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Dislocation motion and vertical vorticity in Rayleigh-Bénard convective structures

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Abstract. The behaviour of an isolated dislocation in a Rayleigh-Bénard roll structure is studied within a linear elasticity theory of topological defects on a model which includes the effect of a large-scale drift flow. The climb velocity is given as a function of the Prandtl number, Rayleigh number and wavenumber for both rigid and stress-free boundary conditions. The effect of a lateral boundary is also briefly discussed.

1. Introduction

Convection in a horizontal layer heated from below provides the simplest example for pattern evolution of non-equilibrium systems. A spatially uniform conducting state becomes unstable at the threshold of a spatially periodic roll structure. However, both convection experiments (Croquette and Pocheau 1984) and numerical simulations (Greenside *et al* 1982, Greenside and Coughran 1984) performed with large-aspect-ratio systems usually show that the structure which develops above the threshold has a texture composed of domains of rolls interspersed with defects such as dislocations, disclinations and grain boundaries. The dynamics of these textured structures is closely connected to that of defects. Several attempts (Siggia and Zippelius 1981a, Newell 1982, Pomeau *et al* 1983, Manneville and Pomeau 1983, Dubois-Violette *et al* 1983, Cross and Newell 1984, Brand and Kawasaki 1984, Kawasaki 1984b, c) have been made recently to develop a theory which can deal with such complicated patterns with topological defects and their dynamics. It now seems that this branch of fluid dynamics is becoming increasingly like a branch of solid state or condensed matter physics requiring the reader to have some familiarity with this field (e.g. Nabarro 1967).

On the other hand, Siggia and Zippelius (1981b, Zippelius and Siggia 1982, 1983) noticed the peculiar roles played by a slowly varying drift flow that is generated by the vertical vorticity. It has been argued since then that the drift-flow effect significantly changes the conclusions obtained previously about the wavenumber selection criterion and stability properties (Cross 1983, Manneville and Piquemal 1983, Busse and Bolton 1984, Bolton and Busse 1985).

To provide a further insight into the large-scale-flow effect, we consider in this work the dynamics of an isolated dislocation‡ in the presence of the vertical vorticity.

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‡ Throughout the paper we consider only the edge-type dislocation with the associated phase jump $+2\pi$.

As analysing the full hydrodynamic equations remains well beyond the capacity of our computing power, we, as others (Cross and Newell 1984, Greenside and Cross 1985), elect to concentrate on suitable model systems which reproduce all of the qualitative features predicted by the Oberbeck-Boussinesq equations and which also allow the calculation of dynamics, including defects, with greater ease. It is hoped that the details of the dynamics poorly approximated in such model equations are not crucial in understanding the slow pattern evolution of convective systems involving defects. A model which includes the effect of the drift flow will be presented in the next section, where the defect-phase dynamics (Brand and Kawasaki 1984, Kawasaki 1984b, c) proposed recently by one of the present authors is extended to take this effect into account. The defect-phase dynamics is a method that describes combined dynamics of slow deformations of roll pattern (phase) and topological defects in this pattern. The analysis is made simpler if one realises that there exist regions where the basic equations of motion for a defect can be approximated in such a way as to be derivable from a potential even in the presence of the mean-drift flow. In this connection, it should be mentioned that Cross and Newell (1984) have explicitly demonstrated that there are cases where the (non-linear) phase dynamic equation can have potential even when the original full equations have none. To capture the effect more explicitly, we analyse the amplitude equations associated with our model in order to calculate the climb velocity of the dislocation motion. The climb here is defined as the motion of a dislocation along the direction of rolls. We compare the case of convection between free-slip (stress-free) boundaries (§ 3) with the one between no-slip (rigid) boundaries (§ 4). As might be expected, the difference between the boundary conditions leads to relatively distinctive behaviour of climbing near zig-zag instabilities in the two cases. The last section is devoted to several remarks in view of other theoretical and experimental findings. Effects of a lateral boundary on the force acting on a dislocation are also considered (appendix 2).

2. General considerations

We shall work with the equation of motion which is the Swift-Hohenberg model (Swift and Hohenberg 1977) for the local amplitude ψ of the vertical velocity component, supplemented with the z -independent (or vertically averaged) horizontal component of drift flow \mathbf{B} . Our model equation reads

$$\partial_t \psi = -\frac{1}{\tau_0} \frac{\delta H_0}{\delta \psi^*} - \mathbf{B} \cdot \nabla \psi \quad (2.1)$$

where $\nabla = (\partial_x, \partial_y)$ and H_0 is the Swift-Hohenberg functional†

$$H_0 = \iint dx dy \left(-\varepsilon |\psi|^2 + \frac{\xi_0^2}{4q_0^2} |(\nabla^2 + q_0^2)\psi|^2 + \frac{1}{2} \tilde{g} q_0^2 |\psi|^4 \right). \quad (2.2)$$

The parameter ε characterises the fluid properties: $\varepsilon = (R - R_c)/R_c$ with the Rayleigh number R , having critical value R_c , and the constants ξ_0 and τ_0 set the length and

† As a matter of fact the original Swift-Hohenberg model has a real order parameter. In this sense this is more closely related to the model studied by Cross and Newell (1984). However, in the main part of this paper we work with the amplitude equation for the roll structure containing a complex amplitude (e.g. Zippelius and Siggia 1983) which is derived from the hydrodynamic equations for Rayleigh-Bénard convection.

time scales of the periodic roll structures with wavelengths close to $2\pi/q_0$, respectively. These constants as well as \hat{g} naturally appear when equation (2.1) is derived from the original hydrodynamic equations and they depend on the boundary conditions on the top and bottom surfaces which we assume to be perfect conductors throughout this work. The actual values of these constants are evaluated in the literature (e.g. Newell and Whitehead 1969, Cross 1980). The presence of the slowly varying drift velocity field generates the z-independent component of vertical vorticity $\omega_z = \hat{z} \cdot (\nabla \times \mathbf{B})$, which is governed by the equation (Manneville 1983a)

$$(\partial_t - \sigma \Delta^\alpha) \omega_z = (1/2q_0^2) \hat{z} \cdot [\nabla \psi^* \times \nabla \nabla^2 \psi + c.c.], \tag{2.3}$$

where σ is the Prandtl number, \hat{z} the unit vertical vector opposite to the direction of gravity and *cc* denotes the complex conjugate. The operator Δ^α distinguishes the two boundary conditions and is identified as

$$\Delta^\alpha = \begin{cases} \text{constant} & (\alpha = 0) & \text{for rigid boundaries} \\ \nabla^2 & (\alpha = 1) & \text{for free-slip boundaries.} \end{cases} \tag{2.4}$$

Our model is slightly different from that of Manneville (1983a), who derived (2.3) starting from the well known Oberbeck-Boussinesq equations by a procedure similar to the derivation of amplitude equations (Cross 1980). As will be shown later, our model (2.1)-(2.4) reduces to the Siggia-Zippelius amplitude equations (Siggia and Zippelius 1981b, Zippelius and Siggia 1982, 1983).

Most simply, a phase-only approximation may be employed by substituting $\psi(\mathbf{r}, t) = a_0 \exp i[\mathbf{q} \cdot \mathbf{r} + \phi(\mathbf{r}, t)]$, $\mathbf{r} \equiv (x, y)$ in the above set of equations, where a_0 is the eikonal value of the amplitude and ϕ represents a deformation field due to the presence of defects; note that the wavevector \mathbf{q} refers to the roll structures without defects and may, in general, be different from the critical one, q_0 . Furthermore, here we use an analogue of the linear elasticity theory of topological defects (Kawasaki 1984c). Then we have

$$\begin{aligned} \partial_t \phi &= -E_0 \phi - \mathbf{q} \cdot \mathbf{B}, \\ (\partial_t - \sigma \Delta^\alpha) \mathbf{B} &= -(a_0^2/q^2) \mathbf{q} \nabla \cdot \nabla \phi, \end{aligned} \tag{2.5}$$

where E_0 is the differential operator which appears by linearising $-(2a_0^2\tau_0)^{-1} \delta H_0 / \delta \phi$ in the phase gradients due to defects. When we consider the slow steady defect motion, an adiabatic approximation for the drift \mathbf{B} can be utilised to yield a linearised phase equation

$$\partial_t \phi = -E \phi, \quad E \equiv E_0 + \sigma^{-1} a_0^2 (\Delta^\alpha)^{-1} \nabla \cdot \nabla. \tag{2.6}$$

Thus, apart from the fact that ϕ can be singular in the presence of the defect, the phase dynamics possesses a potential, H , within the framework of the present approximation; $\partial_t \phi = -(2a_0^2)^{-1} \delta H / \delta \phi$ †. Therefore, the formalism developed by Kawasaki (1984c) can be transcribed to describe the defect-phase dynamics of our model as follows.

Consider the steady dislocation motion with velocity v_0 . For slow motion we take

$$\partial_t \phi = -v_0 \cdot \nabla \phi \tag{2.7}$$

where $\phi = \phi(\mathbf{r} - \mathbf{R}(t))$ is the phase around the moving defect at $\mathbf{R}(t)$ with $v_0 = \dot{\mathbf{R}}$. Then

† The parameter τ_0 has been absorbed into H to render the phase equation of the same form as in Kawasaki (1984c).

we obtain the defect equation of motion (Kawasaki 1984c):

$$\mathcal{D}^0 \cdot \mathbf{R} = \mathbf{X}_l(\mathbf{R}) \equiv 2\pi\tilde{\mathbf{w}}(\mathbf{R}) \times \hat{\mathbf{z}}, \quad (2.8)$$

where \mathcal{D}^0 is the bare friction tensor and

$$\tilde{\mathbf{w}}(\mathbf{r}) \equiv \frac{\delta H}{\delta \nabla \phi} - \left(\frac{\delta H}{\delta \nabla \phi} \right)_0, \quad (2.9)$$

the subscript 0 referring to the stationary state. In (2.8) \mathbf{X}_l is the local force acting on the defect and is a generalisation of the Peach-Koehler force. As was shown by Kawasaki (1984c) and is discussed in appendix 1, for slow or steady defect motions, \mathbf{X}_l consists of two parts:

$$\mathbf{X}_l = \mathbf{X}_s + \mathbf{X}_{fr}. \quad (2.10a)$$

The static force \mathbf{X}_s is given by

$$\mathbf{X}_s = -dH/d\mathbf{R}, \quad (2.10b)$$

in which the phase variable is taken to follow adiabatically the defect motion, while the frictional force \mathbf{X}_{fr} arises from the deviation of ϕ from its adiabatic value due to the defect motion. The latter takes the form

$$\mathbf{X}_{fr} = -\mathcal{D}^*(\mathbf{v}_0) \cdot \mathbf{v}_0 \quad (2.10c)$$

with a new tensor parameter \mathcal{D}^* which renormalises the bare friction tensor:

$$\mathcal{D}^*(\mathbf{v}_0) = -8\pi^2 a_0^2 (\hat{\mathbf{z}} \times \hat{\mathbf{E}})(\hat{\mathbf{z}} \times \hat{\mathbf{E}})(E - \mathbf{v}_0 \cdot \nabla)^{-1}(E + \mathbf{v}_0 \cdot \nabla)^{-1} \delta(\mathbf{r} - \mathbf{R})|_{\mathbf{r}=\mathbf{R}}. \quad (2.11)$$

Here the operator $\hat{\mathbf{E}}$ is defined by

$$E = \hat{\mathbf{E}} \cdot \nabla = \nabla \cdot \hat{\mathbf{E}}. \quad (2.12)$$

A related expression for the friction tensor has been found by Dubois-Violette *et al* (1983). The equation of motion is thus given by

$$[\mathcal{D}^0 + \mathcal{D}^*(\mathbf{v}_0)] \cdot \mathbf{v}_0 = \mathbf{X}_s. \quad (2.13)$$

As expected, the same friction tensor \mathcal{D}^* also enters the energy dissipation rate, Φ (see appendix 1)

$$\Phi = \mathbf{v}_0 \cdot [\mathcal{D}^0 + \mathcal{D}^*(\mathbf{v}_0)] \cdot \mathbf{v}_0. \quad (2.14)$$

The defect equation of motion (2.13) is then also expressed in the form of the conservation law of energy (Siggia and Zippelius 1981a, Kawasaki 1984a); the rate of decrease of potential is equal to the energy dissipation rate:

$$-\mathbf{v}_0 \cdot dH/d\mathbf{R} = \Phi, \quad (2.15)$$

which enables one to evaluate the defect velocity \mathbf{v}_0 .

The arbitrariness in $\tilde{\mathbf{w}}$ discussed in Kawasaki (1984c) will not matter here since the original Swift-Hohenberg model without drift flow has a potential and the drift flow merely convects the phase field, i.e. it does not produce an extra force on the defect core centre.

The general ideas sketched above will be pursued in the subsequent sections to calculate the climb velocity of an isolated dislocation near the convective threshold.

3. Climb motion for free-slip boundaries

In order to implement the analysis, we shall study our model in the limit of small positive ε for a laterally unbound system with the rolls parallel to the y axis. Then,

introducing the scaled coordinates (Newell and Whitehead 1969, Segel 1969) as

$$\underline{X} = \varepsilon^{1/2}x, \quad \underline{Y} = \varepsilon^{1/4}y, \quad \underline{T} = \varepsilon t \tag{3.1}$$

and also the complex envelope function A that describes the slow modulation of the basic pattern through

$$\psi(x, y, t) = A(x, y, t) \exp(iq_0x), \quad A(x, y, t) = \varepsilon^{1/2}A^{(1/2)}(\underline{X}, \underline{Y}, \underline{T}) + O(\varepsilon^{3/4}), \tag{3.2}$$

with $\omega_z(x, y, t) = \varepsilon^{5/4}\omega_z^{(5/4)}(\underline{X}, \underline{Y}, \underline{T}) + O(\varepsilon^{3/2})$, we obtain from (2.1) and (2.3) the amplitude equations at the first non-trivial order in ε . For the stress-free boundary condition, they read

$$\begin{aligned} \tau_0 \partial_t A &= [\varepsilon - \xi_y^2(\partial_y^2 + i2q_0 \partial_x)^2]A - 2\tilde{g}q_0^2|A|^2A - iq_0\tau_0 B_x A, \\ (\partial_t - \sigma \nabla^2)\omega_z &= 2\partial_y\{A^*[\partial_x + (1/i2q_0)\partial_y^2]A + CC\}, \\ \partial_y\omega_z &= -\nabla^2 B_x, \end{aligned} \tag{3.3}$$

where $\xi_y = (\xi_0/2q_0)^{1/2}$. When the parameters are specified as (Newell and Whitehead 1969)

$$\tilde{g} = \frac{1}{3\pi^4}, \quad q_0^2 = \frac{\pi^2}{2}, \quad \xi_0^2 = \frac{8}{3\pi^2}, \quad \tau_0 = \frac{2(1 + \sigma)}{3\pi^2\sigma} \tag{3.4}$$

with the units $\kappa = d = 1$ (κ is the thermal diffusivity and d the layer depth), the above equations (3.3) are nothing other than the amplitude equations derived by Siggia and Zippelius (1981b, Zippelius and Siggia 1982, 1983). It is convenient to rewrite (3.3) in terms of the scaled variables:

$$\begin{aligned} (\varepsilon^{1/2}/\xi_0)x &\rightarrow X, & (\varepsilon^{1/4}/\xi_y)y &\rightarrow Y, & (\varepsilon/\tau_0)t &\rightarrow T \\ A/A_0 &\rightarrow A, & B_x/B_0 &\rightarrow B_x, & \omega_z/\omega_0 &\rightarrow \omega_z, \end{aligned} \tag{3.5}$$

where $A_0 = (\varepsilon/2\tilde{g}q_0^2)^{1/2}$, $B_0 = \varepsilon/q_0\tau_0$ and $\omega_0 = \varepsilon^{5/4}/q_0\tau_0\xi_y$. Then (3.3) becomes

$$\partial_T A = A + (\partial_X - i\partial_Y^2)^2 A - |A|^2 A - iB_x A, \tag{3.6a}$$

$$\gamma \partial_T \omega_z = (\partial_Y^2 + \delta \partial_X^2)\omega_z + g \partial_Y [A^*(\partial_X - i\partial_Y^2)A + CC], \tag{3.6b}$$

$$\partial_Y \omega_z = -(\partial_Y^2 + \delta \partial_X^2)B_x, \tag{3.6c}$$

with†

$$\gamma = \frac{\xi_0 \varepsilon^{1/2}}{2q_0 \tau_0 \sigma}, \quad \delta = \frac{\varepsilon^{1/2}}{2q_0 \xi_0}, \quad g = \frac{\tau_0}{2\tilde{g}q_0^2 \sigma}. \tag{3.7}$$

In the presence of a dislocation, we set

$$A = A_s [1 + u(X, Y, T)] \exp[i\phi(X, Y, T)] \tag{3.8}$$

with the static solution

$$A_s = (1 - Q^2)^{1/2} e^{iQX} \quad Q \equiv (\xi_0/\varepsilon^{1/2})(q - q_0). \tag{3.9}$$

At this stage, we follow Siggia and Zippelius (1981b, Zippelius and Siggia 1982, 1983) and introduce the following approximations‡: (i) linearisation in u , B_x and gradients

† The parameter g should not be confused with the acceleration of gravity.

‡ As Siggia and Zippelius (1981a) themselves pointed out, this linearisation approximation breaks down in the region $Y^2 \leq 4|X|$ where the distortion field becomes significant around the dislocation at $X = Y = 0$. See also the last comment in § 5.

of ϕ which describe perturbations due to a dislocation, (ii) adiabatic approximation for u and ω_z in the long-wavelength limit. One then finds

$$\begin{aligned} \partial_T \phi &= \left(\frac{1-3Q^2}{1-Q^2} \partial_x^2 + 2Q \partial_y^2 - \partial_y^4 \right) \phi - B_x, \\ (\partial_y^2 + \delta \partial_x^2)^2 B_x &= \partial_y^2 [2g(1-Q^2) \partial_y^2 - 2gQ \partial_x^2] \phi, \end{aligned} \tag{3.10a}$$

or, equivalently,

$$\partial_T \phi = \{ D_{\parallel}(Q) \partial_x^2 + D_{\perp}(Q) \partial_y^2 - \partial_y^4 - (\partial_y^2 + \delta \partial_x^2)^{-2} \partial_y^2 [2g(1-Q^2) \partial_y^2 - 2gQ \partial_x^2] \} \phi \tag{3.10b}$$

where

$$D_{\parallel}(Q) \equiv (1-3Q^2)/(1-Q^2), \quad D_{\perp}(Q) \equiv 2Q. \tag{3.11}$$

This linearised (non-local) phase equation (3.10) involves the following instabilities (Siggia and Zippelius 1981b, Zippelius and Siggia 1982, 1983).

- (i) Eckhaus instability for $Q^2 \geq \frac{1}{3}$.
- (ii) Zig-zag instability for $Q < 0, 2g \leq Q^2/(1-Q^2)$.
- (iii) Skewed-varicose instability for $Q \geq 0$.

Hence one should take note of the non-existence of the (positive) transverse diffusion coefficient in the stability domain of the roll pattern. It is also worth remarking that retention of the coupling of B_x to u (represented by the term $-2gQ \partial_x^2 \phi$ in (3.10)) is essential to cause the skewed-varicose instability.

It is enlightening to rewrite (3.10b) further by the use of the rescaled variables

$$\underline{x} = \frac{-D_{\perp}}{\sqrt{D_{\parallel}}} X, \quad \underline{y} = \sqrt{-D_{\perp}} Y, \quad \underline{t} = D_{\perp}^2 T. \tag{3.12}$$

It gives

$$\partial_{\underline{t}} \phi = [\partial_{\underline{x}}^2 - \partial_{\underline{y}}^2 - \partial_{\underline{y}}^4 - (\partial_{\underline{y}}^2 + \lambda^2 \partial_{\underline{x}}^2)^{-2} \partial_{\underline{y}}^2 (\mu \partial_{\underline{y}}^2 + \nu \partial_{\underline{x}}^2)] \phi \tag{3.13}$$

with

$$\begin{aligned} \lambda^2 &\equiv \frac{-D_{\perp} \delta}{D_{\parallel}} = \frac{(q-q_0)/q_0}{D_{\parallel}}, \\ \mu &\equiv \frac{g}{2Q^2/(1-Q^2)} \geq \frac{1}{4}, \\ \nu &\equiv \frac{g}{D_{\parallel}}. \end{aligned} \tag{3.14}$$

Although the $\nu \partial_{\underline{x}}^2$ term is indispensable for inducing the skewed-varicose instability, we may neglect this term at high Prandtl numbers as long as we limit ourselves to the climb motion in the stability domain which lies far away from the skewed-varicose instability line (cross-hatched region in figure 1(a)). We can also drop the $\lambda^2 (\ll 1)$ term to obtain

$$\partial_{\underline{t}} \phi = (\partial_{\underline{x}}^2 - \partial_{\underline{y}}^2 - \partial_{\underline{y}}^4 - \mu) \phi - 2\pi \delta'(\underline{x}) \theta(\underline{y} - \nu_0 \underline{t}), \tag{3.15}$$

where $\phi = \phi(\underline{x}, \underline{y} - \nu_0 \underline{t})$, and the phase variable is made single-valued by adding a source term where $\theta(x)$ is the unit step function, as is often done (Siggia and Zippelius

1981a). The parameter μ represents the effect of the generation of the vertical vorticity and, at the same time, the degree of proximity to the zig-zag instability which occurs at $\mu = \frac{1}{4}$. Since the phase equation now possesses the potential†, the climb velocity v_0 is easily found from (2.13) or (2.15) as in Siggia and Zippelius (1981a) to be given by the equation

$$\sqrt{2}v_0 \int_0^\infty \frac{dp}{\{-p^2 + p^4 + \mu + [(-p^2 + p^4 + \mu)^2 + v_0^2 p^2]^{1/2}\}^{1/2}} = 1. \tag{3.16}$$

The resulting v_0 as a function of μ is plotted in figure 1(b). Note that the velocity in physical units (with $\kappa = d = 1$) is given by

$$v = (2^{3/2}\xi_y/\tau_0)\epsilon^{3/4}|Q|^{3/2}v_0. \tag{3.17}$$

It is not entirely meaningless to extend, in figure 1(b), the curve to the left of the axis of ordinates; since the zig-zag instability takes a long time to develop when one is just slightly on the unstable side of the zig-zag instability line, it is still possible (Pocheau and Croquette 1984, Croquette and Pocheau 1984) to observe the steady dislocation motion. In particular, in the $\mu \rightarrow 0$ limit (absence of mean-drift flow), the climb velocity remains finite

$$v_0 = 2^{-7/4}[K(\sin \frac{3}{8}\pi)]^{-1} = 0.1098 \tag{3.18}$$

where K is the complete elliptic integral of the first kind.

It is of great interest to test our theoretical results experimentally since the free-slip boundary condition is also experimentally realisable (Goldstein and Graham 1969).

4. Rigid boundaries

In the case of the no-slip boundary condition, one finds that the vertical vorticity now obeys the following amplitude equation:

$$(\partial_t - c\sigma)\omega_z = 2\partial_y\{A^*[\partial_x + (1/i2q_0)\partial_y^2]A + cC\}, \tag{4.1}$$

with a constant c which may depend on σ in general and is as yet undetermined. Scaling as before (see (3.5)), we obtain (3.6a), (3.6c) and, instead of (3.6b), the following equation

$$\left(\frac{\epsilon}{\tau_0}\partial_T - c\sigma\right)\omega_z = \frac{\tau_0\epsilon^{1/2}}{\tilde{g}q_0\xi_0}\partial_Y[A^*(\partial_X - i\partial_Y^2)A + cC], \tag{4.2}$$

with, of course, the appropriate parameters for rigid boundaries. In considering slow steady dislocation motion, the first term on the left-hand side of (4.2) can be dropped‡.

† It reads

$$H = \frac{1}{2} \iint d\mathbf{x} d\mathbf{y} [\partial_x \phi + (\partial_x \phi)^2 - (\partial_y \phi)^2 + (\partial_y^2 \phi)^2 + \mu \phi^2],$$

where the restriction $\iint d\mathbf{x} d\mathbf{y} \phi = 0$ is to be understood to preserve the gauge invariance.

‡ This is justified for $v\epsilon^{1/4}/\xi_y \ll c\sigma$ where v is the dislocation climb velocity. This v is evaluated below and is found to behave as $\epsilon^{3/4}$, see (4.13). Thus the condition for this adiabatic approximation is well borne out.

Thus, we consider the amplitude equations of the following form

$$\partial_T A = A + (\partial_X - i\partial_Y^2)^2 A - |A|^2 A - iB_x A, \tag{4.3a}$$

$$(\partial_Y^2 + \delta\partial_X^2) B_x = -c_1 \sqrt{\varepsilon} \partial_Y^2 [A^* (\partial_X - i\partial_Y^2) A + c.c.], \tag{4.3b}$$

where

$$c_1 \equiv -\sigma^{-1} \tau_0 / c\tilde{g}q_0\xi_0. \tag{4.4}$$

With the following choice of the parameters (Cross 1980):

$$\begin{aligned} q_0 &= 3.117, & \xi_0^2 &= 0.148, & \tau_0 &= (0.5117 + \sigma) / 19.65\sigma, \\ \tilde{g} &= 0.6995 - 0.0047\sigma^{-1} + 0.0083\sigma^{-2}, \end{aligned} \tag{4.5}$$

one restores the amplitude equations introduced first by Siggia and Zippelius (1981b, Zippelius and Siggia 1982, 1983). It should be stressed, however, that (4.3b) is not systematic in any small parameter, and other non-linearities are present to the same order in ε which have not been retained. Nonetheless we adhere to this ansatz, originally due to Siggia and Zippelius (1981b, Zippelius and Siggia 1982, 1983), and expect the ansatz to capture the main effects of vertical vorticity.

We now proceed with the same approximations as in the free-slip case and we find the linearised equation

$$\begin{aligned} \partial_T \phi &= \{[(1 - 3Q^2)/(1 - Q^2)]\partial_X^2 + 2Q\partial_Y^2 - \partial_Y^4\} \phi \\ &\quad - (\partial_Y^2 + \delta\partial_X^2)^{-1} \partial_Y^2 [2g'(1 - Q^2)\partial_Y^2 - 2g'Q\partial_X^2] \phi, \end{aligned} \tag{4.6}$$

where $g' \equiv -c_1 \sqrt{\varepsilon}$. The non-local term arises from the generation of the vertical vorticity. Note that this term is already of $O(\varepsilon^{1/2})$. Together with this fact, recall that the parameter δ should be retained to give rise to either the Eckhaus or skewed-varicose instabilities (Siggia and Zippelius 1981b, Zippelius and Siggia 1982, 1983). However, at moderate Prandtl numbers these two instabilities (as well as the cross-roll instability (Busse and Whitehead 1971)) can be neglected near the convective threshold. Therefore, so long as we are restricted to a moderate Prandtl number regime, we only have to be concerned with the zig-zag and knot instabilities (Busse and Clever 1979, in particular their figure 1), the latter being associated with disturbances of large wavenumbers, which cannot be described by our phase dynamics. Thus we may set $\delta = 0$, and we assume in the following that the stability domain of our interest near the zig-zag instability remains unaffected by the knot instability. The phase equation is then greatly simplified as

$$\partial_T \phi = [\tilde{D}_\parallel(Q)\partial_X^2 + \tilde{D}_\perp(Q)\partial_Y^2 - \partial_Y^4] \phi \tag{4.7}$$

where \tilde{D}_\parallel and \tilde{D}_\perp are the longitudinal and transverse diffusion coefficients defined by

$$\begin{aligned} \tilde{D}_\parallel(Q) &\equiv (1 - 3Q^2)/(1 - Q^2) + 2g'Q, \\ \tilde{D}_\perp(Q) &\equiv 2Q - 2g'(1 - Q^2). \end{aligned} \tag{4.8}$$

Since the zig-zag instability occurs for $\tilde{D}_\perp < 0$, we take hereafter $\tilde{D}_\perp > 0$.

The calculation of the climb velocity is almost the same as in the free-slip case. That is, making use of the rescaled variables

$$x = (\tilde{D}_\perp / \sqrt{\tilde{D}_\parallel}) X, \quad y = \sqrt{\tilde{D}_\perp} Y, \quad t = \tilde{D}_\perp^2 T \tag{4.9}$$

(4.7) reduces to

$$\partial_x \phi = (\partial_x^2 + \partial_y^2 - \partial_z^2) \phi - 2\pi \delta'(x) \theta(y - v_0 t) \tag{4.10}$$

with $\phi = \phi(x, y - v_0 t)$. Therefore, v_0 satisfies the equation

$$\sqrt{2} v_0 \int_0^\infty \frac{dp}{\{p^2 + p^4 + [(p^2 + p^4)^2 + v_0^2 p^2]^{1/2}\}^{1/2}} = 1, \tag{4.11}$$

which yields

$$v_0 = 2^{-7/4} [K(\sin \frac{1}{8} \pi)]^{-1} = 0.1684. \tag{4.12}$$

Thus, the climb velocity is given in physical units (with $\kappa = d = 1$) by†

$$v = (\xi_y / \tau_0) \varepsilon^{3/4} \tilde{D}_\perp^{3/2} v_0 \tag{4.13a}$$

$$= \beta \frac{6.4098}{1 + 0.5117 \sigma^{-1}} \left(\frac{q - q_0}{q_0} + \varepsilon \tilde{N}(\sigma) \right)^{3/2}, \tag{4.13b}$$

where in going to (4.13b) from (4.13a) we have used the scaling factors (4.5), and

$$\beta \equiv 2\sqrt{2} v_0, \quad \tilde{N}(\sigma) \equiv c_1 / 2q_0 \xi_0. \tag{4.14}$$

It follows as a consequence of (4.13) that the zero-velocity criterion is $\tilde{D}_\perp = 0$, i.e. it falls upon the zig-zag instability line. If the as yet undetermined parameter c (and hence c_1) is specified as

$$\tilde{N}(\sigma) \rightarrow N(\sigma) \equiv \frac{0.1659 + 23.0395 \sigma^{-1} + 6.1961 \sigma^{-2}}{10.7580 - 0.0726 \sigma^{-1} + 0.1281 \sigma^{-2}} \tag{4.15}$$

so as to make our transverse diffusion coefficient \tilde{D}_\perp coincide with that of Manneville and Piquemal (1983), we obtain from (4.13b)

$$v = \beta \frac{6.4098}{1 + 0.5117 \sigma^{-1}} \left(\frac{q - q_0}{q_0} + \varepsilon N(\sigma) \right)^{3/2}. \tag{4.16}$$

The dislocation velocity of this form was conjectured by Pocheau and Croquette (1984) where β was experimentally determined to be 0.78. The reason for the discrepancy with our theoretical value 0.4762 is not well understood at this moment and may well signal an inadequacy of the linear elasticity treatment of the phase equation for dislocation. Note that in this treatment the only effect of the drift flow is to modify the diffusion coefficients and hence the value of β should remain unaffected. It is thus interesting that the value $\beta = 0.84$ found by numerical simulation of the amplitude equation without the drift flow (Siggia and Zippelius 1981a) is close to the experimental value as noted by Pocheau and Croquette (1984).

Another interesting point to notice in the experimental observations of Croquette and Pocheau (Pocheau and Croquette 1984, Croquette and Pocheau 1984) is the fact that the climb motion slows down near the sidewall (perpendicular to rolls). Such behaviour can be understood as being caused by the repelling force on the dislocation exerted by the rigid sidewall. The detailed study of this force, however, will be presented in appendix 2. There we show that the condition that rolls are perpendicular to the lateral boundary is responsible for the repulsion.

† In contrast with the free-slip case where the transverse diffusion coefficient is rendered non-existent, for rigid boundaries the presence of vertical vorticity just renormalises the bare diffusion coefficients as (4.8). Thus, the result of Siggia and Zippelius (1981a), who neglected the drift flow induced by the vertical vorticity, can simply be carried over in this case with their diffusion coefficients replaced by the renormalised ones (4.8). Note, however, that their equations (3.10) and (3.11a) should be corrected; their parameters α and β correspond to our v_0^2 and β , respectively.

5. Concluding remarks

We have demonstrated how the presence of the slow drift flow generated by the vertical vorticity affects the dislocation motion. Indeed our results demonstrate significant modifications of the original theoretical prediction of Siggia and Zippelius (1981a) by the drift flow.

It might be pointed out that our analyses in this paper are greatly facilitated by our restriction to the cases with potentials. In particular, in the free-slip boundary case where the stability of the roll pattern itself is found in a small fraction of the stability diagram (Busse and Bolton 1984, Bolton and Busse 1985), the domain of validity of our approximate calculation is rather limited. Nonetheless, we expect that the result presented in § 3 can be meaningfully compared with experiments.

Since our prediction (4.16) for the dislocation climb for rigid boundaries seems to have been well verified by the experiment of Croquette and Pocheau (Pocheau and Croquette 1984, Croquette and Pocheau 1984), we comment on the free-slip case by comparison with the numerical simulations of the Boussinesq equations performed by Siggia and Zippelius (1981a). Firstly, in their results one can clearly see the ϵ dependence of the climb velocity, which differs from their result of analytic calculations based on the amplitude equation without the effect of the drift flow, but in accord with our result, figure 1(b). Secondly, their simulation data were for $Q \geq 0$, where existing theories (Siggia and Zippelius 1981b, Zippelius and Siggia 1982, 1983, Busse and Bolton 1984, Bolton and Busse 1985) predict the loss of stability of the roll patterns. At the same time, our analysis in § 3 is not expected to be valid for $Q \approx 0$ where the proximity to the skewed-varicose instability should be taken into account. With these reservations, both the Prandtl number dependence and the order of magnitude of the climbing velocity obtained by the simulation (table II of Siggia and Zippelius 1981a) are in qualitative agreement with our result. It is of prime importance for the approach presented here to examine the neglected non-linearities in deformations as well as to explore a possibility of extending the results to situations that cannot be described by

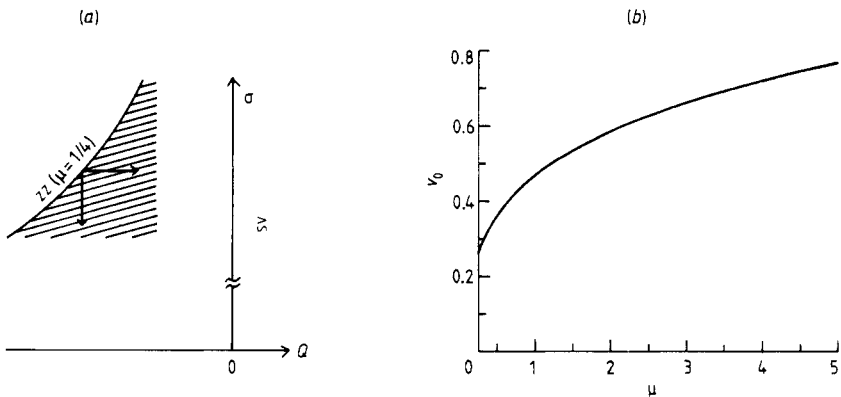


Figure 1. (a) Typical stability diagram for our model at high Prandtl numbers as a function of the Prandtl number σ and $Q = (\xi_0/\epsilon^{1/2})(q - q_0)$ for the free-slip boundary condition. ZZ and SV stand for the zig-zag and skewed-varicose instabilities respectively. The stable roll pattern falls between the two curves. The arrows indicate two representative paths of increasing the parameter μ . (b) Dimensionless climb velocity v_0 as a function of the parameter $\mu \propto \sigma^{-1}/Q^2$.

a potential. Lastly, in the simulation two blobs of vertical vorticity of opposite sign were observed near the dislocation core. Although the experiment (with the cylindrical container) of Croquette *et al* (1983) failed to see these blobs, it might well be that the amplitude variations (such as an amplitude overshoot as suggested by Manneville (Croquette *et al* 1983)) are involved in its generation. In that case, the rapid spatial (and possibly temporal) variations of the amplitude around the core region should be considered, a description of which is beyond the scope of our present approach.

It has been suggested by several workers (Toner and Nelson 1981, Guazzelli *et al* 1983, Dubois-Violette *et al* 1983) that there should be a close analogy between the thermoconvective motion of roll structures and the dynamics of the layered smectic A liquid crystals. In fact, a slight modification of our model (2.1) and (2.3) can give the equations of motion for the smectic A liquid crystals. They read, in appropriate units,

$$\partial_t \phi = -\lambda_p \delta H_0 / \delta \phi - \mathbf{B} \cdot \nabla \phi, \tag{5.1}$$

$$\partial_t (\nabla \times \mathbf{B}) + \nabla \times (\hat{\zeta} \cdot \mathbf{B}) = -\nabla \phi \times \nabla \delta H_0 / \delta \phi, \quad \nabla \cdot \mathbf{B} = 0 \tag{5.2}$$

with the smectic elastic energy H_0 . Here ϕ represents the phase of the one-dimensional mass-density wave along the x direction (perpendicular to the layers). Equation (5.1) describes the permeation process characterised by the parameter λ_p . Equation (5.2) for the velocity field \mathbf{B} now involves the viscosity tensor (Martin *et al* 1972) η via the differential tensor operator $\hat{\zeta}$ as

$$(\hat{\zeta} \cdot \mathbf{B})_i \equiv \nabla_j \eta_{ijkl} \nabla_k B_l. \tag{5.3}$$

If we take the y axis to point along the layering, the diagonal tensor operator $\hat{\zeta}$ has components

$$\begin{aligned} \hat{\zeta}_{xx} &= (\eta_1 - \eta_3 - \eta_5) \partial_x^2 + \eta_3 \partial_y^2, \\ \hat{\zeta}_{yy} &= \eta_3 \partial_x^2 + (\eta_2 - \eta_3 + \eta_4 - \eta_5) \partial_y^2. \end{aligned} \tag{5.4}$$

Equations (5.1) and (5.2) are the simple generalisation of the constitutive equations proposed by Dubois-Violette *et al* (1983). Work on the smectic A phase has so far been conducted with the conventional linearised description. However, recent theoretical studies (Mazenko *et al* 1982, 1983) of (5.1) and (5.2), and experiments (Bhattacharya and Ketterson 1982, Marcerou *et al* 1984, Galloni and Martinoty 1985, Baumann *et al* 1985) as well, reveal that certain non-linearities demanded by rotational invariance cause the breakdown of the conventional treatment. In this connection, it will be fruitful to pursue the question of whether, in the convection problem too, non-linear terms in hydrodynamic modes (Newell 1982, Manneville 1983b, Cross and Newell 1984, Kuramoto 1984, Brand 1984, Greenside and Cross 1985) and/or the Euclidean invariance exert such profound effects on the picture presented in this paper.

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Appendix 1

In this appendix, the frictional force X_r will be calculated for steady defect motion. For that purpose, a single-valued phase variable is used, so that we introduce a line

of phase jump $\zeta(\mathbf{r}) = 0, \eta(\mathbf{r}) > 0$, emerging from $\mathbf{r} = \mathbf{R}$ (or $\zeta = \eta = 0$) or otherwise arbitrary (Brand and Kawasaki 1984, Kawasaki 1984b, c).

The phase equation (2.6) with (2.7) can be solved readily to give

$$\phi(\mathbf{r}) = 2\pi(E - \mathbf{v}_0 \cdot \nabla)^{-1} \hat{\mathbf{E}} \cdot \theta(\eta) \nabla \theta(\zeta) + \phi'(\mathbf{r}) \tag{A1.1}$$

with ϕ' satisfying $(E - \mathbf{v}_0 \cdot \nabla)\phi' = 0$. The differential operator $\hat{\mathbf{E}}$ is defined by (2.12) and $\theta(x)$ is the unit step function. Equivalently we can take

$$\mathbf{m}(\mathbf{r}) \equiv \nabla \phi(\mathbf{r}) = 2\pi \nabla (E - \mathbf{v}_0 \cdot \nabla)^{-1} \hat{\mathbf{E}} \cdot \theta(\eta) \nabla \theta(\zeta) - 2\pi \theta(\eta) \nabla \theta(\zeta) + \nabla \phi', \tag{A1.2}$$

since \mathbf{m} should have a singularity only at $\mathbf{r} = \mathbf{R}$. The function ϕ' can be ignored hereafter because it gives rise to the static force. Then

$$\begin{aligned} \mathbf{m} &= 2\pi(E - \mathbf{v}_0 \cdot \nabla)^{-1} [\nabla(\hat{\mathbf{E}} - \mathbf{v}_0) - \mathbf{1} \cdot \nabla(\hat{\mathbf{E}} - \mathbf{v}_0) + \nabla \mathbf{v}_0] \cdot \theta(\eta) \nabla \theta(\zeta) \\ &= 2\pi(E - \mathbf{v}_0 \cdot \nabla)^{-1} [\hat{\mathbf{z}} \times (\hat{\mathbf{E}} - \mathbf{v}_0) \delta(\mathbf{r} - \mathbf{R}) + \nabla(\theta(\eta) \mathbf{v}_0 \cdot \nabla \theta(\zeta))] \end{aligned} \tag{A1.3}$$

where $\mathbf{1}$ is the unit tensor, and we have used the following identities (Kawasaki 1984c): for any two-component vectors \mathbf{B}_1 and \mathbf{B}_2

$$\mathbf{B}_1 \mathbf{B}_2 - (\mathbf{B}_1 \cdot \mathbf{B}_2) \mathbf{1} = -(\hat{\mathbf{z}} \times \mathbf{B}_2)(\hat{\mathbf{z}} \times \mathbf{B}_1), \tag{A1.4a}$$

and

$$(\hat{\mathbf{z}} \times \nabla) \cdot \theta(\eta) \nabla \theta(\zeta) = -\zeta(\mathbf{r} - \mathbf{R}). \tag{A1.4b}$$

Here we make use of the arbitrariness of the direction of the line $\zeta = 0$ to choose $\mathbf{v}_0 \cdot \nabla \theta(\zeta) = 0$. Thus we obtain

$$\mathbf{m}(\mathbf{r}) = 2\pi \hat{\mathbf{z}} \times (\hat{\mathbf{E}} - \mathbf{v}_0)(E - \mathbf{v}_0 \cdot \nabla)^{-1} \delta(\mathbf{r} - \mathbf{R}). \tag{A1.5}$$

Now we calculate the frictional force \mathbf{X}_{fr} , which is (Kawasaki 1984c)

$$\mathbf{X}_{fr} = 2\pi \omega_{fr} \times \hat{\mathbf{z}} \tag{A1.6a}$$

with

$$\omega_{fr} = 2a_0^2 \mathbf{K} \cdot \mathbf{v}_{fr}, \quad \mathbf{v}_{fr} \equiv \mathbf{m}(\mathbf{R}) - \mathbf{m}(\mathbf{R})|_{\mathbf{v}_0=0}, \tag{A1.6b}$$

where the tensor operator \mathbf{K} is defined by

$$\hat{\mathbf{E}} = -\nabla \cdot \mathbf{K} = -\mathbf{K} \cdot \nabla. \tag{A1.7}$$

It is easy to prove the following property for any differential operator $\hat{Q}(\nabla)$:

$$\hat{Q}(\nabla) \delta(\mathbf{r} - \mathbf{R})|_{\mathbf{r}=\mathbf{R}} = \hat{Q}(-\nabla) \delta(\mathbf{r} - \mathbf{R})|_{\mathbf{r}=\mathbf{R}}. \tag{A1.8}$$

Since $\hat{\mathbf{E}}(\nabla) = -\hat{\mathbf{E}}(-\nabla)$, $E(\nabla) = E(-\nabla)$ and $\mathbf{K}(\nabla) = \mathbf{K}(-\nabla)$, we then find that

$$\begin{aligned} \mathbf{m}(\mathbf{R}) &= -2\pi \hat{\mathbf{z}} \times (\hat{\mathbf{E}} + \mathbf{v}_0)(E + \mathbf{v}_0 \cdot \nabla)^{-1} \delta(\mathbf{r} - \mathbf{R})|_{\mathbf{r}=\mathbf{R}} \\ &= -2\pi \hat{\mathbf{z}} \times [\nabla \times (\mathbf{v}_0 \times \hat{\mathbf{E}})](E - \mathbf{v}_0 \cdot \nabla)^{-1} (E + \mathbf{v}_0 \cdot \nabla)^{-1} \delta(\mathbf{r} - \mathbf{R})|_{\mathbf{r}=\mathbf{R}} \\ &= 2\pi \nabla \mathbf{v}_0 \cdot (\hat{\mathbf{z}} \times \hat{\mathbf{E}})(E - \mathbf{v}_0 \cdot \nabla)^{-1} (E + \mathbf{v}_0 \cdot \nabla)^{-1} \delta(\mathbf{r} - \mathbf{R})|_{\mathbf{r}=\mathbf{R}}. \end{aligned} \tag{A1.9}$$

Note that $\mathbf{m}(\mathbf{R})$ has no part independent of \mathbf{v}_0 . Therefore, we immediately find that

$$\omega_{fr} = -4\pi a_0^2 \hat{\mathbf{E}} \mathbf{v}_0 \cdot (\hat{\mathbf{z}} \times \hat{\mathbf{E}})(E - \mathbf{v}_0 \cdot \nabla)^{-1} (E + \mathbf{v}_0 \cdot \nabla)^{-1} \delta(\mathbf{r} - \mathbf{R})|_{\mathbf{r}=\mathbf{R}}, \tag{A1.10}$$

to obtain the result (2.10c) with the expression (2.11).

Alternatively, we can start with (2.19) of Kawasaki (1984c) which we write as

$$\mathbf{X}_l = \mathbf{X}_s + \mathbf{X}_{fr}, \quad \mathbf{X}_{fr} = \int d\mathbf{r} \mathbf{A}(\mathbf{r}) \nabla \cdot \tilde{\omega}(\mathbf{r}), \tag{A1.11}$$

where $\tilde{\omega}$ is defined by (2.9). Here, however, \mathbf{A} must be taken to be $\nabla \phi$ of the moving defect, i.e. \mathbf{m} . Then it follows, with the help of (A1.8) and $\nabla \cdot \tilde{\omega} = 2a_0^2 \partial_t \phi = -2a_0^2 \mathbf{v}_0 \cdot \mathbf{m}$,

that

$$\begin{aligned} \mathbf{X}_{fr} &= -2a_0^2 \int d\mathbf{r} \mathbf{m}(\mathbf{r}) \mathbf{v}_0 \cdot \mathbf{m}(\mathbf{r}) \\ &= 8\pi^2 a_0^2 [\hat{\mathbf{z}} \times (\hat{\mathbf{E}} + \mathbf{v}_0)] (E + \mathbf{v}_0 \cdot \nabla)^{-1} [\hat{\mathbf{z}} \times (\hat{\mathbf{E}} - \mathbf{v}_0)] (E - \mathbf{v}_0 \cdot \nabla)^{-1} \delta(\mathbf{r} - \mathbf{R}) \Big|_{\mathbf{r}=\mathbf{R} \cdot \mathbf{v}_0} \\ &= 8\pi^2 a_0^2 (\hat{\mathbf{z}} \times \hat{\mathbf{E}}) (\hat{\mathbf{z}} \times \hat{\mathbf{E}}) (E + \mathbf{v}_0 \cdot \nabla)^{-1} (E - \mathbf{v}_0 \cdot \nabla)^{-1} \delta(\mathbf{r} - \mathbf{R}) \Big|_{\mathbf{r}=\mathbf{R} \cdot \mathbf{v}_0} \end{aligned} \quad (\text{A1.12})$$

leading to the result (2.11). Equation (A1.12) with (2.10c) also gives the expression

$$\mathcal{D}^*(\mathbf{v}_0) = 2a_0^2 \int d\mathbf{r} \mathbf{m}(\mathbf{r}) \mathbf{m}(\mathbf{r}). \quad (\text{A1.13})$$

The energy dissipation rate Φ is now obtained as

$$\Phi = \mathbf{X}_l \cdot \mathbf{v}_0 - \int d\mathbf{r} \partial_t \phi \delta H / \delta \phi \quad (\text{A1.14})$$

which consists of dissipations occurring at the defect core and in the surrounding phase field. Use of the phase equation $\delta H / \delta \phi = 2a_0^2 \partial_t \phi$ yields

$$\Phi = \mathbf{X}_l \cdot \mathbf{v}_0 - 2a_0^2 \mathbf{v}_0 \cdot \int d\mathbf{r} \mathbf{m}(\mathbf{r}) \mathbf{m}(\mathbf{r}) \cdot \mathbf{v}_0. \quad (\text{A1.15})$$

This leads to (2.14) with the use of (2.8) and (A1.13).

Appendix 2

This appendix is devoted to considering how the presence of a rigid sidewall affects the strength of the local force on the dislocation.

The static distortion of the phase field due to a single dislocation a distance $y_0/2$ away from the rigid surface ($y=0$) in the negative y direction is determined by the following boundary-value problem (see (4.7); throughout this appendix we write $D_{\parallel}(D_{\perp})$ and $x(y)$ in place of $\tilde{D}_{\parallel}(\tilde{D}_{\perp})$ and $X(Y)$):

$$(D_{\parallel} \partial_x^2 + D_{\perp} \partial_y^2 - \partial_y^4) \phi(\mathbf{r}) = 2\pi s D_{\parallel} \delta'(x) \theta(y + \frac{1}{2} y_0) \quad (\text{A2.1a})$$

with the Neumann boundary condition† (Cross 1982)

$$\partial_y \phi = 0 \quad \text{at } y = 0, \quad (\text{A2.1b})$$

where the parameter s specifies the sign of the phase jump 2π of the dislocation, and $\theta(x)$ is the usual unit step function. The appropriate Green function for the bounded space ($y \leq 0$), $G_B(\mathbf{r}, \mathbf{r}')$, is given in terms of the one for the unbounded space, $G(\mathbf{r}, \mathbf{r}')$, as

$$G_B(\mathbf{r}, \mathbf{r}') = G(\mathbf{r} - \mathbf{r}') + G(\mathbf{r} - \mathbf{r}'_1), \quad G(\mathbf{r} - \mathbf{r}') \equiv G(\mathbf{r}, \mathbf{r}') \quad (\text{A2.2})$$

where $\mathbf{r}' = (x', y')$, $\mathbf{r}'_1 = (x', -y')$ and G satisfies the equation

$$(D_{\parallel} \partial_x^2 + D_{\perp} \partial_y^2 - \partial_y^4) G(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'). \quad (\text{A2.3})$$

Therefore, the boundary-value problem (A2.1) can be solved by locating an image dislocation of the same type directly above the true dislocation situated at a distance

† In the absence of boundary forcing, the phase ϕ at the boundary is arbitrary up to a constant.

$y_0/2$ above the boundary surface. The dislocation will then experience a force due to the image dislocation. Accordingly, we turn to the problem of obtaining an interaction force between two dislocations in the unbounded domain.

Within the theory linearised in the extra phase gradient $\nabla\phi$ due to dislocations, the phase distortion exerts on the dislocation (with its sign s_1) at \mathbf{r} the local force (Kawasaki 1984c)

$$\mathbf{X}(x, y) \equiv \mathbf{X}_l(\mathbf{r}) = 2\pi a_0^2 s_1 [\hat{x}(D_\perp - \partial_y^2)\partial_y\phi(\mathbf{r}) - \hat{y}D_\parallel\partial_x\phi(\mathbf{r})], \quad (\text{A2.4})$$

where a_0 is the eikonal value of the amplitude and \hat{x} (or \hat{y}) is the unit vector along the x (or y) axis. The phase distortion $\phi(x, y)$ at a point \mathbf{r} when a dislocation with sign s_2 is located at the origin can be obtained, once $G(\mathbf{r})$ is known, as

$$\begin{aligned} \phi(x, y) &= -2\pi s_2 D_\parallel \int_0^\infty dy' \partial_x G(x, y - y') \\ &= s_2 \operatorname{sgn} x \left[\frac{\pi}{2} + \int_0^\infty dp \frac{\sin py}{p} \exp\left(-\frac{|x|}{\sqrt{D_\parallel}} p (D_\perp + p^2)^{1/2}\right) \right], \end{aligned} \quad (\text{A2.5})$$

where the term $\pi/2$ in the square brackets arises from taking the upper limit of the integration over y' to infinity at the last step of the calculation and represents the phase jump associated with the dislocation. The well known expressions (Siggia and Zippelius 1981a, Guazzelli *et al* 1983) for the phase distortion field in the two limiting cases may be recovered by approximating the integral in (A2.5) as follows:

$$\int_0^\infty dp \frac{\sin py}{p} \exp\left(-\frac{|x|}{\sqrt{D_\parallel}} p^2\right) = \frac{\pi}{2} \operatorname{erf}\left(\frac{D_\parallel^{1/4} y}{2\sqrt{|x|}}\right) \quad (\text{A2.6a})$$

for $D_\perp^{1/2} y \ll 1$ (smectic regime (de Gennes 1972, Pershan 1974, Toner and Nelson 1981, Kawasaki† 1984c))

$$\int_0^\infty dp \frac{\sin py}{p} \exp\left(-\left(\frac{D_\perp}{D_\parallel}\right)^{1/2} |x| p\right) = \tan^{-1}\left(\left(\frac{D_\parallel}{D_\perp}\right)^{1/2} \frac{y}{|x|}\right)$$

for $D_\perp^{1/2} y \gg 1$ (xy regime‡). (A2.6b)

However, in calculating the interaction force the approximation should be employed with circumspection since (A2.4) involves gradients of ϕ . In fact, except for the case $D_\perp = 0$ where the replacement (A2.6a) becomes exact, the approximant (A2.6a) fails to reproduce the correct behaviour of the force in the smectic regime as given by (A2.12a) below.

Now the force acting on a dislocation at \mathbf{r}_1 due to another at \mathbf{r}_2 is readily found, by inserting (A2.5) into (A2.4), to be

$$\begin{aligned} X_x(x, y) &= 2\pi a_0^2 s_1 s_2 \cdot \operatorname{sgn} x \cdot D_\perp^{3/2} \int_0^\infty dp e^{-|x|p\sqrt{1+p^2}} (1+p^2) \cos py, \\ X_y(x, y) &= 2\pi a_0^2 s_1 s_2 \cdot \sqrt{D_\parallel} D_\perp \int_0^\infty dp e^{-|x|p\sqrt{1+p^2}} (1+p^2)^{1/2} \sin py, \end{aligned} \quad (\text{A2.7})$$

† In equations (4.17b) and (4.19) of this reference, $k|x|^{-1/2}$ and $|z| \operatorname{erfc}|z|$ should be replaced by $k^{1/2}|x|^{-1/2}$ and $-|z| \operatorname{erfc}|z|$, respectively.

‡ Note that this terminology implies an analogy to the superfluid with regard to the strain field, not to the force between vortices. (In (A2.4) higher spatial derivatives in x were dropped, which must be restored to recover an xy symmetry of the force.)

where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \equiv (x, y)$, $\underline{x} \equiv (D_{\perp}/\sqrt{D_{\parallel}})x$, $\underline{y} \equiv \sqrt{D_{\perp}}y$, and s_1 and s_2 are the signs of phase jumps of the two dislocations. In particular[†],

$$X_x(0, y) = 0 \tag{A2.8}$$

and

$$X_y(y) \equiv X_y(0, y) = 2\pi a_0^2 s_1 s_2 \sqrt{D_{\parallel}} D_{\perp} \int_0^{\infty} dp e^{-\delta p} (1+p^2)^{1/2} \sin py \tag{A2.9}$$

where it is understood that the limit $\delta \rightarrow 0+$ be taken after integration. Carrying out the integration and through a little calculation, we finally find (we take $y \geq 0$ for convenience)

$$X_y(y) = 2\pi a_0^2 s_1 s_2 \sqrt{D_{\parallel}} D_{\perp} S(\underline{y}) \tag{A2.10}$$

with

$$S(z) \equiv \int_0^1 dt e^{-zt} (1-t^2)^{1/2} = \frac{\pi}{2z} [I_1(z) - L_1(z)]. \tag{A2.11}$$

Here $I_n(z)$ and $L_n(z)$ are the modified Bessel function of the first kind and the modified Struve function, respectively. Both large- and small-distance behaviour of X_y can be deduced from inspection of (A2.11) as

$$X_y(y) = 2\pi a_0^2 s_1 s_2 \sqrt{D_{\parallel}} D_{\perp} \times \begin{cases} \pi/4 - \underline{y}/3 + O(\underline{y}^2) & \underline{y} \ll 1 \\ 1/\underline{y} - 1/\underline{y}^3 + O(\underline{y}^{-5}) & \underline{y} \gg 1. \end{cases} \tag{A2.12a}$$

$$\tag{A2.12b}$$

In figure 2, the image force on the dislocation, $X_y(y_0)$ with $s_1 s_2 = 1$, or the function $S(\underline{y}_0)$ is illustrated as a function of its separation from the sidewall, $y_0/2$. As expected, the force is repulsive, and the closer the dislocation lies to the sidewall, the stronger it is repelled by the wall.

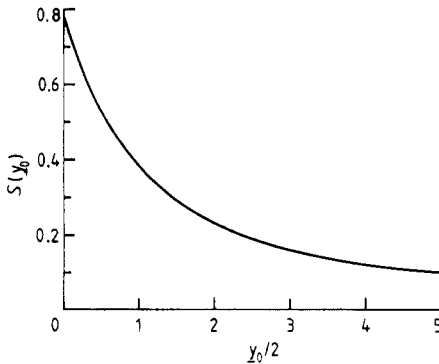


Figure 2. Image force $X_y(y_0)$ on the dislocation at a distance $y_0/2$ from the rigid sidewall; $\underline{y}_0 \equiv \sqrt{D_{\perp}}y_0$, $S(\underline{y}_0) = X_y(y_0)/2\pi a_0^2 \sqrt{D_{\parallel}} D_{\perp}$ with $s_1 s_2 = 1$.

[†] The integral in the expression for X_x in (A2.7) is examined and is found to vanish smoothly at $x = 0$.

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