Dynamics of line singularities

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Abstract

The dynamics of line singularities in three different physical systems are considered, namely vortices in an inviscid fluid, vortices in a type-II supercondctor, and dislocations in an elastic crystal. When the core of the singularity can be regularised with a continuum model, as is the case for superconducting and fluid vortices, the dynamics can be derived systematically in the asymptotic limit as the core radius tends to zero. The asymptotic analysis is more difficult when the core of the singularity is so small as to demand an atomic model, as is the case for dislocations, where the derivation of a law of motion is still an open problem in the mathematical sense.

1 Introduction

Almost all the physical problems discused in this volume have the common theme that they can be crudely modelled by fairly straightforward partial differential equations whose solutions in three-dimensional space are singular along certain lines. However, the position of those lines is not known a priori but needs to be determined as part of the problem[1]. This aspect of the problem introduces nonlinearity and demands the existence of some regularising mechanism that is active only in the core of the singularity: mathematical analysis is then necessary to quantify the long-range effect of this regularising mechanism and hence deduce the dynamics of the line singularity.

[1]Thus they can be thought of as "codimension-two" free boundary problems [10].

The aim of this paper is to demonstrate the basic steps in finding models for the dynamics of vortices in fluids, superconductors and dislocations in crystals. The basic mathematical idea is the same in all three cases but the last example is much the most complicated technically because it is the only case in which the regularising effects in the core occur on an atomistic scale. Indeed, the difficulty of arranging the marriage between a discrete core and a continuum model further away seems to be the principal mathematical obstacle to further understanding of several aspects of metal plasticity.

2 Vortices in an inviscid fluid

A line vortex lying along a curve Γ in an incompressible, inviscid and otherwise irrotational fluid is a solution of the following equations:

$$\begin{aligned} \operatorname{div} \boldsymbol{u} &= 0, & (1)\\ \operatorname{curl} \boldsymbol{u} &= \omega_0 \boldsymbol{\delta}_\Gamma(\boldsymbol{x}). & (2) \end{aligned}$$

Here $\boldsymbol{u}$ is the fluid velocity, $\omega_0 = 2\pi\gamma$ is the circulation around the vortex, where γ is the vortex strength, and

$$\boldsymbol{\delta}_\Gamma(\boldsymbol{x}) = \int_\Gamma \delta(x - x')\delta(y - y')\delta(z - z')\, d\boldsymbol{x}', \tag{3}$$

where $\delta(x)$ is the Dirac δ-function. By virtue of (1), we may define a vector stream function $\boldsymbol{\Omega}$ satisfying:

$$\begin{aligned} \operatorname{curl} \boldsymbol{\Omega} &= \boldsymbol{u}, & (4)\\ \operatorname{div} \boldsymbol{\Omega} &= 0, & (5) \end{aligned}$$

(for two-dimensional flows $\boldsymbol{\Omega} = (0, 0, \psi)$ where ψ is the usual stream function). We then find that

$$-\nabla^2 \boldsymbol{\Omega} = \omega_0 \boldsymbol{\delta}_\Gamma(\boldsymbol{x}), \tag{6}$$

and hence, using the Green's function for the Laplacian in $\mathbb{R}^3$,

$$\begin{aligned} \boldsymbol{\Omega} &= \frac{\omega_0}{4\pi} \int_\Gamma \frac{1}{s}\, d\boldsymbol{x}', & (7)\\ \boldsymbol{u} &= \frac{\omega_0}{4\pi} \int_\Gamma \nabla\left(\frac{1}{s}\right) \wedge d\boldsymbol{x}' = -\frac{\omega_0}{4\pi} \int_\Gamma \frac{\boldsymbol{s} \wedge d\boldsymbol{x}'}{s^3}, & (8) \end{aligned}$$

where $\boldsymbol{s} = \boldsymbol{x} - \boldsymbol{x}'$ and $s = |\boldsymbol{s}|$. This is the familiar Biot-Savart law.

The motion of the vortex is determined by the local fluid velocity. Asymptotically expanding (8) as the point $\boldsymbol{x}$ approaches the vortex gives [17][2]

$$\boldsymbol{u} \sim \frac{\omega_0}{2\pi r}\boldsymbol{e}_\theta - \frac{\omega_0}{4\pi}K\ \log(r)\,\boldsymbol{b} + \cdots, \tag{9}$$

where r and θ are local polar coordinates, $\boldsymbol{e}_\theta$ is the unit vector in the azimuthal direction, K is the curvature of the vortex line, and $\boldsymbol{b}$ is the unit binormal. Since the vortex moves with the fluid we must evaluate (9) as $r \to 0$. The first term describes the rotation of the fluid about the vortex line and does result in any translation of the vortex. The second term suggests that the vortex moves in the binormal direction with infinite speed, but, of course, the inviscid approximation breaks down in the vortex core, since the fluid velocity is approaching infinity, and an inner core region needs to be introduced in which viscous forces are not negligible (the core radius is $\mathrm{Re}^{-1/2}$ when viscous forces are the regularising mechanism, where Re is the Reynolds number [1, 11, 15, 17, 18])[3]. Although the full Navier-Stokes equations need to be solved in the core, at leading order the solution may be assumed to be two-dimensional and radially symmetric. At the next order, the Fredholm alternative may be applied to find a solvability condition. When the first-order solution is matched back with the outer solution (9) the result is the law of vortex motion:

$$\boldsymbol{v} \sim -\frac{\omega_0}{4\pi}K\ \log(\epsilon)\,\boldsymbol{b}, \tag{10}$$

where ϵ is the core radius of the vortex relative to a typical radius of curvature of its centerline. Further terms in this expansion of the vortex velocity $\boldsymbol{v}$ can be calculated; the nonlocal effects of the "arms" of the vortex, and the details of the core structure (such as vortex stretching) all give order one contributions. However, for the purposes of highlighting the analogy with superconducting vortices and dislocations we will concentrate on the leading term here. We note though that if there is a large background fluid velocity $\boldsymbol{u}_0$ (of any magnitude greater than $\omega_0 K \log\epsilon$), then a similar analysis gives the leading order vortex velocity as

$$\boldsymbol{v} \sim \boldsymbol{u}_0. \tag{11}$$

Having completed our brief review of vortices in an inviscid fluid, let us now consider vortices in a type-II superconductor, where a similar framework exists.

[2] The singular terms in this expansion can also be found by expanding (6) directly as the vortex is approached.

[3] Alternatively the core may be regularised in a purely inviscid manner by postulating that it comprises a thin region of distributed vorticity. This also results in the law of motion (10).

3 Vortices in a type-II superconductor

3.1 Homogeneous superconductors

A line vortex lying along a curve Γ in a type-II superconductor may be described by the dimensionless London equations [13]:

$$(\mathrm{curl})^2\boldsymbol{H} + \boldsymbol{H} = 2\pi\boldsymbol{\delta}_\Gamma(\boldsymbol{x}), \tag{12}$$

$$\mathrm{div}\,\boldsymbol{H} = 0, \tag{13}$$

where $\boldsymbol{H}$ is the magnetic field, and $\boldsymbol{\delta}_\Gamma$ is as before. Despite the similarity with fluid vortices, there are two differences which are apparent even at this stage.

The first is the absence of the parameter ω_0: superconducting vortices have quantised strengths, and it is thought that the only stable vortex is that containing exactly one quantum. The second is that equation (12) has a natural lengthscale associated with it, known as the penetration depth; the magnetic field decays exponentially away from a vortex over this natural lengthscale. This scale has been used to nondimensionalize (12), so it is unity here.

The magnetic field $\boldsymbol{H}$ is analogous to the vector stream function $\boldsymbol{\Omega}$. The variable analogous to the fluid velocity $\boldsymbol{u}$ is the electric current $\boldsymbol{J} = \mathrm{curl}\,\boldsymbol{H}$. Using the Green's function for the modified Helmholtz equation in $\mathbb{R}^3$ we may write

$$\boldsymbol{H} = \frac{1}{2}\int_\Gamma \frac{e^{-s}}{s}\,d\boldsymbol{x}', \tag{14}$$

$$\boldsymbol{J} = \frac{1}{2}\int_\Gamma \nabla\left(\frac{e^{-s}}{s}\right)\wedge d\boldsymbol{x}' = -\frac{1}{2}\int_\Gamma e^{-s}\left(\frac{1}{s^3}+\frac{1}{s^2}\right)\boldsymbol{s}\wedge d\boldsymbol{x}'. \tag{15}$$

Expanding (15) as the point $\boldsymbol{x}$ approaches the vortex we find

$$\boldsymbol{J} \sim \frac{1}{r}\boldsymbol{e}_\theta - \frac{1}{2}K\ \log r\,\boldsymbol{b} + \cdots, \tag{16}$$

where r, θ, $\boldsymbol{e}_\theta$, K and $\boldsymbol{b}$ are as in (9).

A third difference between fluid vortices and superconducting vortices arises in the law of motion. A physically based argument, which will be rationalised below, suggests that superconducting vortex will move in response to the "Lorentz force" generated on the magnetic field in its core by the local electric current. Thus $\boldsymbol{v} \propto \boldsymbol{J}\wedge\boldsymbol{t}$ where $\boldsymbol{t}$ is the unit tangent to the vortex line, since the vortex carries a unit amount of magnetic flux. Equation (16) then suggests that the vortex will move with an infinite speed in the normal direction.

However, as in the fluid case, the London equations cease to be valid as the vortex core is approached. The regularising model in this case is the time-dependent Ginzburg-Landau (Gor'kov-Eliashburg) model [7]. Again, the leading order inner problem is two-dimensional and radially symmetric, and the Fredholm alternative can be used to derive a solvability condition for the first order core equations. Matching this first order inner solution with the outer solution (16) gives the law of vortex motion:

$$\boldsymbol{v} \sim -\frac{1}{\beta} K \, \log \epsilon \, \boldsymbol{n}, \tag{17}$$

where $\boldsymbol{n}$ is the unit normal, β is an order one constant which depends on the core structure, and ϵ is the nondimensional core radius, which is $1/\kappa$ in this case, where κ is the so-called Ginzburg-Landau parameter [4]. It is the matching with the inner region which justifies the "Lorentz force" argument above for the law of motion, and which gives the constant of proportionality.

As in the fluid case, further terms in this expansion of the vortex velocity $\boldsymbol{v}$ can be calculated [4]. The nonlocal effects of the "arms" of the vortex again produce an order one contribution. However, the simplicity of the Ginzburg-Landau (Gor'kov-Eliashburg) equations in comparison to the Navier-Stokes equations, and the quantisation of the vortex strength, means that there are no terms due to deformation of the vortex core in this case.

As in the fluid case, if there is a large background electric current $\boldsymbol{J}_0$ (of magnitude greater than $\log \epsilon$), then a similar analysis gives the leading order vortex velocity as

$$\boldsymbol{v} \sim \boldsymbol{J}_0 \wedge \boldsymbol{t}. \tag{18}$$

However, we note that this law of motion is ill-posed (in the sense that an arbitrarily small perturbation may grow arbitrarily quickly) if there is a component of $\boldsymbol{J}_0$ lying along the vortex line [16]. In such cases, the law (18) may be regularised by retaining the curvature term (17).

3.2 Inhomogeneous superconductors

Since vortices carry magnetic field, vortex motion produces an electric field which in turn leads to dissipation and an effective resistance. In practice, attempts are made to stop vortices moving by introducing inhomogeneities into the material such as impurities, dislocations and grain boundaries. The idea is that such inhomogeneities will weaken the superconducting capabilities of the material at those points, which will then act as pinning sites for the vortices.

Inhomogeneities can be built into the Ginzburg-Landau and London models by allowing the equilibrium number density of superconducting electrons N_s to vary spatially. The London equations then become [5]

$$\begin{aligned} \mathrm{curl}\left(\frac{1}{N_s(\boldsymbol{x})}\,\mathrm{curl}\,\boldsymbol{H}\right) + \boldsymbol{H} &= 2\pi\boldsymbol{\delta}_\Gamma(\boldsymbol{x}), && (19) \\ \mathrm{div}\,\boldsymbol{H} &= 0. && (20) \end{aligned}$$

Because of the coupling between the three components of the magnetic field in (19) we cannot now explicitly use the Green's function to obtain a Biot-Savart-type solution. However, it is still straightforward to obtain the singular terms in the expansion of $\boldsymbol{J}$ as the vortex line is approached, and as we have seen, it is these which dominate the motion. We find [5]

$$\boldsymbol{J} \sim \frac{N_s}{r}\boldsymbol{e}_\theta - \frac{K\,N_s}{2}\log r\,\boldsymbol{b} + \frac{1}{2}\nabla N_s\cdot n\,\log r\,\boldsymbol{b} - \frac{1}{2}\nabla N_s\cdot b\,\log r\,\boldsymbol{n}. \tag{21}$$

As before, the law of motion comes from matching with an inner solution of the full Ginzburg-Landau equations in the vicinity of the core, giving

$$\boldsymbol{v} \sim (K\boldsymbol{n} - \nabla\log N_s)\,\frac{\log(1/\epsilon)}{\beta(\boldsymbol{x})}. \tag{22}$$

We see that the variation in N_s acts like a pinning potential: vortices are attracted to the local minima of N_s. Note also that the "mobility" β may now also be a function of position.

3.3 Thin films

If the superconducting material does not occupy the whole of space then we must solve the London equations (12), (13) in the material, together with the Maxwell equations

$$\begin{aligned} \mathrm{curl}\,\boldsymbol{H} &= \boldsymbol{0}, && (23) \\ \mathrm{div}\,\boldsymbol{H} &= 0, && (24) \end{aligned}$$

in the external region (assuming there are no external currents), with continuity conditions on the interface and an applied magnetic field at infinity, say. The problem is simplified considerably if the superconducting material is a thin film, given by $-\delta g(x,y) \le z \le \delta g(x,y)$, $\delta \ll 1$. We assume that the film is symmetric for ease of exposition; it is easy to generalise the results to the nonsymmetric case.

To leading order as $\delta \to 0$ we find that the magnetic field is simply equal to the applied field. This is to be expected since an order one current density in a region of width $O(\delta)$ can

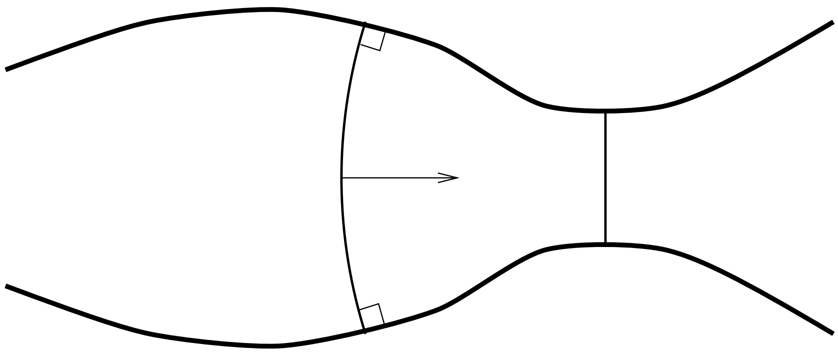

Figure 1: A vortex meeting the walls of a thin film normally and moving under curvature.

only produce an $O(\delta)$ magnetic field. To leading order the current density in the film lies in the x-y plane, and satisfies

$$\boldsymbol{e}_z \cdot \operatorname{curl} \boldsymbol{J}^{(0)} + H_A^{(0)} = 2\pi\delta(\boldsymbol{x} - \boldsymbol{x}_0), \tag{25}$$

$$\operatorname{div}(g\boldsymbol{J}^{(0)}) = 0, \tag{26}$$

where $H_A^{(0)}$ is the leading order component of the applied field in the z-direction, $\boldsymbol{x} = (x, y)$, and $\boldsymbol{x}_0$ is the position of the vortex, which lies in the z-direction to leading order.

As the point $\boldsymbol{x}$ approaches $\boldsymbol{x}_0$ we find

$$\boldsymbol{J}^{(0)} \sim \frac{1}{r}\boldsymbol{e}_\theta - \frac{\log r}{2g}\left(\frac{\partial g}{\partial y}, -\frac{\partial g}{\partial x}\right) + \cdots. \tag{27}$$

As before, we need to match with a core region described by the full Ginzburg-Landau (Gor'kov-Eliashburg) equations. The resulting law of motion is

$$\boldsymbol{v} \sim \frac{\log \epsilon}{\beta}\nabla \log g. \tag{28}$$

Thus we see that variations in thickness also act as a pinning potential, and vortices are attracted to local minima of the film thickness.

This result can be interpreted in the following way. It can be shown that superconducting vortices must meet a boundary normally. If the vortex forms an arc of a circle under this constraint, then the law (28) is equivalent to the resulting motion by curvature [3] (see Fig. 1).

4 Dislocations in an elastic crystal

In metal plasticity, we can define an outer length scale as that on which dislocations can be regarded as a line singularity, i.e., the outer equations are the Navier equations of linear elasticity. The second order strain tensor is defined as

$$\boldsymbol{e} = (\nabla \boldsymbol{u})^S , \tag{29}$$

where $\boldsymbol{u}$ is the elastic displacement, and the superscript S denotes the "symmetric part of". The strain tensor is related to the stress tensor through Hooke's law:

$$\boldsymbol{\sigma} = \lambda \mathrm{trace}(\boldsymbol{e})\, \boldsymbol{I} + 2\mu \boldsymbol{e}, \tag{30}$$

where λ and μ are the Lamé constants. Finally, the equations of elastic equilibrium are

$$\mathrm{div}\, \boldsymbol{\sigma} = \boldsymbol{0}. \tag{31}$$

An isolated dislocation can be modelled as a singular solution of these equations in which the displacement is not single valued (this is the classical Volterra model of dislocations [8]).

A more graphic framework in which to think of dislocations is that of "cut-and-weld" operations. By arming a metal worker with a very fine saw which wastes no material, a welding torch and a virgin crystal in which certain parallel crystallographic planes (later to be interpreted as the slip planes) are inscribed, a macroscopic dislocation can be created by asking him to saw along an arbitrary region in one of the planes, then subject the cut metal to a constant jump in tangential displacement across the cut, and finally weld the metal together again. The boundary of the cut is then called a slip dislocation, and the constant displacement jump across the cut is called the Burgers vector.

Since the cut and weld operation generates no holes or interpenetration, a "total" displacement from the undislocated state $\boldsymbol{u}^T$ exists. There are two ways to think about $\boldsymbol{u}^T$. If we consider this displacement as obtained by integrating the strain, we has the advantage of not needing to know the reference configuration, then $\boldsymbol{u}^T$ is not single valued and is analogous to the velocity potential in an inviscid fluid ϕ, which will also be multivalued when vortices are introduced (for a rectilinear vortex the velocity potential is proportional to θ, the polar angle). On the other hand, if we wish to work with a single valued displacement, we must choose a particular branch of $\boldsymbol{u}^T$, which will then jump across the branch cut (which can naturally, but need not be, identified with the metal worker's cut above; like the branch cut, the metal worker's cut is not constrained to lie in the slip plane, but any other cut will result in a gap or overlap region after the displacement jump is imposed, which will require the addition or removal of material before welding the sides together again)[4]. We may further define the "distortion" tensor $\boldsymbol{\beta} = \nabla \boldsymbol{u}^T$ as the generalized derivative of this single valued total displacement. As shown in [9], this tensor is the sum of two components: the plastic component $\boldsymbol{\beta}^P$ which is due to the jumps across the cuts, and the elastic component $\boldsymbol{\beta}^E$ which results from the elastic response to the cut and weld process. Note that although $\boldsymbol{\beta}^P$ depends on our choice of branch cuts (which are arbitrary), its row curl is single-valued. By direct differentiation of the displacement jump it can be shown that:

$$\mathrm{curl}\boldsymbol{\beta}^P = -\boldsymbol{\delta}_\Gamma \otimes \boldsymbol{b}, \tag{32}$$

where the dislocation lies along the curve Γ, $\boldsymbol{b}$ is the Burger's vector, and $\otimes$ is the tensor product. Since $\mathrm{curl}\boldsymbol{\beta} = 0$ we therefore have

$$\mathrm{curl}\boldsymbol{\beta}^E = \boldsymbol{\delta}_\Gamma \otimes \boldsymbol{b}. \tag{33}$$

The physical variable in elasticity which is analogous to the fluid velocity is the strain tensor $\boldsymbol{e}$ which is given by $\boldsymbol{e} = (\boldsymbol{\beta}^E)^S$. We may describe an isolated line dislocation lying along a curve Γ by integrating (33) to give

$$\boldsymbol{e} = (\boldsymbol{Q} \otimes \boldsymbol{b} + \nabla \boldsymbol{u}^E)^S \tag{34}$$

where

$$\mathrm{curl}\,\boldsymbol{Q} = \boldsymbol{\delta}_\Gamma(\boldsymbol{x}), \tag{35}$$

and to fix the gauge we set

$$\mathrm{div}\,\boldsymbol{Q} = 0. \tag{36}$$

The variable $\boldsymbol{Q}$ is thus mathematically equivalent to the fluid velocity in (1),(2). The elastic displacement $\boldsymbol{u}^E$ depends upon the choice of gauge for $\boldsymbol{Q}$ and will be single-valued but will not in general be regular.

The analogy with fluids and superconductors could be closer if $\boldsymbol{u}^E$ were zero. Unfortunately, it is $\boldsymbol{\sigma}$ and not $\boldsymbol{e}$ which satisfies (31), so this will not in general be the case. However, the dislocation equivalent of the Biot-Savart integral can still be formulated, and is known as the Peach-Koehler formula [8]. This formula gives the stress generated by an arbitrary dislocation curve.

[4] It is reassuring to note that for a given set of dislocations, any two sets of branch cuts, with associated distortion tensors, give rise to the same stress and strain fields.

Whereas fluid vortices move in response to fluid velocity, and superconducting vortices move in response to electric current, dislocations will move in response to stress. In the same way that fluid velocities and electric currents have singularities the elastic stress diverges like $1/r$ as $r \to 0$ and, as usual, we need to regularise to model in the core of the dislocation.

Here we find a major difference between dislocations and the other line singularities we have been considering. In an undislocated crystal, the stresses and strains are sufficiently small for conventional linear elasticity theory to be applied so that we may approximate the discrete lattice by a continuum and the interatomic forces by elastic forces.

In a crystal containing a dislocation, the atoms are displaced from their perfect lattice sites and the resulting distortion produces a stress field in the crystal around the dislocation. However, the stresses and strains in the bulk of the crystal are only small enough for linear elasticity theory to be applied when we study regions that are at least several atom spacings from any dislocation. At a length scale of a few atom spacings from the core of the dislocation the effects of the interatomic potentials can neither be approximated by linear elastic forces nor can the lattice be thought of as a continuum. Therefore, the core of the dislocation is intrinsically discrete and in it a nonlinear atomistic model must be used. This model should be capable of being matched directly onto an outer linear elastic model whose solution has divergent stresses. This matching will clearly require a careful choice of dependent variables that make sense both in the core and outside. This choice must be compatible with, say, an atomistic simulation involving a dislocated array of atoms under the action of, say, Lennard-Jones potentials. In order to get a feel for the possible behaviour of such a model we now consider some simple paradigm models; for simplicity we will now concentrate on a pure edge dislocation [8], which is necessarily rectilinear.

4.1 The Frenkel-Kontorova model

The Frenkel-Kontorova model [6] is a one-dimensional model which effectively assumes that the dislocation is one atom wide in the direction perpendicular to the slip plane; thus the atomic mismatch is confined to two chains of atoms. One of these chains is taken to be fixed, while the model solves for the position of the atoms in the other chain. The model balances the forces on each atom due to its neighbours on either side in the same chain with the potential it feels due to the mismatch with the neighbouring chain (see Fig. 2) resulting in

$$u_{n+1} - 2u_n + u_{n-1} = \frac{hA}{2\pi} \sin\left(\frac{2\pi u_n}{h}\right), \tag{37}$$

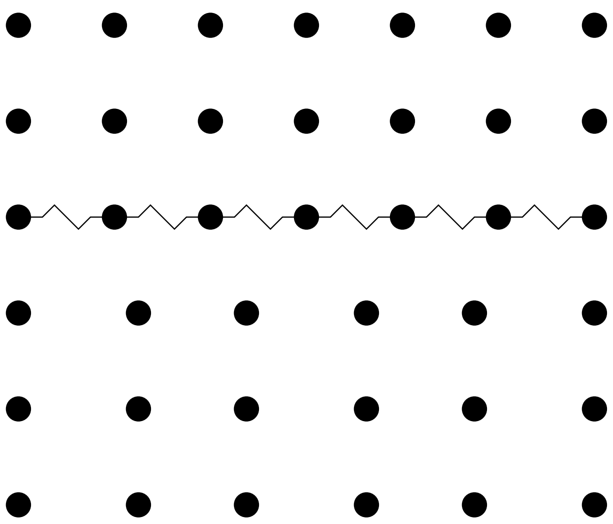

Figure 2: Diagram illustrating the Frenkel-Kontorova model.

where u_n is the displacement in the x-direction of the nth atom, h is the atomic spacing, and A is constant. The right-hand side here can be any periodic function with period h, and would properly be the result of summing an infinite series of, say, Lennard-Jones potentials; however, since the model is already very simplistic we choose (37).

We note that A in (37) measures the relative strength of the neighbouring chain of atoms. If A is small then $u_{n+1} \approx u_n$ and we can consider the continuum approximation. If we let $x = nh$ and $v = 2\pi u/h$ then we find that as A and h tend to zero

$$\frac{d^2 v}{dx^2} = \left(\frac{A}{h^2}\right) \sin v. \tag{38}$$

The width of the core is then $h/\sqrt{A}$, so that the number of atoms in the core is approximately $1/\sqrt{A}$. Thus, the uniformly continuum approximation is only valid when the core contains many atoms, as we would expect.

A uniform applied shear force may be modelled in this simple situation by adding a constant driving force F to the right-hand side of (37). To add time dependence to model wave propagation we should add a term proportional to d^2u_n/dt^2 and such a term will produce elastic waves which will radiate out from the moving dislocation. Such waves dissipate energy, and if we work on a much longer timescale than the timescale for their motion we might model the effect of this dissipation to by including a term proportional to du_n/dt in (37). Thus we arrive at the following equation describing the motion of the dislocation:

$$\frac{du_n}{dt} = u_{n+1} - 2u_n + u_{n-1} - \frac{hA}{2\pi} \sin\left(\frac{2\pi u_n}{h}\right) - F. \tag{39}$$

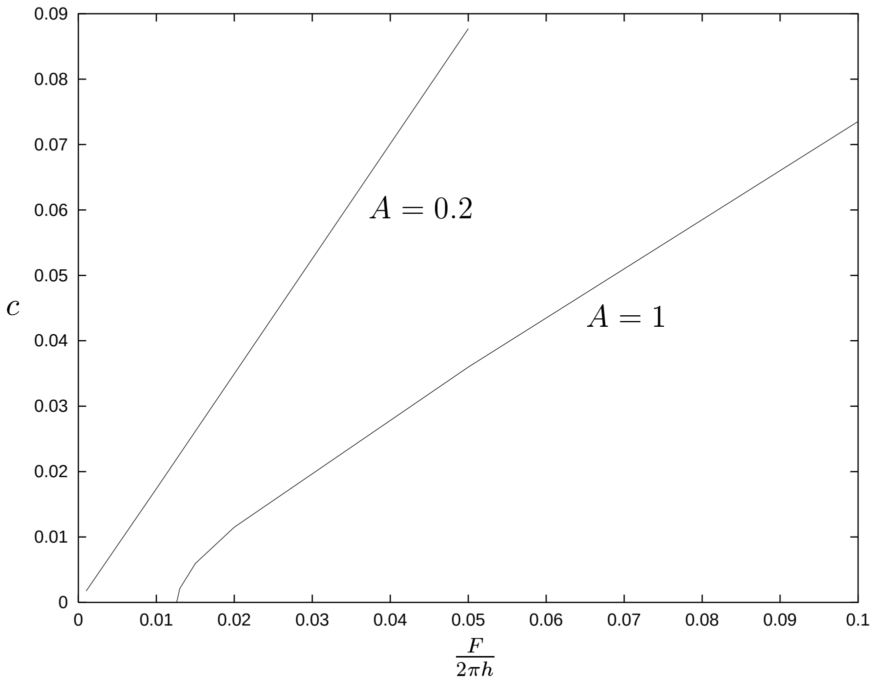

Figure 3: The speed of a dislocation c as a function of the applied force F.

What we would like now is an equation relating the speed of the dislocation to the applied stress F. To this end we seek travelling wave solutions $u_n = u(n - ct)$, giving

$$-c\frac{du}{d\eta} = u(\eta + 1) - 2u(\eta) + u(\eta - 1) - \frac{hA}{2\pi}\sin\left(\frac{2\pi u(\eta)}{h}\right) - F. \tag{40}$$

This equation appears to have the following propertiy : There exists F_{crit} such that if $F < F_{crit}$ then $c = 0$ and $F_{crit} \to 0$ as $A \to 0$. Thus there is a critical applied stress required to get a dislocation to move. In the continuum model there is no such critical stress; the ability to remain steady under small stresses is a result of the discrete nature of the model.

Computational experiments seem to confirm these statements (see Fig 3 and 4)

4.2 The Peierls-Nabarro Model

The Peierls-Nabarro model (see [8]) assumes the dislocation is one atom wide in one direction, but continuous in the other direction (i.e. many atoms wide). However, unlike the one-dimensional Frenkel-Kontorova model the Peierls-Nabarro model does try to take account of the elastic stresses in the bulk of the material. The model solves the equations of linear elasticity in each of two halfspaces and balances the stress generated with the interatomic

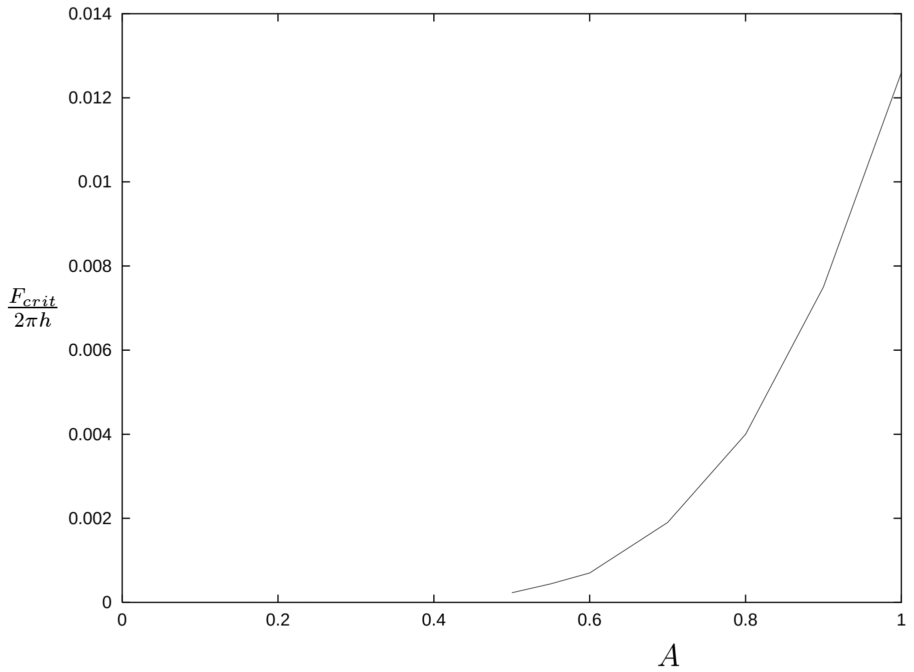

Figure 4: The critical stress F_{crit} as a function of A.

stress due to the mismatch of atoms at the join (the so-called disregistry) (see Fig. 5), giving

$$\int_{-\infty}^{\infty} \left.\frac{du}{dx}\right|_{x=x'} \frac{1}{x-x'}\, dx' = \frac{hA}{2\pi} \sin\left(\frac{2\pi u_n}{h}\right). \tag{41}$$

Solving this equation we see that there is no divergence in the displacements and strains, although the displacement jumps across the x axis. Thus, the Peierls-Nabarro model removes the artificial divergence at the core that is associated with the idealized dislocation of Volterra. Nevertheless, for the Peierls dislocation the strains in the core region are so large that it is questionable whether Hooke's law applies. On the other hand, it is questionable whether it is mathematically consistent to match an atomistic right-hand side in (41) with the continuum response on the left-hand side.

4.3 The two-dimensional Frenkel-Kontorova model

The Frenkel-Kontorova model in two dimensions [2] considers a two-dimensional cubic lattice of atoms which are allowed to be displaced in both the x and y-directions (that is, both slip and glide motion are allowed in principle). In the far field (which corresponds to letting $h \to 0$) a continuum approximation holds which (for an appropriate choice of constants in

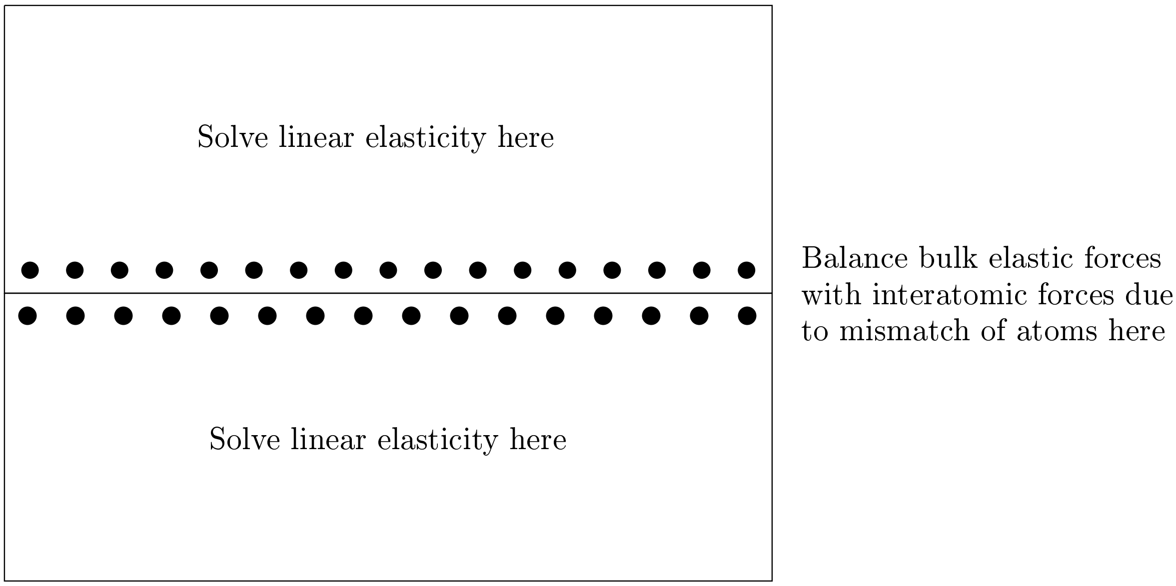

Figure 5: Diagram illustrating the Peierls-Nabarro model.

the Frenkel-Kontorova model) is the Navier equations. Thus we now have a model of the core which can match back into our far field model.

The applied stress now appears through this matching as a boundary condition (at infinity) on the Frenkel-Kontorova model. We have used this model to simulate edge dislocations (Fig. 6). When the applied stress is larger than a threshold stress the dislocations glide in the x direction, so that travelling wave solutions are expected to exist. If we could relate the speed of travelling wave solutions to the behaviour at infinity we would have our law of motion for dislocations.

A question still under study is whether climb of dislocations, which is in principle allowed by the model, can be observed in practice.

Finally, let us comment on the possibility of obtaining a continuum limit of the Frenkel-Kontorova model for dislocation cores in two dimensions for simple cubic lattices. To simplify the argument, let us assume that the atoms are only allowed to be displaced in the x-direction (it can be seen for Fig. 6 that this is not such a bad assumption). Then we have [12]

$$u_{n+1,m} - 2u_{n,m} + u_{n-1,m} = \frac{hA}{2\pi}\left(\sin\left(\frac{2\pi(u_{n,m+1} - u_{n,m})}{h}\right) + \sin\left(\frac{2\pi(u_{n,m} - u_{n,m-1})}{h}\right)\right), \tag{42}$$

where $u_{n,m}$ is the displacement of the nth atom in the mth row. Now, if A is very small, $u_{n+1,m} \approx u_{n,m}$, and the core will be continuous in the x-direction. If A is very large, $u_{n,m+1} - u_{n,m} \approx k$, $k \in \mathbf{Z}$, the gap created by the extra halfplane of atoms will take many rows to close, and the core will be continuous in the y-direction. However, since it is impossible for

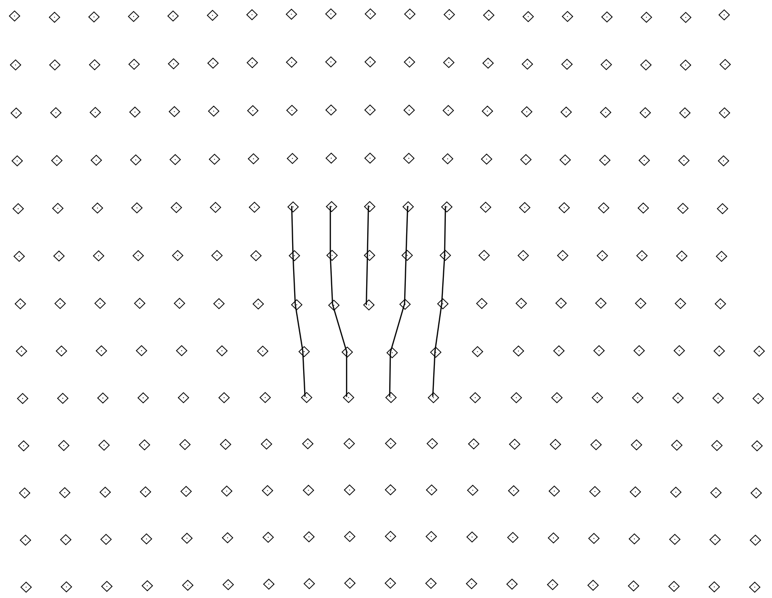

Figure 6: Steady dislocation in the two-dimensional Frenkel-Kontorova model.

A to be both small and large, there will always be a direction in which the core is discrete.

The discreteness of the core is effectively a geometrical constraint. The displacement in the x-direction u must jump by an atom spacing as we circle the dislocation *at any radius*, however small. Thus it is impossible to have a continuum model of the core in which displacement gradients are bounded.

5 Conclusion

We have examined the dynamics of line singularities in three different physical systems, namely vortices in an inviscid fluid, vortices in a type-II superconductor, and dislocations in an elastic crystal. We have attempted to highlight some of the similarities and differences between these systems.

In each case the derivation of a law of motion for the singularity is approached by the same basic methodology. The outer problem is linear but singular, and the variables of interest diverge at the singularity. This leads to an inner problem near the core of the singularity over which some regularising mechanism acts. The leading order (in the core radius) inner problem is two-dimensional when the line describing the singularity in the outer problem is smooth. Often it is also be radially symmetric. At next order in the inner solution the Fredholm alternative can be applied to derive a solvability condition on the first order equations. When this inner solution is matched back with the outer solution this solvability condition gives the law of motion of the singularity.

This procedure has been successfully carried out for fluid vortices and superconducting vortices, in a variety of situations. For dislocations the problem is made harder by the discrete nature of the core problem.

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