreement with Ref. 6].

The balance between the Peach-Köhler force and the drag gives a condition for v similar to the one found in Sec. II,

$$\frac{\overline{v}}{\delta^{3/2}}\Gamma\left[\frac{\overline{v}^2}{\delta^3}\right] = 64\pi^3\left[\frac{\delta_+ - \delta}{\delta}\right],\qquad(3.9)$$

where $\overline{v} = \pi^3 v / 2\sqrt{2}$, and Γ is defined as in (2.12). If $\delta = 0$, the limit value of \overline{v} is of order $[\delta^+(\sim \epsilon)]^{3/2}$ times a number that cannot be really computed analytically, owing to the nonlinearity of the phase equation as large distances.

This condition cannot be taken too literally, as it still implies the neglect of relevant nonlinear terms in the phase diffusion. The only firm conclusion that can be drawn from (3.9) is that v varies as the $\frac{3}{2}$ power of some linear combination of δ and δ^+ (remember that $\delta^+ \sim \epsilon$) and that v does not vanish when $D_{\perp} = 0$.

IV. GLIDING OF DISLOCATIONS

By definition, the gliding of dislocations is the motion *perpendicular* to the roll axis. We show in this section a gliding effect intimately connected

with the nonvariational structure of the equations of the Darcy-Rayleigh convection.

Consider a system of smoothly curved rolls and let χ be the complex amplitude of the unbended structure. Thus, the local complex amplitude of the curved rolls is $\chi(1+i\hat{\gamma}y^2)$, $\hat{\gamma}$ being a small real quantity. Indeed, this equation has a local meaning only, since secular terms as $\hat{\gamma} y^2 \chi$ are not allowed, in general, as steady solutions of the equations. Nevertheless, this solution is sufficient for the moment, as we shall be concerned first with a finite region of space around y=0, such that $i\hat{\gamma}y^2$ is everywhere small therein, and amounts to a small phase change. In Secs. II and III we could have replaced the phase factor $e^{i\delta x}$ by the beginning of its Taylor expansion near $x\delta = 0$, that is, $e^{i\delta x}$ by $1 + i\delta x$, as $x\delta$ is everywhere small around a dislocation of extent of order $e^{-1/2}$ along x when δ is of order ϵ . We can assume (for instance) $\hat{\gamma} \sim \epsilon$, so that $\hat{\gamma} y^2 \sim \epsilon^{1/2}$ around a dislocation extending along y at distances of order $\epsilon^{-1/4}$.

Consider first, in the case of a variational system, a dislocation in rolls with a uniform curvature. No force of variational origin can produce gliding; when the dislocation is shifted of one roll, the potential (if it exists) is unchanged, and no work compensates the viscous loss during this gliding. One consequence of this remark is that no terms in the amplitude equation (3.6) deriving from a potential can contribute to gliding for a uniform curvature. To make this point clearer, let us show first the absence of gliding, when the left part of Eq. (3.6) is retained only, as it derives from a potential. Our starting point is the equation

$$2\chi_t = \Lambda[\chi] \tag{4.1a}$$

with

$$\Lambda[\chi] \equiv \epsilon \chi + 4 \left[\partial_{\mathbf{x}} + \frac{i}{2\pi} \partial_{y^2}^2 \right]^2 \chi - \frac{\pi^4}{4} |\chi|^2 \chi$$
(4.1b)

together with the static dislocation solution χ_0 defined before.

Consider now the perturbed solution

$$\chi_0(x-vt,y)(1+i\hat{\gamma}y^2)+\chi_1+\cdots$$

with (a priori) $\chi_1 \sim v \sim \hat{\gamma}$ (notice that gliding occurs in the x direction—i.e., perpendicular to the roll axis, although climbing was along the y axis). The first-order perturbation χ_1 is given by the solution of Eq. (4.1a) at the order $\hat{\gamma}$:

$$-2v\chi_{0,x} - \frac{D\Lambda}{D\chi} \bigg|_{\chi_{0}} \chi_{1} = 4i\widehat{\gamma} \left[\left[\partial_{x} + \frac{i}{2\pi} \partial_{y^{2}}^{2} \right]^{2} y^{2} \chi_{0} - y^{2} \left[\partial_{x} + \frac{i}{2\pi} \partial_{y^{2}}^{2} \right]^{2} \chi_{0} \right] \\ = 4i\widehat{\gamma} \left[\frac{4i}{2\pi} \chi_{0,x} + \frac{8iy}{2\pi} \chi_{0,y^{2}} - \frac{1}{4\pi^{2}} (8y\chi_{0,y^{2}} + 12\chi_{0,y^{4}}) \right].$$
(4.2)

As the solution depends on x and t through the combination x - vt, the velocity v is determined by taking the scalar product of (4.2) with $\chi_{0,x}$ that is in the kernel of $(D\Lambda/D\chi)|_{\chi_0}$.

After adding the complex conjugate, one has

$$-4v(\chi_{0,x},\chi_{0,x}) = -\frac{16\hat{\gamma}}{\pi} \int dx \, dy \left[|\chi_{0,x}|^2 + y(\chi_{0,x}^*\chi_{0,xy} + \chi_{0,xy}^*\chi_{0,x}) \right] \\ -\frac{\hat{\gamma}}{\pi^2} \int dx \, dy \, i \left[\chi_{0,x}^* (8y\chi_{0,y^3} + 12\chi_{0,y^2}) - \text{c.c.} \right].$$

$$(4.3)$$

By integration by part, and after taking care that the "external" boundary terms do not contribute, one has

$$\int dx \, dy (\chi_x \chi_x^* + 2y \chi_x^* \chi_{xy}) = \int dx \, dy \, \chi(-\chi_{xx}^* + 2y \chi_{x^2y}^*)$$

and

where

$$\int dx \, dy (\chi_x \chi_x^* + 2y \chi_x \chi_{xy}^*) = \int dx \, dy \, \chi(-\chi_{xx}^* - 2y \chi_{x^2y}^*) ,$$

so that the first integral on the right-hand side of Eq. (4.3) vanishes. The second one vanishes after similar manipulations, and this proves the absence of gliding in an uniformly curved structure described by Eq. (4.1) as stated before.

Now we shall add to the right-hand side of (4.1a) terms of order $\hat{\gamma}$ coming from the action of the right-hand side of Eq. (3.6) (equal to the next-order terms in the amplitude equation) on $\chi_0(1+i\hat{\gamma}y^2)$ at order $\hat{\gamma}$. This gives the following solvability condition (that fixes the gliding velocity):

$$-2\pi^{2}v(\chi_{0,x},\chi_{0,x}) = \int dx \, dy \, \chi_{0,x}^{*} N[\chi_{0}]$$
with
$$N[\chi_{0}] \equiv -i\epsilon\pi \left[\partial_{x} - \frac{i}{\pi} \partial_{y^{2}}^{2}\right] (i\hat{\gamma}y^{2}\chi_{0})$$
(4.4a)

$$+\frac{\pi^{4}}{4}\left[\frac{5}{4}|\chi_{0}|^{2}i\hat{\gamma}\partial_{y^{2}}^{2}(y^{2}\chi_{0})-\frac{i\hat{\gamma}}{4}\chi_{0}^{2}(y^{2}\chi_{0}^{*})_{yy}-i\hat{\gamma}y^{2}\chi_{0}|\chi_{0,y}|^{2}-2i\hat{\gamma}y|\chi_{0}|^{2}\chi_{0,y}+2i\hat{\gamma}y\chi_{0}^{2}\chi_{0,y}^{*}\right]$$
$$-\frac{\hat{\gamma}y^{2}\pi^{5}}{8}(7|\chi_{0}|^{2}\chi_{0,x}-3\chi_{0}^{2}\chi_{0,x}^{*}).$$

We have inserted into the definition of N quantities depending explicitly on y^2 . Actually, the final contribution of these terms must vanish since, to be coherent, we must add to χ_0 the correction coming from the fact that the unbended amplitude is the solution of Eq. (3.6) including its right-hand side. In other terms, the unbended solution remains a possible solution under the infinitesimal phase change $\chi_0 \rightarrow \chi_0(1+i\xi)$ at first order in ξ with real $\xi \sim 0$. This invariance makes vanish any term proportional to $i\gamma y^2$ in (4.4) and yields the new solvability condition

$$-2\pi^2 v(\chi_{0,x},\chi_{0,x}) = \int dx \, dy \, \chi_{0,x}^* N'[\chi_0] , \qquad (4.5a)$$

$$N'[\chi_0] = 2i\hat{\gamma} \left[-\epsilon + \frac{5\pi^4}{16} |\chi_0|^2 \right] (2y\chi_{0,y} + \chi_0) - \frac{i\pi^4}{8} \hat{\gamma}\chi_0^2(\chi_0^* + 2y\chi_{0,y}^*) .$$
(4.5b)

By integrating by parts, it is easy to show that

$$i \int dx \, dy [\chi_{0,x}^*(2y\chi_{0,y} + \chi_0) - \text{c.c.}] = 0 .$$
 (4.6)

Indeed, this expresses the fact that the term $-\epsilon \chi_{y^2}$ on the right-hand side of Eq. (3.6) comes from the Euler-Lagrange functional $\int dx \, dy |\chi_y|^2$.

After some elementary manipulations, and by putting $\chi = ae^{i\varphi}, a, \varphi \in R$ (4.5a) becomes

2718

(**4.4**b)

$$-2\pi^{2}v(\chi_{0,x},\chi_{0,x}) = -\frac{\pi^{4}}{2} \int dx \, dy [3a^{3}a_{x}y\varphi_{y} - a^{3}(2ya_{y} + a)\varphi_{x}] \,. \tag{4.7}$$

The integral on the right-hand side of Eq. (4.7) does not vanish, as it should do in a variational model. Even more, it strongly diverges.

Consider the contribution of the integrand $(-a^4\varphi_x)$. At large y, a is constant so that $\int \varphi_x dx$ is a constant changing from 0 to 2π as y varies from $-\infty$ to $+\infty$ across the dislocation core. This is why the integral $-\int dx dy a^4\varphi_x$ diverges. This divergence has a topological origin, so that it cannot be eliminated by accounting for the finite velocity of the dislocation, as was eliminated the drag divergence for the climbing motion.

Indeed, it is unreasonable to conclude from this that the gliding velocity is physically infinite. The right-hand side of Eq. (4.7) diverges as a linear distance, its order of magnitude is accordingly $\hat{\gamma}a^4 l_y \sim \hat{\gamma}\epsilon^2 l_y$, where l_y is some typical "cut length." This length comes from the torsion of rolls at large distances; in this domain the phase change $i\hat{\gamma}y^2$ becomes finite, so that $l_y \sim \hat{\gamma}^{-1/2}$, which means that the right-hand side of (4.7) is actually of order $\hat{\gamma}^{1/2}\epsilon^2$. Owing to the quite strong divergence of the integral under consideration, the actual expression should depend in a nonlocal way on $\hat{\gamma}$. The exact calculation of this quantity needs an amplitude equation making obvious the geometric invariance of the equation, to account for a finite change in the roll orientation.

The estimate of the gliding velocity is still obtained from the solvability condition, in the form of Eq. (4.7). One may readily verify that $\int dx \, dy |\chi_{0,x}|^2$ converges at large distances, even even at $v = \delta = 0$, no divergence arises from the phase deformation (contrary to what happens for climbing). Thus, one gets the estimate $(x \sim \epsilon^{-1/2}, y \sim \epsilon^{-1/4}, \chi_0 \sim \epsilon^{1/2})$

$$\int dx \, dy \, |\, \chi_{0,x} \,|^2 \sim \epsilon^{5/4}$$

And, in order of magnitude, Eq. (4.7) yields

$$v\epsilon^{5/4} \sim \hat{\gamma}^{1/2}\epsilon^2$$
$$v \sim \hat{\gamma}^{1/2}\epsilon^{3/4}.$$

or

It is not obvious to compare the magnitude of this velocity with the climb velocity, owing to the fact that $\hat{\gamma}$ and δ (introduced in Secs. II and III) are quite different quantities. Nevertheless, one may reason as follows: The phase change in the dislocation region due to δ is $\delta l_x \sim \delta \epsilon^{-1/2}$, as $l_x \sim \epsilon^{-1/2}$ is the size of the dislocation along x. Similarly the phase change due to $\hat{\gamma}$ is

$$l_{y}^{2}\hat{\gamma} \sim (\epsilon^{-1/4})^{2}\hat{\gamma} \simeq \hat{\gamma} \epsilon^{-1/2}$$

Thus $\delta \sim \epsilon$ implies $l_x \delta \sim \epsilon^{1/2}$. Imposing a similar phase change due to bending yields

or
$$\hat{\gamma} \sim \epsilon^{-1/2} \gamma \sim \epsilon^{1/2}$$

With these (somewhat arbitrary) estimates, the climb velocity is $v_{\text{climb}} \sim \delta^{3/2} \sim \epsilon^{3/2}$ if $\delta \sim \epsilon$, although the glide velocity is

$$v_{\text{glide}} \sim \epsilon^{3/4} \gamma^{1/2} \sim \epsilon^{5/4} \gg v_{\text{climb}}(\sim \epsilon^{6/4})$$

This a (possible) explanation for the experimental $fact^{12}$ that climbing is much more frequent than gliding in Rayleigh-Bénard convection.

V. CONCLUSION

The amplitude equation describes slow variations in cellular structures as the rolls generated in Rayleigh-Bénard instabilities. The variational structure of these equations is generally limited to the lowest relevant order in ϵ (approximately equal to the distance of the control parameter to its critical value). Thus the climb of dislocations is no more governed by a Peach-Köhler force with a simple form in nonvariational problems.

This may lead to frustration effects maintaining the structure in a permanent unsteady state, even near the threshold; a supplementary layer finishing at a dislocation may tend to disappear, to decrease the wave number of the structure that becomes even more unstable against perpendicular phase diffusion. When the equations of motion have a variational structure climb of dislocations always tends to put the structure into a state of marginal stability with respect to the perpendicular phase diffusion.

APPENDIX A: GENERAL PROPERTIES OF VARIATIONAL MODELS OF CELLULAR STRUCTURES

In this appendix, we derive some specific properties of variational models, which are very similar to the ones of an elastic crystal in its ground state. In these models, a function, called "potential," is minimal when the wave number of the structure qtakes an optimal value q_{opt} . This wave number can be seen as the one of the structure without external

<u>27</u>

2719

pressure. For steady states with a different wave number, a Taylor expansion of the potential can be made around q_{opt} , and we define V_{per} (as in Sec. II) as the potential per unit dimension (length or square length) of the structure. With the help of this potential, the phase diffusion coefficients⁴ D_{\perp} and D_{\parallel} can be computed, as elastic moduli of an elastic structure. Then we perform a new nonperturbative calculation of the dislocation velocity, as a function of D_{\perp} and D_{\parallel} .

Other specific properties of variational models are sketched in the second part of this appendix.

1. Peach-Köhler force in variational models

Our starting point is the following evolution equation for a scalar field A(x,t), x being a twodimensional vector and t the time:

$$A_t = -\frac{\delta \underline{V}}{\delta A} , \qquad (A1)$$

where \underline{V} is a functional (as the one introduced in Sec. II) that will be left unspecified below. We want to calculate the velocity of a dislocation. The domain is a channel Ω defined by

$$-\frac{l}{2} < x < \frac{l}{2}$$

and

$$-l' < y < l'$$

with l' very large. The rolls are parallel to the y direction. There are n + 1 rolls for y > 0 and n rolls for y < 0. Far from the dislocation the rolls are periodic, their wave number being approximately $q = (2\pi n)/l$.

A displacement δx of the dislocation causes a variation of the potential. We express it formally. From (A1)

$$\delta \underline{V} = -\int_{\Omega} A_t \delta A \, dx \, dy \, . \tag{A2}$$

We define as usual the phase displacement φ by

$$A(x) = A_0(x + \varphi) + \cdots$$

where $A_0(x)$ is the one-dimensional stationary periodic solution of wave number q. As the dislocation moves slowly, φ will be of the form $\varphi(x, y - vt)$. From (A2)

$$\delta \underline{V} = \int_{\Omega} \varphi_t A_x^2 \delta \varphi \, dx \, dy \; .$$

As the rate of variation of $\delta \varphi$ is assumed to be much smaller than the one of the amplitude A, we have

$$\delta \underline{V} = -\langle A_x^2 \rangle \int_{\Omega} \delta \varphi \, \varphi_t dx \, dy \, , \qquad (A3)$$

 $\langle A_x^2 \rangle$ being the mean value of A_x^2 .

The left-hand side of this equation can be evaluated by noting that, during the evolution, a region of wave number q have been replaced by a region of wave number $q - 2\pi/l$. Then

$$\delta \underline{V} = -2\pi \frac{dV_{\text{per}}}{dq} \tag{A4}$$

is the energy change as the dislocation move of δy along the rolls. Whence, finally,

$$2\pi \frac{dV_{\text{per}}}{dq} = -v \langle A_x^2 \rangle \int_{\Omega} \varphi_y^2 dx \, dy \,. \tag{A5}$$

This fixes the climb velocity through the balance between the Peach-Köhler force [left-hand side of Eq. (A5)] and the dissipation rate due to the large distance phase behavior. Making now l and l' tend to infinity, we get a problem almost identical to the one considered in Sec. II, with the exception that it is not confined to weak nonlinearities. It is possible to relate dV_{per}/dq to the phase diffusion coefficients. Let us recall that the starting point of the calculation of these quantities is the change of $A_0(x)$ in a small constant phase perturbation

 $A'_{0}(x) = A_{0}(x) + \varphi A_{0,x}$.

When φ is nonuniform this becomes the beginning of an expansion in the gradient of φ :

$$A(x,t) = A_0(x) + A_{0,x}\varphi + A_1 + A_2 + \cdots$$

where A_1 is of order $(\vec{\nabla} \varphi)$, etc. The solvability conditions for this expansion lead to the phase diffusion equation.

We now consider A(x,t) to be the perturbed field. The time evolution of A(x,t) is then given by the deviation of the potential from its minimum. At first order in the perturbation we have, of course, $\delta V=0$; since the basic field A_0 is a stationary solution, we must hence calculate δV at the next order in $\nabla \varphi$.

To obtain it, we notice that the perturbation consists at lowest order in a local compression and rotation of the rolls. (Because of the rotational invariance of the basic equation, only the compression must be considered.) The associated wave number variation is

$$\delta q = q \left[1 + \varphi_x + \frac{\varphi_y^2}{2} + \frac{\varphi_x^2}{4} \right]. \tag{A6}$$

As the compression is of second order in φ_y , there is no term in φ_y in A_1 . We also assume that there is no variation of the field outside some closed domain Ω' , which we can divide into squares of

2720

DISLOCATION MOTION IN CELLULAR STRUCTURES

side $2\pi/q$. As φ varies slowly any of these squares, say S, is linearly transformed by the perturbation into a parallelogram S'. There are, hence, contributions to δV of the form

$$\Delta_S \underline{V} = \int_{S'} V[A] dx \, dy - \int_S V[A_0] dx \, dy \; .$$

There is no boundary term, as the perturbation vanishes outside Ω' . The field A is approximately periodic in S' with a wave number $q + \delta q$. We can make a Taylor expansion of the periodic potential $V_{per}(q)$ and

$$\Delta_{S} \underline{V} = \frac{1}{2} \int_{S} \left[q \frac{dV_{\text{per}}}{dq} \varphi_{y}^{2} + q \frac{dV_{\text{per}}}{dq} \frac{\varphi_{x}^{2}}{2} + q^{2} \frac{d^{2}V_{\text{per}}}{dq^{2}} \varphi_{x}^{2} \right] dx \, dy + T_{A_{1}}$$

This expression allows one to connect dV_{per}/dq with the diffusion coefficients introduced before.

First-order terms are irrelevant, as explained before, and T_{A_1} denotes the second-order terms in φ_x^2 coming from A_1 . Finally, from (A3), the total variation of the potential is

$$\delta \underline{V} = -\langle A_x^2 \rangle \int_{\Omega'} \left[\frac{D_\perp}{2} \varphi_y^2 + \frac{D_{||}}{2} \varphi_x^2 \right] dx \, dy$$

with $\varphi = 0$ on $\partial \Omega'$. This allows one to write

$$\varphi_t = D_{||}\varphi_{xx} + D_{\perp}\varphi_{yy}$$

with

$$D_{\perp} = -\frac{q}{\langle A_{0,x}^2 \rangle} \frac{dV_{\text{per}}}{dq} . \qquad (A7a)$$

A careful examination of the expansion of Ref. 4 leads to the estimation of the T_{A_1} terms. We conjecture here that they are of order $O(\epsilon)$ for $\delta \sim \epsilon$. Another relation can hence be written

$$D_{\perp} \sim \frac{\delta}{q_{\text{opt}}} D_{\parallel} + O(\epsilon)$$
 . (A7b)

We can rewrite (A7a)

$$2\pi D_{\perp} = \frac{v}{q} \int \theta_y^2 dx \, dy$$

where $\theta = q\varphi$ is the dimensionless phase of the perturbation around the dislocation. We can now proceed as before to calculate the dislocation speed. It becomes, if one neglects the nonlinear terms in the phase diffusion as explained in Sec. II,

$$\left[\frac{D_{\parallel}v^2}{4q^2D_{\perp}^3}\right]^{1/2}\Gamma\left[\frac{v^2}{D_{\perp}^3}\right]=1,$$

 Γ being the function defined in Sec. II.

2. Other properties of the one-dimensional model

a. Existence of an invariant quantity.

Let us consider the expression

$$K = (\epsilon - q_0^4) \frac{A^2}{2} + \frac{3}{4} A_x^4 - q_0^2 A_x^2 - A_x A_{xxx} + \frac{1}{2} A_{xx}^2 .$$
(A8)

We have

wh

$$K_{\mathbf{x}} = L(A)A_{\mathbf{x}}$$
,
ere

$$L(A) = [\epsilon - (\partial_{x^2}^2 + q_0^2)^2] A + (A_x^3)_x .$$

This means that if A is a one-dimensional stationary solution of (2.1) K is a constant of the "motion" in the x direction. This invariant can also be expressed in terms of the slowly varying amplitude χ . The expression (2.2) allows us to express it at order $O(\epsilon^2)$:

$$K_{1} = \frac{\epsilon}{4} |\chi|^{2} - iq_{0}^{3}(\chi^{*}\chi_{x} - \chi\chi_{x}^{*}) + 2q_{0}^{2}|\chi_{x}|^{2}$$
$$-q_{0}^{2}(\chi_{xx}\chi^{*} + \chi_{xx}^{*}\chi) + \frac{9}{32}q_{0}^{4}|\chi|^{4}$$

and $K = K_1 + O(\epsilon^{5/2})$.

Now K_1 is also an approximate invariant for the amplitude equation at second order. This can be verified by multiplying the x-dependent part of Eq. (2.6) by $(\chi_x^* - i\chi^* q_0)$ and adding the complex conjugate to get

$$\epsilon \chi \chi_{x}^{*} - 4iq_{0}^{3} \chi^{*} \chi_{xx} + 4q_{0}^{2} \chi_{xx} \chi_{x}^{*} - 4q_{0}^{2} \chi_{xxx} \chi^{*} + \frac{9}{4} |\chi|^{2} \chi \chi_{x}^{*} + 4iq_{0} \chi_{x}^{*} \chi_{xxx} + c.c. = 0$$

The left-hand side of this equation is equal to $4K'_{1x}$ with

$$K_1' = K_1 + iq_0(\chi_x^* \chi_{xx} - \chi_x \chi_{xx}^*) .$$

 K'_1 is the exact invariant for the amplitude equation at order ϵ^2 and it is equal to K at the same order. A similar result can be found for the amplitude equation at order $\epsilon^{3/2}$.

For the steady solution of (2.1) defined by (2.4), K can be calculated at lowest order in ϵ and δ , utilizing (A6)

$$K(\epsilon,\delta) = \frac{\epsilon}{6q_0^4} (5\epsilon + 16q_0^3\delta) \; .$$

b. Existence of a potential.

In fact, such an invariant exists for any variational equation. To quote Ref. 13 "all the equations which arise from problems in the calculus of variation with one independent variable, can be expressed in the Hamiltonian form." Reference to the original work of Ostrogradsky can be found in Ref. 13. To give an example of the derivation of this sort of invariant, let us consider a functional

$$\underline{V}[A] = \int_0^{l''} dx \ V(A, A_x, A_{xx}) = \int_0^{l''} V[A] dx$$

where A is a real function of x, $x \in [0, l'']$ with the boundary conditions

$$A = A_x = 0$$

at
$$x = 0, l''.$$

The Euler-Lagrange equation for V[A] reads

$$L[A] = 0 \tag{A9}$$

with

$$L[A] = \frac{\partial V}{\partial A} - \frac{\partial \dot{V}}{\partial A_x} + \frac{\partial \ddot{V}}{\partial A_{xx}} , \qquad (A10a)$$

where the dot denotes, as usual, the total derivative with respect to x.

The constant of the motion then writes

$$K(A, A_x, A_{xx}) = V - A_x \frac{\partial V}{\partial A_x} - A_{xx} \frac{\partial V}{\partial A_{xx}} + \frac{\partial \dot{V}}{\partial A_{xx}} A_x$$
(A10b)

and

$$K_{\mathbf{x}} = L[A]A_{\mathbf{x}} \; .$$

The amplitude equation (2.6) can also be written in a variational form, as mentioned in the text. This variational form is

$$\chi_t = -\frac{\delta U_2}{\delta \chi^*}$$

and

$$\chi_t^* = -\frac{\delta U_2}{\delta \chi}$$

with

$$U_{2} = U_{1} - \int \left[\frac{1}{8} q_{0}^{2} (\chi_{y}^{2} \chi^{*2} + \chi_{y}^{*2} \chi^{2}) - \frac{1}{2} q_{0}^{2} |\chi_{y}|^{2} |\chi|^{2} + \frac{3iq_{0}^{3}}{2} |\chi|^{2} \chi^{*} \chi_{x} - 4iq_{0} \chi_{xxx} \chi^{*} - 2 |\chi_{yx}|^{2} \right] dx dy$$

c. Relation between the potential and the invariant for periodic structures.

We now assume that the solution of (A9) is approximately periodic in the bulk. In the limit $l'' \rightarrow \infty$, one can find a central interval $(l_1, l'' - l_1)$ in which the solution is exponentially close to a periodic solution, of wave number q. (Except perhaps for a finite number of values of q.) Therefore, we will consider that A is approximately periodic.

We now make a dilatation of ratio $1 + \eta$. The perturbed field is

$$A'(\mathbf{x}) = A\left[(1+\eta) \left[\mathbf{x} - \frac{l''}{2} \right] + \frac{l''}{2} \right]$$

and we match A'(x) smoothly to be boundaries. The new central interval is then

$$(l_2, l'' - l_2)$$

with

$$l_2 = l_1 - \frac{\eta l''}{2}$$

and

$$\delta \underline{V} = \delta B + \delta C = 0$$

with

$$\delta B = \left(\int_{0}^{l_{2}} + \int_{l''-l_{2}}^{l''} \right) V[A'] - \left(\int_{0}^{l_{2}} + \int_{l''-l_{2}}^{l''} \right) V[A] dx,$$

$$\delta C = \int_{l_{2}}^{l''-l_{2}} V[A'] dx - \int_{l_{1}}^{l''-l_{1}} V[A] dx - \left(\int_{l_{2}}^{l_{1}} + \int_{l''-l_{1}}^{l''-l_{2}} \right) (V[A] dx).$$

27

(A11)

For this variation, one has for $x = l_1$

$$\delta A = -\frac{\eta L'}{2}A_x ,$$

hence from (A10a) (remember that L[A]=0)

$$\delta B = \eta L' \left[\frac{\partial V}{\partial A_x} A_x + \frac{\partial V}{\partial A_{xx}} A_{xx} - \frac{\partial \dot{V}}{\partial A_{xx}} A_x \right]_{x=l_1},$$

where $L' = l'' - 2l_1$. The other term reads

$$\delta C = \frac{1}{(1+\eta)} \int_{l_2}^{l''-l_2} V[A'] dx - \int_{l_1}^{l''-l} V[A] dx + \eta \left[\int_{l_1}^{l''-l_1} V[A] dx - \frac{V[A(l_1)] + V[A(l''-l_1)]}{2} L' \right].$$

The second term vanishes with an appropriate choice of l_1 which just requires $A(l_1)$ to be equal to its bulk mean value,

$$\delta C = \eta L' q \frac{dV_{\rm per}}{dq}$$

From (A10b), and with the same choice of A, it comes

$$\delta B = \eta L' [V_{\text{per}}(q) - K]$$

and (A11) now reads

$$q \frac{dV_{\rm per}}{dq} = K - V_{\rm per}(q)$$
.

This is a nonperturbative result. We can now develop the two sides of the equation using (A7) and the fact that K is restricted to the order $O(\epsilon^2)$ by the boundary conditions, as shown in Ref. 14 for a particular case. At lowest order we get $\delta \sim \epsilon$, which expresses again the wave number selection through the boundaries. To give an intuitive picture of what happens in a variational model, it can be said that $q(dV_{per}/dq)$ plays the role of a pressure which is responsible of the accommodation of the wave number q, although dislocations move to make the wave number closer to the optimal one in the bulk. As shown in Sec. III, this variational picture may be lost in other models of cellular structure.

APPENDIX B: EXAMINATION OF THE FORM OF EQ. (3.5)

In this appendix, we briefly explain some checks which we have made concerning the form of Eq. (3.5). For the model of Darcy-Rayleigh convection, the curve $D_{\perp}(q,\epsilon) = 0$ starts⁶ vertically from $(\pi,0)$ in the (q,ϵ) Cartesian plane. This must follow from Eq. (3.5). Consider a y-dependent linear perturbation superposed on a roll system of horizontal wave number $\pi + \delta$, $\delta \sim \epsilon$; that is, a perturbation $ie^{i\gamma y}e^{i\delta x}\hat{\chi},\hat{\chi} \in \mathbb{R}$ to a basic solution $(4\epsilon/\pi^4)^{1/2}e^{i\delta x}$ (the factor i in the perturbation expresses the fact that the diffusive motion under consideration is close to a small translation of the ground solution). If we limit ourselves to quantities of order γ^2 (that is, correct to describe phase diffusion), the contribution of the right-hand side of (3.5) that is linear with respect to $\hat{\chi}$ reads

$$i\epsilon\hat{\chi}\gamma^{2} - \frac{i\pi^{4}}{4}\gamma^{2}\left[\frac{5|\chi|^{2}}{4}\hat{\chi} - \frac{1}{4}|\chi|^{2}\hat{\chi}\right]$$

and this vanishes since $|\chi|^2 = (4\epsilon)/\pi^4$.

If one follows the derivation of D_{\perp} of Ref. 4, the vanishing of this quantity implies that the curve $D_{\perp}=0$ starts vertically near (ϵ,π) , a result obtained already⁶ by a direct analysis of the Darcy-Boussinesq equations. The other check we have imagined is the computation of the "invariant" (in the sense of Refs. 5 and 11) for periodic solutions. This invariant is obtained from (3.5) as follows: Let us consider first a situation where χ depends on x only, and not on y and t. This gives

$$-\pi^{2}\left[\epsilon\chi+4\chi_{xx}-\frac{\pi^{4}}{4}|\chi|^{2}\chi\right]=-i\epsilon\pi\chi_{x}+\frac{i\pi^{5}}{2}|\chi|^{2}\chi_{x}-\frac{3i\pi^{5}}{8}(\chi^{2}\chi_{x}^{*}-|\chi|^{2}\chi_{x})$$

Now multiply both sides of this equation by $(\chi_x^* - i\pi \chi^*)$ and add the complex conjugate. Then

(A12)

$$\left|\frac{\pi^6}{4} |\chi|^2 + \epsilon \pi^2 \right| (\chi \chi_x^* + \chi^* \chi_x) - 4\pi^2 (\chi_{xx} \chi_x^* + \chi_{xx}^* \chi_x) + 4i\pi^3 (\chi_{xx} \chi^* - \chi \chi_{xx}^*) = \frac{\pi^6}{2} |\chi|^2 (\chi_x \chi^* + \chi \chi_x^*) .$$

This can be equally put into the form dK/dx = 0 with

$$K \equiv \left[\frac{\pi^6}{16} |\chi|^2 + \frac{\epsilon \pi^2}{2} \right] |\chi|^2 - \pi^2 |\chi_x|^2 + 2i\pi^2 (\chi_x \chi^* - \chi \chi_x^*) - \frac{\pi^6}{8} |\chi|^4 .$$

For steady roll solution

$$\chi = e^{i\delta x} \left[\frac{4\epsilon}{\pi^4} \right]^{1/2} (\delta \sim \epsilon)$$

and

$$K \simeq \left[\frac{\epsilon \pi^2}{4} - 4\pi^3 \delta\right] |\chi|^2 .$$

This expression is in agreement with the one obtained by expanding the exact invariant¹¹ of the Darcy-Boussinesq equations near $\epsilon \sim \delta \sim 0_+$.

APPENDIX C: NUMERICAL SOLUTION OF THE AMPLITUDE EQUATION

In this appendix we present some results obtained by simulation of the amplitude equation. Such simulations have already been developed by Siggia



FIG. 1. Limiting velocity of the dislocation in function of the number (n+1) of wavelengths in the initial state.

and Zippelius who concentrated their attention on the verification of the law $v \sim \delta^{3/2}$.² Here, we are mostly interested by the explicit form of the solution and the way we reach it. To this end, we have developed the most obvious and simplest finite difference explicit scheme. Boundary conditions and spatial resolution were the same as those of Ref. 2 and the time step was chosen in order to avoid linear numerical instabilities. As a standard initialization we have chosen to feed the system with a system of n or n+1 pairs of rolls the amplitude of which goes to zero along a line perpendicular to the roll axis at t=0. This procedure gives an adequate degree of freedom for growing solutions with a phase which is singular somewhere. Simulations have been performed for transitions $n+1 \rightarrow n$ pairs of rolls where the final state is at the critical wave vector and with n = 3, 4, 6, 9, 12 aiming at a reliable extrapolation $n \rightarrow \infty$. Let us examine first the problem of how one can numerically reach the solution for an isolated dislocation in an infinite medium. At $n \to \infty$ the velocity of the dislocation is zero and from Fig. 1 it is clear that $v_{\rm lim} \sim 1/n^2$, a



FIG. 2. Slowing down rate $-\delta v / \delta t$ in function of the velocity v of the dislocation for the transition $7 \rightarrow 6$.



FIG. 3. Relaxation rate of the velocity as a function of the width displays a diffusive character.

fact which can easily be derived from Eq. (A5). Here we present v_{lim} against $1/(n+1)^2$ which is equivalent for *n* large but gives a better fit for *n* small.

The second feature to be considered is the final evolution of the velocity $v \rightarrow v_{\lim}$ at fixed *n*. The general trend is similar to that depicted by Fig. 4 of Ref. 2. Here the velocity is determined with great accuracy in noting the instants at which the amplitude node passes through a point of the lattice. The plot of $-\delta v / \delta t$ against v for the transition $7 \rightarrow 6$ (Fig. 2) clearly demonstrates an exponential relaxation towards the limiting value v_{\lim} . This is expected, since the final evolution is governed by the relaxation of the phase of diffusive character. This



FIG. 4. (a) Real and (b) imaginary part of the dislocation solution for the transition $7 \rightarrow 6$.



FIG. 5. (a) Modulus and (b) phase of the dislocation solution of Fig. 4.

diffusive process is confirmed by the plot of the inverse relaxation time against the inverse the square of lateral size of the system (Fig. 3). Figures 4(a) and 4(b) display the real and imaginary part of the complex amplitude while Figs. 5(a) and 5(b) display the modulus and the phase for the solution of the $7 \rightarrow 6$ transition. One can attempt to reconstruct the hydrodynamic fields from the amplitude function but the amplitude equation is invariant in a multiplication of the solution by $e^{i\varphi}$, where φ is a constant, so Fig. 6 presents the two extreme cases $\varphi = 0$ [Fig. 6(a): symmetric defect] and $\varphi = \pi/2$ [Fig. 6(b): antisymmetric defect] which have the same dynamics at this order. Having explicitly the numerical solution, one can calculate any desired quantity. Figure 7 displays the evolution with



FIG. 6. Reconstructed hydrodynamic fields showing the effect of the multiplication by $\exp i\varphi$ (φ const) of the amplitude of Fig. 4.



FIG. 7. Integrals α and α' function of the number n+1 of wavelengths in the initial state.

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(n + 1) of the integrals α and α' of Sec. III. Multiplicative factors appropriate to the Darcy-Rayleigh problem are $64\sqrt{3}/\pi$ and $128/\pi$ for α and α' , respectively, leading to figures quoted in the text. Extrapolation is difficult especially for α' which has not monotonous variations with *n* small, while the stationary state for *n* large is difficult to obtain.

Finally, simulations of the amplitude equation stress on two facts which should not be underestimated. First, it is unlikely that the symmetric and antisymmetric defects have the same dynamics and this limitation of the lowest-order equation should be relaxed. Second, and more important, is the observation of the difficulty one has to reach the stationary state since the underlying process is the diffusion of phase. To this respect one can say that the isolated dislocation in an infinite medium is a concept valid at the long time limit.

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FIG. 6. Reconstructed hydrodynamic fields showing the effect of the multiplication by $\exp i\varphi$ (φ const) of the amplitude of Fig. 4.