This is to certify that the

dissertation entitled

ESTIMATION OF THE FORCE ON SCREW DISLOCATIONS
IN FINITE ELASTICITY USING THE J-INTEGRAL

presented by

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has been accepted towards fulfillment
of the requirements for

Ph.D degree in Mechanics

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Date 5/5/87

ESTIMATION OF THE FORCE ON SCREW DISLOCATIONS IN FINITE ELASTICITY USING THE J-INTEGRAL

by

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A DISSERTATION

Submitted to

Michigan State University

in Partial Fulfillment of the Requirements

for the Degree of

DOCTOR OF PHILOSOPHY

in

Mechanics

Department of Metallurgy, Mechanics and Material Science

1987

ABSTRACT

ESTIMATION OF THE FORCE
ON SCREW DISLOCATIONS
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This study is concerned with estimating the value of the force between two screw dislocations in an elastic solid. Since the linear theory of elasticity predicts unbounded strains at a dislocation, the results predicted by such a theory are suspect. The present study is carried out within the fully nonlinear theory of elasticity.

Since the force between two dislocations is defined as the rate of change of energy with respect to the separation between the dislocations, one way to calculate this force is to first calculate the total energy stored in the body. This is an almost impossible task to carry out exactly in a fully nonlinear theory. However, we observe that the value of the J-integral evaluated along a path surrounding one dislocation is precisely equal to the magnitude of this force. We exploit the path-independence of the J-integral in order to obtain accurate estimates of the force between two dislocations in the presence of nonlinearity.

We first carry this out in the context of the linear theory, for illustrative purposes, and then carry it out in the context of nonlinear theory.

To my father and mother

for the example and inspiration

they have provided throughout my life.

ACKNOWLEDGMENTS

I would like to express my sincere appreciation to my teachers: Professor Rohan Abeyaratne of Massachusetts Institute of Technology for his guidance throughout this work and for his inspiration and teaching of finite elasticity, nonlinear fracture mechanics and instabilities while he was at Michigan State University.

I would also like to thank Professor Cornelius O. Horgan who taught me continuum mechanics, elasticity, variational calculus and discussed many challenging problems in nonlinear continuum mechanics.

Grateful thanks are extended to Professor David H.Y. Yen who taught me applied mathematics in support of the elasticity theory, and Professor Nicholas J. Altiero who taught me elastic stability and computational mechanics. Finally, I would like to thank Dean David L. Sikarskie of Michigan Technological University, formerly chairman of the Metallurgy, Mechanics and Materials Science Department at Michigan State University for his guidance, teaching and support throughout my entire education at the University of Michigan and Michigan State University.

A final note of appreciation must go to U.S. National Science Foundation for their support of this work under Grant MEA 86-96034.

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CHAPTER 1

INTRODUCTION

The theory of dislocations has received a large amount of attention in the materials science literature. In particular, solutions to the problems of straight dislocations in an infinite continuous medium have been found within the linear theory of elasticity. The displacement field and the stress field have both been obtained in the presence of a single dislocation and multiple dislocations. The results of these investigations are unsatisfactory within the linearized theory since the results predict infinite strains at the dislocations, contrary to the assumption upon which the theory rests. These results can be found in the theory of dislocations literature, e.g. Hirth and Lothe [1] and Lardner [2], cite these findings. We recapitulate these results in Chapter 3.

In recent years investigators have employed some nonlinearities in the formulation of the problem of dislocations. In particular, Kachanov [3], solves a screw dislocation problem in an infinite medium under the assumption that the stress-strain relations are nonlinear; however, he assumes that the displacement gradients are small. The problem of dislocations in nonlinear elasticity is also described in an article by Gairola [4]. The formulation is described in general tensorial notation and the problem of a screw dislocation in an infinitely long and straight cylinder bounded by two circles is treated by the method of successive approximation (Signorini's method [4]).

There is also an interest among material scientists to obtain the force on a dislocation. The force on a dislocation, or in general the "force on a defect", is defined to be the rate of change of the total energy of the body (which is composed of the elastic strain energy of the material containing the "defect" and the potential energy of any external loading mechanism,) with respect to a change of the position of a defect. In the case of the screw dislocations this is the force tending to make the screw glide in the x-direction (chapter 3). We also note that the force acting on a dislocation is not a true mechanical force but it has the dimensions of a force. It may be viewed as a "driving force" in the thermodynamic sense. This is discussed in detail in Eshelby's article "The Continuum Theory of Lattice Defects" [5].

The J-integral is a path independent integral which plays a central role in nonlinear fracture mechanics [6]. As shown by Rice [7], one can readily verify that J reduces to the energy release rate, which in turn leads to the stress intensity factor in linear elastic fracture mechanics. It is also stated by Eshelby [8] and Rice [9] that, in general, the J-integral can be used to define the "force on a defect", the defect being the dislocation in the present case.

In the present study, the theory of dislocations is studied within the context of finite elasticity, and attention is restricted to screw dislocations. The exact displacement field and stress field are obtained analytically for a single screw dislocation in an infinite region. Further, the results are extended in an approximate manner to two screw dislocations in a nonlinearly elastic region by using the theory of "small deformations superposed on a large deformation". The force between the dislocations is calculated via J-integral. Even though the analysis is approximate, the results for the force are expected to be good, for the reasons explained below.

Consider, for example, the case of two screw dislocations in an infinite medium. If one were to assume that the presence of a second dislocation only causes a small perturbation, one can then carry out an analysis based on the theory of small deformations superposed on a large deformation. Clearly this assumption is invalid in the vicinity of the dislocation but it is expected to be reasonable at points far from the dislocation. Our interest here lies solely in evaluating the value of J which represents the force on a dislocation. Since the J-integral is path-independent, we can evaluate it at points distant to the dislocation. We expect to get reasonable results for our purpose.

We will note that for a screw dislocation in an infinite medium, the value of J becomes zero, but for the two screw dislocations in an infinite medium J is calculated to be nonzero.

The chapters and discussions are presented in the following sequence:

Chapter 2 summarizes results from finite elasticity theory, the notion of the J-integral and finally the notion of a screw dislocation. In Chapter 3 the formulation and results for a single screw dislocation and two screw dislocations in an infinite <u>linear</u> elastic region are discussed. The calculation of the force on a dislocation, using two different techniques, is then carried out and finally the results of the two techniques are compared to one another. Chapter 4 covers similar issues in the nonlinearly elastic case. Chapter 5 summarizes and discusses the results.

Finally, we note that after the first draft of this dissertation was written, we received a paper by P.J. Rosakis and A.J. Rosakis [24] in which they independently solved the problem of a <u>single</u> screw dislocation in incompressible finite elastostatics. Their results for this problem are more general than ours, since ours are restricted to generalized neo-Hookean materials and theirs aren't. However, they do <u>not</u> address the problem of two dislocations nor do they consider the force between dislocations.

CHAPTER 2

PRELIMINARIES ON FINITE ELASTICITY AND THE DISLOCATION PROBLEM

In Section 2.1 of this chapter, certain pertinent results from the equilibrium theory of finitely deformed, homogeneous and isotropic elastic solids are summarized. The complete theory and general results from the continuum theory of finite elasticity may be found in [10]. Herein the theory is first presented in 3-dimensions. Then in Section 2.2, it is specialized in two ways: The case of finite anti-plane shear deformation (which provides the setting for discussing the screw dislocation) is considered first and then, this is further specialized to the case of infinitesimal anti-plane shear deformation.

The J-integral, with some historical notes, is described in Section 2.3 of this chapter. The proof for the path independency of the J-integral is omitted from the section but may be found in [7]. The relationship between the path independent integral J and the notion of a force on a defect is discussed. Finally, in section 2.4 we formulate and discuss the notion of a screw dislocation.

2.1 Finite Elasticity

Let R be an open region occupied by the interior of a body in its undeformed configuration and denote by $\underset{\sim}{x}$ the position vector of a material point in R. A deformation is described by

$$\underset{\sim}{y} = \underset{\sim}{y}\,(\underset{\sim}{x}) = \underset{\sim}{x} + \underset{\sim}{u}\,(\underset{\sim}{x}) \qquad \text{for all } \underset{\sim}{x} \in R, \tag{2.1}$$[1]

which is a mapping of R onto a domain R^*; $\underset{\sim}{u}\,(\underset{\sim}{x})$ represents the displacement field associated with this deformation. The transformation (2.1) is assumed to be invertible and suitably smooth.

Let $\underset{\sim}{F}$ be the deformation gradient tensor field,

$$\underset{\sim}{F}\,(\underset{\sim}{x}) = \nabla\,\underset{\sim}{y}\,(\underset{\sim}{x}) \qquad \text{for all } \underset{\sim}{x} \in R; \tag{2.2}$$

the determinant of $\underset{\sim}{F}$ is called the Jacobian determinant and is denoted by J,

$$J\,(\underset{\sim}{x}) = \det \underset{\sim}{F}\,(\underset{\sim}{x}) > 0 \qquad \text{for all } \underset{\sim}{x} \in R. \tag{2.3}$$

The deformation of an <u>incompressible</u> material must be locally volume preserving, hence

$$J\,(\underset{\sim}{x}) = \det \underset{\sim}{F}\,(\underset{\sim}{x}) = 1 \qquad \text{for all } \underset{\sim}{x} \in R. \tag{2.4}$$

Define the tensor fields $\underset{\sim}{C}$ and $\underset{\sim}{G}$ by

---

[1]Letters underlined by a tilde represent three-dimensional vectors and tensors.

$$\underset{\sim}{C} = \underset{\sim}{F}^T \underset{\sim}{F} , \quad \underset{\sim}{G} = \underset{\sim}{F} \underset{\sim}{F}^T , \tag{2.5}$$

and their common principal scalar invariants I_1, I_2, and I_3 by

$$\begin{aligned} I_1 &= \mathrm{tr}\,(\underset{\sim}{C}) , \\ I_2 &= \frac{1}{2} \left[(\mathrm{tr}(\underset{\sim}{C}))^2 - \mathrm{tr}(\underset{\sim}{C}^2) \right] , \\ I_3 &= \det \underset{\sim}{C} . \end{aligned} \tag{2.6}$$

From (2.4) - (2.6) one concludes that

$$I_3 (\underset{\sim}{x}) = J^2 (\underset{\sim}{x}) = 1 \qquad \text{for all } \underset{\sim}{x} \in R. \tag{2.7}$$

The Lagrangian strain tensor field is given by

$$\underset{\sim}{E} = \frac{1}{2} (\underset{\sim}{C} - \underset{\sim}{1}). \qquad (2.8)^{1}$$

The stresses are denoted by $\underset{\sim}{\tau} (\underset{\sim}{y})$ for the actual (Cauchy) stress tensor field on R^* and $\underset{\sim}{\sigma} (\underset{\sim}{x})$ for the corresponding nominal (Piola)

---

[1] $\underset{\sim}{1}$ stands for the idem tensor.

stress tensor field on R. They are, in general, related to each other by

$$\underset{\sim}{\tau} = \frac{1}{J}\,\underset{\sim}{\sigma}\,\underset{\sim}{F}^T,$$

$$\underset{\sim}{\sigma} = J\,\underset{\sim}{\tau}\,\underset{\sim}{F}^{-T}. \tag{2.9}$$

In the absence of body forces, the local equilibrium equations are

$$\operatorname{div} \underset{\sim}{\tau} = \underset{\sim}{0} \qquad \text{on } R^*,$$

$$\operatorname{div} \underset{\sim}{\sigma} = \underset{\sim}{0} \qquad \text{on } R, \tag{2.10}$$

together with $\underset{\sim}{\tau} = \underset{\sim}{\tau}^T$ on R^*, and $\underset{\sim}{\sigma}\underset{\sim}{F}^T = \underset{\sim}{F}\underset{\sim}{\sigma}^T$ on R. To continue, let $\underset{\sim}{s}$ be the nominal surface traction and $\underset{\sim}{t}$ the corresponding true surface traction. Then

$$\underset{\sim}{s} = \underset{\sim}{\sigma}\,\underset{\sim}{n} \qquad \text{on } S\ ,$$

$$\underset{\sim}{t} = \underset{\sim}{\tau}\,\underset{\sim}{n}^* \qquad \text{on } S^*, \tag{2.11}$$

where $\underset{\sim}{n}$ is a unit normal to the surface S in R, and $\underset{\sim}{n}^*$ is a unit normal to S^*, the image of S after deformation. It can be shown that

$$\underset{\sim}{t} = \underset{\sim}{0} \text{ on } S^* \quad \text{if and only if} \quad \underset{\sim}{s} = \underset{\sim}{0} \quad \text{on } S. \tag{2.12}$$

This is useful in the case of a traction-free surface S^*, since it enables the boundary condition on the unknown deformed surface to be specified on the known undeformed surface S.

Let W be the elastic potential, characteristic of the given elastic material, the value of W represents the stored strain energy per unit undeformed volume. For homogeneous, isotropic and incompressible elastic materials, W can be shown to depend on the deformation solely through the invariants I_1, and I_2 i.e. $W = \hat{W}(I_1, I_2)$. The corresponding constitutive law takes the form

$$\underset{\sim}{\tau} = 2\left[\frac{\partial\hat{W}}{\partial I_1}\underset{\sim}{G} + \frac{\partial\hat{W}}{\partial I_2}(I_1\underset{\sim}{1} - \underset{\sim}{G})\underset{\sim}{G}\right] - P\underset{\sim}{1}, \tag{2.13}$$

or, equivalently,

$$\underset{\sim}{\sigma} = 2\left[\frac{\partial\hat{W}}{\partial I_1}\underset{\sim}{F} + \frac{\partial\hat{W}}{\partial I_2}(I_1\underset{\sim}{1} - \underset{\sim}{G})\underset{\sim}{F}\right] - P\underset{\sim}{F}^{-T}, \tag{2.14}$$

where P is a scalar field required to maintain the constraint of incompressibility (2.4).

2.2 Anti-Plane Shear

Next, we consider the special case of finite anti-plane shear deformations. The development that follows is based on the analysis by

Knowles [11]. Assume the region R occupied by the undeformed body to be cylindrical and a fixed cartesian coordinate frame is chosen so that the x_3 - axis is parallel to the generators of R. Let D be the cross-section of R in the plane $x_3 = 0$.

The deformation (2.1) on R is said to be an anti-plane shear if it is of the form

$$y_\alpha = x_\alpha, \; y_3 = x_3 + u\,(x_1, x_2). \qquad (2.15)^1$$

Thus in an anti-plane shear deformation, particles in the body are displaced purely in the axial direction by an amount $u(x_1, x_2)$. In the absence of body forces, the deformation (2.15) can, in general, be sustained only in materials for which the strain energy density takes a more restricted form, (Knowles [12]). A class of such materials are those characterized by,

$$W = \hat{W}\,(I_1) \quad \text{for all} \quad I_1 \geq 3, \quad \hat{W}\,(3) = 0, \qquad (2.16)^2$$

and referred to as "Generalized Neo-Hookean Materials". We assume that W conforms to the Baker-Ericksen inequality (see [13]):

---

[1]Greek subscripts take the range 1, 2 while Latin subscripts assume the values 1, 2, 3. Repeated subscripts are summed.

[2]Note that $I_1 = 3$ in the undeformed state.

$$\hat{W}'(I_1) > 0 \quad \text{for all} \quad I_1 > 3, \tag{2.17}$$

where $\hat{W}'$ is the derivative of $\hat{W}$ with respect to the argument. This can be shown to be equivalent to requiring a positive modulus of shear at all deformations.

The infinitesimal shear modulus is

$$\mu = 2\,\hat{W}'(3) > 0. \tag{2.18}$$

For the class of deformations given by (2.15), the components of the deformation gradient tensor are calculated from (2.2) to be

$$\begin{aligned} F_{\alpha\beta} &= \delta_{\alpha\beta}\,, \\ F_{\alpha 3} &= 0, \\ F_{3\alpha} &= u_{,\alpha}\,, \\ F_{33} &= 1 \quad \text{on } D. \end{aligned} \qquad (2.19)^{1}$$

In viewing (2.19), one can conclude that J, the determinant of $\underset{\sim}{F}$, becomes 1 automatically. Now calculating $\underset{\sim}{F}^{-1}$, its components denoted by F^{-1}_{ij}, we find

---

[1] Subscripts preceded by a comma indicate partial differentiation with respect to the corresponding material cartesian coordinate.

$$
\begin{aligned}
F^{-1}_{\alpha\beta} &= \delta_{\alpha\beta} , \\
F^{-1}_{\alpha 3} &= 0, \\
F^{-1}_{3\alpha} &= - u_{,\alpha} , \\
F^{-1}_{33} &= 1 \quad \text{on } D.
\end{aligned}
\tag{2.20}
$$

Next the tensor fields $\underset{\sim}{C}$ and $\underset{\sim}{G}$ given by (2.5) are calculated to be,

$$
\begin{aligned}
C_{\alpha\beta} &= \delta_{\alpha\beta} + u_{,\alpha} \; u_{,\beta} , \\
C_{\alpha 3} &= C_{3\alpha} = u_{,\alpha} , \\
C_{33} &= 1 \quad \text{on } D,
\end{aligned}
\tag{2.21}
$$

and,

$$
\begin{aligned}
G_{\alpha\beta} &= \delta_{\alpha\beta} , \\
G_{\alpha 3} &= G_{3\alpha} = u_{,\alpha} , \\
G_{33} &= 1 + u_{,\alpha} \, u_{,\alpha} \quad \text{on } D.
\end{aligned}
\tag{2.22}
$$

The principal scalar invariants I_1, I_2, and I_3 are given by (2.6) and for anti-plane shear deformations are

$$\begin{aligned} I_1 &= I_2 = 3 + |\nabla u|^2 , \\ I_3 &= 1 \quad \text{on } D . \end{aligned} \tag{2.23}$$

The components of the Lagrangian strain tensor are obtained from equations (2.8), (2.21):

$$\begin{aligned} E_{\alpha\alpha} &= \frac{1}{2} u_{,\alpha} u_{,\alpha} \qquad \text{(no sum)}, \\ E_{33} &= \frac{1}{2} |\nabla u|^2 , \\ E_{\alpha\beta} &= \frac{1}{2} u_{,\alpha} u_{,\beta} , \\ E_{3\alpha} &= E_{\alpha 3} = \frac{1}{2} u_{,\alpha} \quad \text{on } D. \end{aligned} \tag{2.24}$$

Recalling from equation (2.16) that W is only a function of I_1, and using equations (2.13) - (2.14), the constitutive equation becomes

$$\underset{\sim}{\tau} = 2\,\hat{W}'(I_1)\,\underset{\sim}{G} - P\,\underset{\sim}{1},$$
$$\underset{\sim}{\sigma} = 2\,\hat{W}'(I_1)\,\underset{\sim}{F} - P\,\underset{\sim}{F}^{-T}. \tag{2.25}$$

For anti-plane shear deformations, the components of $\underset{\sim}{\tau}$ and $\underset{\sim}{\sigma}$ are found from (2.25), (2.22) and (2.21) to be

$$\begin{aligned} \tau_{\alpha\beta} &= \left\{ 2\,\hat{W}'(I_1) - P \right\} \delta_{\alpha\beta} , \\ \tau_{\alpha 3} &= 2\,\hat{W}'(I_1)\, u,_{\alpha} , \\ \tau_{33} &= 2\,\hat{W}'(I_1)\,(1 + |\nabla u|^2) - P. \end{aligned} \tag{2.26}$$

Similarly,

$$\begin{aligned} \sigma_{\alpha\beta} &= \left\{ 2\,\hat{W}'(I_1) - P \right\} \delta_{\alpha\beta} , \\ \sigma_{\alpha 3} &= P\, u,_{\alpha} , \\ \sigma_{3\alpha} &= 2\,\hat{W}'(I_1)\, u,_{\alpha} , \\ \sigma_{33} &= 2\,\hat{W}'(I_1) - P . \end{aligned} \tag{2.27}$$

The equilibrium equations in the absence of body forces are given by (2.10). Substituting (2.27) into (2.10) gives the three equations

$$\left\{ 2\,\hat{W}'(I_1) - P \right\}_{,\alpha} + P,_{3}\, u,_{\alpha} = 0 \quad \text{on } D \tag{2.28}$$

and

$$\left\{2\, \hat{W}'(I_1)\, u_{,\alpha} \right\}_{,\alpha} - P_{,3} = 0 \quad \text{on } D. \tag{2.29}$$

From equations (2.29), (2.15) and (2.23) one concludes that $P_{,3}$ must be a function of x_1 and x_2 only; therefore

$$P_{,3} = \hat{P}\,(x_1, x_2)\ . \tag{2.30}$$

Using (2.30) in (2.28) and differentiating with respect to x_3, indicates that

$$\hat{P}_{,\alpha 3} = 0, \tag{2.31}$$

which implies that $\hat{P}$ must be a constant-valued function, say,

$$\hat{P}\,(x_1, x_2) = P_1 = \text{constant.} \tag{2.32}$$

Therefore

$$\hat{P}\,(x_1, x_2, x_3) = P_1\, x_3 + \overset{o}{P}\,(x_1, x_2). \tag{2.33}$$

Substituting (2.33) into (2.28) and (2.29), leads to the conclusion that,

$$P(x_1, x_2, x_3) = 2\,\hat{W}'(I_1) + P_1\,[u + x_3] + P_2, \tag{2.34}$$

and,

$$[2\,\hat{W}'(I_1)\,u,_{\alpha}\,]_{,\alpha} = P_1 \tag{2.35}$$

where P_1 and P_2 are constants.

Equation (2.35) is the <u>governing differential equation</u> for an anti-plane shear deformation. Once it is solved (with the appropriate boundary conditions) for the displacement field u, the stress field can then be obtained from (2.26) and (2.27).

If the body contains a traction-free surface S^*, then

$$\underset{\sim}{t} = \underset{\sim}{0} \quad \text{on } S^* , \tag{2.36}$$

and from equation (2.11) one concludes that

$$\underset{\sim}{\sigma}\,\underset{\sim}{n} = \underset{\sim}{0} \quad \text{on } S. \tag{2.37}$$

Note from equation (2.34) and the first of (2.27), that

$$\sigma_{22} = - [P_1 (u (x_1, x_2) + x_3) + P_2], \tag{2.38}$$

$$\sigma_{12} = 0.$$

By applying the boundary condition (2.37) and using (2.38), one finds that the constants P_1 and P_2 must vanish

$$P_1 = P_2 = 0. \tag{2.39}$$

Finally, on substituting (2.39) into (2.26) and (2.27), the stresses become

$$\tau_{\alpha\beta} = \sigma_{\alpha\beta} = 0,$$

$$\tau_{\alpha 3} = \tau_{3\alpha} = \sigma_{\alpha 3} = \sigma_{3\alpha} = 2\, \hat{W}' (3 + |\nabla u|^2)\, u_{,\alpha}\, , \tag{2.40}$$

$$\tau_{33} = 2\, \hat{W}' (3 + |\nabla u|^2)\, |\nabla u|^2,$$

and the differential equation (2.35) can be written as

$$[2\, \hat{W}' (3 + |\nabla u|^2)\, u_{,\alpha}\,]_{,\alpha} = 0 \quad \text{on } D\, . \tag{2.41}$$

We now consider the particular solution

$$u (x_1, x_2) = \kappa_\alpha\, u_\alpha \quad \text{on } D, \tag{2.42}$$

which satisfies the differential equation (2.41); a deformation of this type is termed simple shear. We let κ and τ be

$$\kappa = |\nabla u| = (\kappa_\alpha \kappa_\alpha)^{\frac{1}{2}}, \tag{2.43}$$

$$\tau = (\tau_{3\alpha} \tau_{3\alpha})^{\frac{1}{2}},$$

so that τ is the resultant shear stress and κ is the resultant amount of shear. From equation (2.40) we can write

$$\tau = \tau(\kappa) \equiv 2\,\hat{W}'(3 + \kappa^2)\,\kappa. \tag{2.44}$$

The function $\tau(\kappa)$ characterizes the material response in shear.

In summary, the displacement field $u(x_1, x_2)$ associated with a finite anti-plane shear deformation is to satisfy the governing differential equation (2.41). The corresponding stress components are given by (2.40).

Next consider the special case of an infinitesimal anti-plane shear deformation. In this case, a linearization of the nonlinear equations is carried out under the assumption that $|\nabla u|$, the gradient of the displacement is small, i.e.,

$$\frac{\partial u}{\partial x_\alpha} << 1. \tag{2.45}$$

On linearizing equation (2.24), the components of the Lagrangian strain tensor become

$$E_{\alpha\beta} = 0 \,, \; E_{33} = 0,$$

$$E_{3\alpha} = E_{\alpha 3} = \frac{1}{2} u,_\alpha \,. \tag{2.46}$$

Next, the stored energy function $\hat{W}$ approximates to

$$\hat{W}\,(3 + |\nabla u|^2) \sim \frac{\mu}{2} \; |\nabla u|^2, \tag{2.47}$$

so that by (2.40), the stresses are calculated to be

$$\begin{aligned} &\tau_{\alpha\beta} = 0 \,, \; \tau_{33} = 0, \\ &\tau_{\alpha 3} = \tau_{3\alpha} = \mu u,_\alpha \,, \end{aligned} \tag{2.48}$$

on D. The governing differential equation (2.41) reduces to Laplace's equation,

$$\nabla^2 u = 0 \qquad \text{on D.} \tag{2.49}$$

Thus in the case of infinitesimal anti-plane shear, the displacement field $u(x_1, x_2)$ is to satisfy the differential equation (2.49). The corresponding stress and strain components are given by (2.48) and (2.46) respectively.

2.3 J-Integral

The concept of the path independent J-integral was first introduced by Eshelby [8] in the course of determining the "energetic force" on an "elastic defect" such as a void or an inclusion. It was subsequently exploited by Rice [9] in the context of fracture mechanics. Additional path independent integrals were discovered by Knowles and Sternberg [14], and more recently by Abeyaratne and Knowles [15]. In a general three-dimensional setting, $\underset{\sim}{J}$ is given by the surface-independent integral

$$\underset{\sim}{J} = \int_S (\hat{W}\,\underset{\sim}{n} - \underset{\sim}{F}\,\underset{\sim}{\sigma}\,\underset{\sim}{n})\, d A\,, \tag{2.50}$$

where $\hat{W}$ is the elastic potential, $\underset{\sim}{n}$ is the outward normal to the regular closed surface S, $\underset{\sim}{F}$ is the deformation gradient tensor and $\underset{\sim}{\sigma}$ is the nominal (Piola) stress tensor. If the body does not contain any holes or inclusions within S, the value of $\underset{\sim}{J}$ is zero. If it does, the value is non-zero, and this value can be interpreted as a "force" on the hole or defect (see below). Similarly, Rice [7], Budiansky and Rice [16] have shown that a similar situation occurs if the region inside S contains a crack-tip. In this thesis we consider the case where the region inside S contains a dislocation.

Let the total energy of a body under the prescribed loads be denoted by E. Suppose that the body contains a "defect" (a singularity in the elastostatic field) at the position $\underset{\sim}{\xi}$. Then, the change in the total energy with respect to a change of the position of a defect can be shown to be (Eshelby [7], Budiansky and Rice [15])

$$\Delta E = J_i \, \Delta \xi_i, \tag{2.51}$$

where J_i is the ith component of $\underset{\sim}{J}$ taken on a surface S enclosing the defect. Since ΔE has the dimensions of work and $\Delta\xi_i$ the dimensions of length, it follows that J_i may be thought of as a "<u>force on the defect</u>". For example, in fracture mechanics, J_i is referred to as the force on a crack-tip. From (2.51) we can write $J_i = \partial E/\partial \xi_i$. This latter expression leads to the alternative interpretation of J_i as an <u>energy release rate</u>. According to most theories of fracture mechanics, crack propagation occurs when the energy release rate J_1 reaches a critical value.

In an entirely analogous manner, if we have a dislocation in an elastic material located at $\underset{\sim}{\xi}$, $\underset{\sim}{J}$ becomes the <u>force on the dislocation</u> due to the elastic field. It is known to be an important and useful parameter in predicting dislocation motion.

For the case of finite anti-plane shear deformations, the x_α component of the force on a defect is obtained from,

$$J_\alpha = \int_\Gamma (\hat{W} n_\alpha - n_\beta \sigma_{\beta 3} u_{,\alpha})\, ds, \tag{2.52}$$

which is the appropriate restricted form of (2.50) in anti-plane shear; ds is arc length along a closed contour Γ enclosing the defect. Our purpose in this thesis is to emphasize the fact that the force on a dislocation is a concept analogous to, and possibly as important as, the force on a crack-tip; that it can be calculated using the path-independent J-integral, and to calculate explicitly the force between two screw-dislocations in the linear and the non-linear theory of elasticity. We will exploit the path independence of (2.52) for this latter purpose.

2.4 Dislocation

Consider an infinite two-dimensional region D and view D as the cross-section of an infinite body in its undeformed (reference) configuration. Suppose that a cut is made on the half line $x_2 = 0$, $x_1 > 0$, the top face of the cut is denoted by Γ^+, while the bottom face by Γ^-. The upper face Γ^+ is now displaced by an amount b (relative to Γ^-) in the x_3-direction and the two faces are fused back together. If $u(x_1, 0^+)$ and $u(x_1, 0^-)$ denote the x_3-components of displacement on Γ^+ and Γ^- then (see fig. 3.1).

$$u\,(x_1,\,0^+) - u\,(x_1,\,0^-) = b \qquad \text{for } x_1 > 0. \tag{2.53}$$

The vector $b\,\underset{\sim}{e}_3$, where $\underset{\sim}{e}_3$ is a unit vector in the x_3-direction is known as the <u>Burgers vector</u> associated with this dislocation.

Traction continuity across the line $x_2 = 0$, $x_1 > 0$ requires

$$\tau_{32}\,(x_1,\,0^+) - \tau_{32}\,(x_1,\,0^-) = 0 \qquad \text{for } x_1 > 0. \tag{2.54}$$

In <u>summary</u>, let D_o denote the entire $(x_1,\,x_2)$-plane with the line $x_2 = 0$, $x_1 \geq 0$ deleted. We wish to find a displacement field $u\,(x_1,\,x_2)$, twice continuously differentiable on D_o such that

$$\left(2\,\hat{W}'\,(3 + |\nabla u|^2)\,u_{,\alpha}\right)_{,\alpha} = 0 \qquad \text{on } D_o, \tag{2.55}$$

$$u\,(x_1,\,0+) - u\,(x_1,\,0-) = b \qquad \text{for } x_1 > 0, \tag{2.56}$$

$$\tau_{32}\,(x_1,\,0+) - \tau_{32}\,(x_1,\,0-) = 0 \qquad \text{for } x_1 > 0 \tag{2.57}$$

$$u_{,\alpha} \to 0 \text{ as } x_1^2 + x_2^2 \to \infty\,. \tag{2.58}$$

This is a "weak formulation" of the equations of (anti-plane) elastostatics, since it involves a discontinuity in the displacement (and possibly in the displacement gradient ∇u and the shear stress τ_{31}) across the line $x_2 = 0$, $x_1 > 0$.

An alternative weak formulation, which is in fact _less_ singular than the preceding one, pertains to elastostatic fields involving equilibrium shocks. Here one permits discontinuities in ∇u but _not_ in u itself (see, for example, Knowles and Sternberg [17]). It has been shown ([18], [19]) that if the response curve in shear is monotonically increasing ($\tau'(\kappa) > 0$ for all κ) then equilibrium shocks cannot exist. (The condition $\tau'(\kappa) > 0$ ensures the ellipticity of the partial differential equation (5.55), see Zee and Sternberg [20]).

A minor modification of the arguments used in [18], [19] shows that (in contrast to the situation with equilibrium shocks), even if $\tau'(\kappa) > 0$ one _can_ have weak solutions involving dislocations. However, ∇u and τ_{31} are continuous across the dislocation-line (even though u itself is discontinuous). We will assume throughout that

$$\tau'(\kappa) > 0 \qquad \text{for all } \kappa . \tag{2.59}$$

CHAPTER 3

LINEAR PROBLEM

In this chapter, the linearized problem for a single screw dislocation in an infinite medium is discussed first. This is then extended to the case of two screw dislocations. In section 3.2, the force on a dislocation is found by two different techniques, first by calculating the total elastic energy and taking the rate of change of the energy with respect to the dislocation position; second, by application of the J-integral. Naturally, the results coincide.

3.1 Single Dislocation

Consider a screw dislocation in an infinite region R made of homogeneous isotropic elastic material. Let us suppose that a cut is made along the semi-infinite line $x_2 = 0$, $x_1 > 0$, the top face of the cut ($x_2 = 0^+$) being held fixed and the bottom face displaced in the x_3-direction by the constant amount b; $b\underset{\sim}{e}_3$ is the Burger's vector. See Figure 3.1. The dislocation is said to be a right-handed screw dislocation if b is positive. Let D be the cross section of R in the plane $x_3 = 0$, for a screw dislocation described above, the deformation is one of anti-plane shear and the governing linearized differential equation for the displacement field is Laplace's equation (2.49). We use (r,θ) as polar coordinates ($r>0$, $0<\theta\leq 2\pi$) and formulate the problem in terms of these polar coordinates. There exists a jump in the displacement field across the dislocation line, equation (2.56), but the tractions are continuous across the dislocation line, equation (2.57). We also note that as $r \to \infty$, the stress field and the displacement gradients vanish. Therefore the boundary value problem (2.55) - (2.58) for a single screw dislocation in a linear elastic field is expressed as

$$\left.\begin{aligned}
&\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} = 0, \quad \text{for } r > 0,\ 0 < \theta < 2\pi \\
&u\,(r, 0^+) - u\,(r, 2\pi^-) = b, \quad \text{for } r > 0 \\
&\partial u/\partial\theta\,(r, 0^+) - \partial u/\partial\theta\,(r, 2\pi^-) = 0, \quad \text{for } r > 0 \\
&u_{,\alpha} = 0\left(\frac{1}{r}\right) \quad \text{as} \quad r \to \infty .
\end{aligned}\right\} \tag{3.1}$$

We seek a solution to the boundary value problem (3.1) which is a function of θ alone; $u = u(\theta)$. Upon integration, the general solution for $u(\theta)$ is found to be,

$$u = A\theta + B \qquad \text{on } D. \tag{3.2}$$

Note that the condition at infinity $(3.1)_4$ is automatically satisfied. By applying the boundary conditions $(3.1)_2$, $(3.1)_3$, we evaluate the constants of integration A and B. The resulting solution is found to be.

$$u = \frac{b}{2\pi}\theta \qquad \text{on } D . \qquad (3.3)$$

The corresponding stresses are obtained from equation (2.48),

$$\left.\begin{aligned} \sigma_{31} &= \frac{-\mu b}{2\pi}\,\frac{x_2}{x_1^2 + x_2^2}, \\ \sigma_{32} &= \frac{\mu b}{2\pi}\,\frac{x_1}{x_1^2 + x_2^2}, \end{aligned}\right\} \quad \text{on } D,\ \ r \neq 0, \qquad (3.4)$$

all others being zero. In polar coordinates,

$$\left.\begin{aligned} \sigma_{3r} &= 0 \\ \sigma_{3\theta} &= \frac{\mu b}{2\pi r} \end{aligned}\right\} \quad \text{on } D ,\ (r \neq 0). \qquad (3.5)$$

The force on a single screw dislocation can be calculated by incorporating the stresses found in (3.4) and the displacement gradients obtained from (3.3), in the J-integral of (2.52). It can then be calculated by taking a closed circular contour centered at the dislocation. One readily finds $J_\alpha = 0$. The force on a single screw dislocation in an infinite elastic medium due to the elastic field turns out to be zero. This is due to the fact that there are only the internal stresses (3.4) or (3.5) which are caused by that dislocation itself and there are no other means of raising or lowering the total elastic energy in the elastic field. In order to obtain a force on this dislocation, one can either introduce another dislocation into the body or place the existing screw dislocation at a finite distance from a boundary.

Finally, we discuss the total strain energy in the body. While we have no immediate need for this here, it helps to make clear the need to introduce the notions of <u>core radius</u> and <u>outer radius</u>. These will be utilized in the subsequent sections. In order to calculate the total strain energy associated with the deformation, (3.3), we must first obtain the strain energy density, $\hat{W}$. From (2.47), it becomes,

$$\hat{W} = \frac{\mu b^2}{8\pi^2 r^2} \; . \tag{3.6}$$

Note that there is a singularity at the origin of the order r^{-2}. Thus the total strain energy stored in a disk of radius r centered at the origin becomes unbounded. We follow standard practice (e.g. [1])

and eliminate the singularity at the origin of the dislocation by considering a "Volterra core" assumption that there exists a small radius of r_o centered at the dislocation in which we do not calculate the total energy. Therefore, we consider a core region such that

$$\delta = \left\{ (x_1, x_2) \;\middle|\; 0 \leq x_1^2 + x_2^2 \leq r_o^2 \right\} , \tag{3.7}$$

and integrate the strain energy density on the remaining material $D_S = D - \delta$.

Similarly, the total stored energy has a logarithmic singularity at infinity. This forces one to cut out the far-field by some large radius R ($>r_o$). In summary, when calculating the total energy, one must restrict attention to the region between two finite radius cylinders, the smaller one being the Volterra core and the larger one, a circular cylinder of radius R, see [1]. The total energy is, therefore, written as

$$E = \int_0^{2\pi}\int_{r_o}^{R} \frac{\mu b^2}{8\pi^2 r^2} \, r dr d\theta , \tag{3.8}$$

using (3.6). Integrating (3.8) gives

$$E = \frac{\mu b^2}{4\pi} \ln \frac{R}{r_o} . \tag{3.9}$$

It is important to note that the choice of r_o and R does <u>not</u> affect the energy release rate or dislocation force. This is zero independent of the choice of r_o and R. This feature continues to be true for two dislocations and, therefore, one is able to get useful results for J <u>without</u> having to specify the values of r_o and R.

3.2 <u>Two Dislocations</u>

Consider now two screw dislocations in an infinite region R, made of homogeneous isotropic linear elastic material. The first of the two dislocations is located at $(\ell, 0)$ with the Burger's vector $b_1 \underset{\sim}{e}_3$ and the second one located at $(-\ell, 0)$ with the Burger vector $b_2 \underset{\sim}{e}_3$. We set up three polar coordinate systems, first set (r_1, θ_1), $(r_1>0,\ 0<\theta_1\leq 2\pi)$ centered at $(\ell, 0)$ and the second set of polar coordinates (r_2, θ_2), $(r_2>0,\ -\pi<\theta_2\leq\pi)$ at $(-\ell, 0)$ and finally (r, θ), $(r>0,\ 0<\theta\leq 2\pi)$ centered at the origin. This is illustrated in Figure 3.2.

The displacement field for the two screw dislocations is found immediately by applying the principle of superposition to the displacement field for a single screw dislocation, equation (3.3). The displacement field is therefore given by

$$u = \frac{b_1}{2\pi}\ \theta_1 + \frac{b_2}{2\pi}\ \theta_2\ . \tag{3.10}$$

Observe that u is discontinuous across the lines $x_2 = 0,\ x_1 > \ell$ and $x_2 = 0,\ x_1 < -\ell$. The strains may then be calculated from (2.46) and (3.10)

$$\begin{aligned} 2\,E_{31} &= u_{,1} = \frac{b_1}{2\pi}\ \frac{\partial\theta_1}{\partial x_1}(x_1,\ x_2) + \frac{b_2}{2\pi}\ \frac{\partial\theta_2}{\partial x_1}(x_1,\ x_2), \\ 2\,E_{32} &= u_{,2} = \frac{b_1}{2\pi}\ \frac{\partial\theta_1}{\partial x_2}(x_1,\ x_2) + \frac{b_2}{2\pi}\ \frac{\partial\theta_2}{\partial x_2}(x_1,\ x_2), \end{aligned} \tag{3.11}$$

which reduce to

$$\begin{aligned} 2\,E_{31} &= u_{,1} = -\frac{b_1}{2\pi}\ \frac{\sin\theta_1}{r_1} - \frac{b_2}{2\pi}\ \frac{\sin\theta_2}{r_2}, \\ 2\,E_{32} &= u_{,2} = \frac{b_1}{2\pi}\ \frac{\cos\theta_1}{r_1} + \frac{b_2}{2\pi}\ \frac{\cos\theta_2}{r_2}\ . \end{aligned} \tag{3.12}$$

Next we calculate the strain energy density associated with this deformation from

$$\hat{W} = \frac{\mu}{2}\ |\nabla u|^2\ , \tag{3.13}$$

where μ is the infinitesimal shear modulus and $|\nabla u|^2 = u,_\alpha \; u,_\alpha$.
By substituting (3.12) into (3.13), we can readily show that,

$$\hat{W} = \frac{\mu}{2} \left\{ \frac{b_1{}^2}{4\pi^2 r_1^2} + \frac{b_2{}^2}{4\pi^2 r_2^2} + \frac{2\, b_1 b_2}{4\pi^2 r_1 r_2} \cos (\theta_1 - \theta_2) \right\} . \qquad (3.14)$$

In order to calculate the total strain energy E in the body, we must integrate (3.14) over D. However, it is first necessary to eliminate the singularity at the origin of dislocations and infinity from D which cause the total strain energy to become unbounded as in the case of a single screw dislocation. To do so, we consider two hollow-cores each with a radius of r_o at the center of the dislocations (ℓ,0) and ($-\ell$,0). See Figure 3.2. Let δ_1 and δ_2 denote the so-called core regions,

$$\delta_1 = \left\{ (x_1, x_2) \mid 0 \le (x_1 - \ell)^2 + x_2^2 \le r_o^2 \right\},$$

$$\delta_2 = \left\{ (x_1, x_2) \mid 0 \le (x_1 + \ell)^2 + x_2^2 \le r_o^2 \right\}.$$

Next, let R ($> \ell + r_o$) be a large fixed number and let D_R denote the region inside the circle of radius R:

$$D_R = \left\{ (x_1, x_2) \mid 0 \le x_1^2 + x_2^2 \le R^2 \right\} .$$

Let D_S denote the material inside D_R but outside δ_1, δ_2.

$$D_S = D_R - \delta_1 - \delta_2 \ .$$

The total strain energy in D_S is finite. The strain energy density, $\hat{W}$ from equation (2.14) is now integrated over D_S

$$E = \int_{D_S} \hat{W} \, dA \ . \tag{3.15}$$

Substituting equation (3.14) into equation (3.15) and writing the integral as three separate terms, gives a total strain energy,

$$E = \int_{D_S} \hat{W}_1 \, dA + \int_{D_S} \hat{W}_2 \, dA + \int_{D_S} \hat{W}_3 \, dA, \tag{3.16}$$

where

$$\int_{D_S} \hat{W}_1 \, dA = \frac{\mu b_1^2}{8\pi^2} \int_{D_S} \frac{1}{r_1^2} \, dA,$$

$$\int_{D_S} \hat{W}_2 \, dA = \frac{\mu b_2^2}{8\pi^2} \int_{D_S} \frac{1}{r_2^2} \, dA, \tag{3.17}$$

$$\int_{D_S} \hat{W}_3 \, dA = \frac{\mu b_1 b_2}{8\pi^2} \int_{D_S} \frac{2}{r_1 r_2} \cos(\theta_1 - \theta_2) \, dA \ .$$

In order to evaluate the three integrals in (3.17), we first relate (r_1, θ_1), $(r_1>0,\ 0<\theta\leq 2\pi)$ to (r_2, θ_2), $(r_2>0,\ -\pi<\theta_2\leq\pi)$ by geometry:

$$
\begin{aligned}
r_2 \sin\theta_2 &= r_1 \sin\theta_1 \ , \\
r_2 \cos\theta_2 &= 2\ell + r_1 \cos\theta_1 \ , \qquad\qquad (3.18) \\
r_2 &= 2\ell \left\{ 1 + \frac{r_1}{\ell} \cos\theta_1 + \frac{r_1^{\,2}}{4\ell^2} \right\}^{\frac{1}{2}} .
\end{aligned}
$$

We use (r_1, θ_1) as the independent variables chosen to perform the integration over D_S. The element of area dA is then $r_1 dr_1 d\theta_1$. The integrals (3.17) are evaluated with the aid of (3.18). The first term of the equation (3.16) is written as

$$
\int_{D_S} \hat{W}_1 \, dA = \int_0^{2\pi}\!\!\int_{r_o}^{r_1^*} \frac{\mu b_1^2}{8\pi^2} \frac{1}{r_1^{\,2}} \, r_1 dr_1 d\theta_1 = \frac{\mu b_1^2}{4\pi} \left(\ln \frac{R}{r_o} - \frac{1}{4} \frac{\ell^2}{R^2} \right) + O\left(\frac{\ell^2}{R^2} \right) \qquad (3.19)
$$

where

$$
r_1 = r_1^* (\theta_1) \equiv \sqrt{R^2 - \ell^2 \sin^2 \theta_1} - \ell \cos\theta_1
$$

is the equation of the large circle $x_1^2 + x_2^2 = R^2$.

In evaluating the integral in (3.19) we have used the fact that R is large in comparison to ℓ and r_o. Thus, the final expression in (3.19) holds asymptotically, for large R. The second term of the equation (3.16) is essentially identical to the first and so

$$\int_{D_S} \hat{W}_2 \, dA = \int_0^{2\pi}\int_{r_o}^{r_2^*} \frac{\mu b_2^2}{8\pi^2} \frac{1}{r_2^2} r_2 dr_2 d\theta_2 = \frac{\mu b_2^2}{4\pi}\left(\ln \frac{R}{r_o} - \frac{1}{4} \frac{\ell^2}{R^2}\right) + O\left(\frac{\ell^2}{R^2}\right), \tag{3.20}$$

where

$$r_2 = r_2^*(\theta_2) \equiv \sqrt{R^2 - \ell^2 \sin^2 \theta_2} + \ell \cos \theta_2 .$$

Finally the third term of the equation (3.16) is integrated over D_S by expressing the integrand in terms of r_2, θ_2. Carrying out this integration, the third term of (3.16) becomes

$$\int_{D_S} \hat{W}_3 \, dA = \int_0^{2\pi}\int_{r_o}^{r_2^*} \frac{2\mu b_1 b_2}{8\pi^2 r_1 r_2} \cos(\theta_1 - \theta_2) \, r_2 dr_2 d\theta_2$$

$$= \frac{\mu b_1 b_2}{4\pi}\left(\ln \frac{2\ell}{r_o} - 2\ln \frac{R}{r_o} + \frac{1}{2} \frac{\ell^2}{R^2}\right) + O\left(\frac{\ell^2}{R^2}\right). \tag{3.21}$$

The summation of the three integrals (3.19) - (3.21), will give the total strain energy of the elastic field in the presence of two screw dislocations, with the Burger's vectors b_1 and b_2 respectively,

$$E = \frac{\mu}{16\pi}(b_1 - b_2)^2 \left[4\ln\frac{R}{r_o} - \frac{\ell^2}{R^2} \right] + \frac{\mu b_1 b_2}{4\pi}\ln\frac{2\ell}{r_o} + O\left(\frac{\ell^2}{R^2}\right) \tag{3.22}$$

on D_S. If the two screw dislocations have the same Burger's vectors, $b_1 = b_2 = b$, then the total strain energy E reduces to

$$E = \frac{\mu b^2}{4\pi}\ln\frac{2\ell}{r_o} + O\left(\frac{\ell^2}{R^2}\right). \tag{3.23}$$

Equation (3.23) is in the same form as it is described in [1] and [2], however in the general case $(b_1 \neq b_2)$, (3.22) holds.

Our primary interest lies in finding the force on a dislocation, say, the right-hand one in Figure 3.2. For this purpose, one calculates the rate of change of the total strain energy with respect to the dislocation position, as described previously. One can readily show that from (3.23) and (2.51) the force on a dislocation becomes

$$F = \frac{-\partial E}{\partial(2\ell)} = \frac{\mu b_1 b_2}{4\pi\ell} \quad . \tag{3.24}$$

Equation (3.24) is a classical result which is cited in [1] and [2]. It provides the force on a screw dislocation in a homogeneous, isotropic, linear elastic field in the presence of another screw dislocation. With $b_1 = b_2$, it is also the same result as a force on a single screw dislocation which is placed at a distance ℓ from a traction free surface as is illustrated in Figure 3.3.

We now describe an <u>alternative</u> way of finding the force on a dislocation by utilizing the equivalence between the force on the dislocation and the path independent integral J. The formulation of the J-integral was described and discussed in Chapter 2, section 2.3. For reasons of algebraic convenience we only consider the case b_1=b_2 here.

In order to calculate the force on one of the dislocations, a path of integration for J must be chosen, which encloses that dislocation but not the other. Since the integral is path-independent, we will choose a convenient path to eliminate cumbersome calculation. In this case, a circular path containing the dislocation located at (ℓ , 0) is chosen, (Figure 3.4), centered at the dislocation, with radius r_1 which is taken to be infinitesimal. The element of arc length ds is $r_1 d\theta_1$. Since the dislocations are located on the x_1-axis, by symmetry the force between them must also be in the x_1-direction. Thus, it is the J_1- integral that we must consider. From (2.52) and the path independence

$$J = J_1 = \int_0^{2\pi} (\hat{W}n_1 - \sigma_{3\beta}n_3u_{,1})\, r_1 d\theta_1 . \qquad (3.25)$$

Next, we will approximate the integrand of J for small r_1 by using the binomial expansion in (3.18). The result is, as $r_1 \to 0$ at fixed θ_1,

$$\begin{aligned} r_2 &\sim 2\ell + r_1 \cos\theta_1 , \\ \sin\theta_2 &\sim \frac{r_1 \sin\theta_1}{2\ell} , \qquad (3.26) \\ \cos\theta_2 &\sim \frac{2\ell + r_1\cos\theta_1}{2\ell + r_1\cos\theta_1} = 1. \end{aligned}$$

The displacement gradients of equation (3.12) are likewise approximated and they are, as $r_1 \to 0$ at fixed θ_1

$$u_{,1} \sim \frac{b}{2\pi} \left\{ -\frac{\sin\theta_1}{r_1} + \frac{r_1 \sin\theta_1}{(2\ell)^2} \right\},$$

$$u_{,2} \sim \frac{b}{2\pi} \left\{ \frac{\cos\theta_1}{r_1} - \frac{1}{2\ell} \right\}. \qquad (3.27)$$

By using equation (3.13) and (3.27), we can now calculate the corresponding value of the strain energy density $\hat{W}$, it is, given as

$$\hat{W} \sim \frac{\mu b^2}{8\pi^2} \left\{ \frac{1}{r_1^{\,2}} - 2 \frac{\cos\theta_1 + \sin\theta_1 \dfrac{r_1 \sin\theta_1}{2\ell}}{r_1 \, (2\ell)} \right\}. \qquad (3.28)$$

Similarly the stresses $\sigma_{3\beta}$ are approximated to the appropriate order by using equations (2.48); they become ,

$$\sigma_{31} \sim \frac{\mu b}{2\pi} \left\{ -\frac{\sin\theta_1}{r_1} + \frac{r_1 \sin\theta_1}{(2\ell)^2} \right\},$$

$$\sigma_{32} \sim \frac{\mu b}{2\pi} \left\{ \frac{\cos\theta_1}{r_1} - \frac{1}{2\ell} \right\}. \qquad (3.29)$$

On substituting equations (3.27) - (3.28) into the J-integral (equation (3.25)) and separating the integrals into three parts, the result becomes,

$$J = J_a + J_b + J_c \text{ ,} \tag{3.30}$$

where

$$J_a = \int_0^{2\pi} \hat{W} n_1 r_1 d\theta_1 \text{ ,}$$

$$J_b = \int_0^{2\pi} -n_1 \mu u_{,1}^2 r_1 d\theta_1 \text{ ,} \tag{3.31}$$

$$J_c = \int_0^{2\pi} -n_2 \mu u_{,1} u_{,2} r_1 d\theta_1 \text{ .}$$

Here $n_1 = \cos\theta_1$, $n_2 = \sin\theta_1$. Using equation (3.28) and the first of (3.31), J_a becomes,

$$J_a = \int_0^{2\pi} \frac{\mu b^2}{8\pi^2} \left[\frac{1}{r_1^2} \cos\theta_1 - \frac{2\ell\cos\theta_1 + r_1 \sin^2\theta_1}{2 r_1 \ell^2} \cos\theta_1 \right] r_1 d\theta_1 \text{ ,} \tag{3.32}$$

$$= \frac{\mu b^2}{8\pi^2} \left[0 + \frac{\pi}{\ell} - 0 \right] \text{ ,}$$

$$= \frac{\mu b^2}{8\pi\ell} \text{ .}$$

To calculate J_b, the second of the equations (3.31) we first obtain $u^2{}_{,1}$ from equation (3.27),

$$u_{,1}^{2} = \frac{b^2}{4\pi^2}\left\{-\frac{\sin^2\theta_1}{r_1{}^2} + \frac{r_1{}^2\sin^2\theta_1}{(2\ell)^4} - \frac{2\sin^2\theta_1}{(2\ell)^2}\right\} . \qquad (3.33)$$

On substituting this into J_b, we find

$$J_b = \frac{-\mu b^2}{4\pi^2}\int_0^{2\pi}\left\{-\frac{\sin^2\theta_1}{r_1{}^2} + \frac{r_1{}^2\sin^2\theta_1}{(2\ell)^4} - \frac{2\sin^2\theta_1}{(2\ell)^2}\right\}\cos\theta_1 r_1 d\theta_1 \; . \qquad (3.34)$$

$$= 0$$

Finally the third equation in (3.31), J_c, is calculated by first obtaining $u_{,1}u_{,2}$ from equation (3.27),

$$u_{,1}u_{,2} = \frac{b^2}{4\pi^2}\left\{-\frac{\sin\theta_1\cos\theta_1}{r_1{}^2} + \frac{\sin\theta_1}{2\ell r_1} + \frac{r_1\sin\theta_1\cos\theta_1}{r_1(2\ell)^2}\right\} . \qquad (3.35)$$

We now substitute (3.35) into (3.31) and evaluate it

$$J_c = \frac{-\mu b^2}{4\pi^2} \int_0^{2\pi} \left\{ \frac{-\sin\theta_1 \cos\theta_1}{r_1^{\,2}} + \frac{\sin\theta_1}{(2\ell) r_1} + \frac{\sin\theta_1\cos\theta_1}{(2\ell)^2} \right\} \sin\theta_1 r_1 d\theta_1 \ , \qquad (3.36)$$

$$= \frac{\mu b^2}{4\pi^2} \left\{ 0 + \frac{\pi}{2\ell} + 0 \right\} ,$$

$$= \frac{\mu b^2}{8\pi\ell} \ .$$

We then obtain J by combining (3.32) - (3.34) and (3.36),

$$J = \frac{\mu b^2}{4\pi\ell} \qquad (3.37)$$

which is, of course, identical to the result (3.24) (when $b_1 = b_2 = b$) obtained by the previous direct method.

CHAPTER 4

NON-LINEAR PROBLEM

The boundary value problem for a single screw dislocation in an infinite nonlinearly elastic medium is posed in section 4.1 of this chapter. It is observed that the displacement field has the same form as in the linear elastic case, found in Chapter 3. However, the stress field depends on the particular choice of the constitutive law and therefore, it is different from the one obtained in the previous chapter.

In section 4.2, two screw dislocations are introduced in an infinite nonlinearly elastic medium. The boundary value problem is posed in terms of the field equation (2.41) and the appropriate boundary conditions for the two screw dislocations. An exact solution to this nonlinear boundary value problem is not determined, instead we obtain an approximate solution as follows: our analysis is based on the assumption that the introduction of a second dislocation causes only a small perturbation in the pre-existing nonlinear field induced by the first dislocation. This permits us to use the theory of small deformations superposed on a large deformation to solve the problem. Clearly, this approximation is very good at points far from the second dislocation and is poor near that dislocation. However, since our primary purpose here is to find the force on one of the dislocations and since this can be written in terms of the path-independent J-integral _taken over a path which is far from the dislocations for most of its length,_ we expect that this approximation will provide accurate results for the force. A similar procedure was used by Abeyaratne [21] to calculate the energy release rate in fracture mechanics.

4.1 Single Dislocation

Consider a screw dislocation at the origin of an infinite region R made of homogeneous isotropic and incompressible elastic material. Suppose that a cut is made on the half-plane $x_2 = 0$, $x_1 > 0$, the top face of the cut ($x_2 = 0^+$) is held fixed and the bottom face displaced by b in the x_3-direction. Let D be the cross-section of R, in the undeformed state, in the plane $x_3 = 0$ and D_o is D with the line $x_2=0$, $x_1 \geq 0$ deleted. The resulting deformation is assumed to be one of _finite anti-plane shear_. In order to seek a solution, we set up (r, θ) as polar coordinates ($r>0$, $0<\theta\leq 2\pi$) at the origin. The boundary value problem for a single screw dislocation is then described by

$$\frac{\partial}{\partial r}\left(r\,\hat{W}'\,(3+|\nabla u|^2)\,u_{,r}\right)+\frac{\partial}{\partial\theta}\left(\hat{W}'\,(3+|\nabla u|^2)\,\frac{u_{,\theta}}{r}\right)=0 \quad \text{on } D_o,$$

$$u\,(r, 0+) - u\,(r, 2\pi-) = b, \quad r>0,$$

$$u_{,\alpha} \to O\left(\frac{1}{r}\right) \text{ as } r \to \infty, \tag{4.1}$$

$$\sigma_{32}\,(r, 0+) - \sigma_{32}\,(r, 2\pi^-) = 0, \; r>0.$$

The first of the boundary conditions in (4.1) insures that there exists a jump in the displacement equal to the amount b; the second boundary condition states that the displacement gradient vanishes as we further move away from the dislocation; the third states that the tractions must be continuous across the dislocation line. Motivated by the nature of the displacement field in the corresponding linearized problem, we again seek a solution of the form,

$$u = \hat{u}\,(\theta). \tag{4.2}$$

Substituting equation (4.2) into the boundary-value problem (4.1), reduces it to

$$\begin{aligned} &\frac{d}{d\theta}\left(\hat{W}'(3 + |\nabla\hat{u}|^2)\,\frac{\hat{u}_{,\theta}}{r} \right) = 0\ , \\ &\hat{u}\,(0+) - \hat{u}\,(2\pi^-) = b\ . \end{aligned} \tag{4.3}$$

Traction continuity condition is automatically satisfied. Integrating (4.3), yields

$$2\,\hat{W}'(3 + |\nabla\hat{u}|^2)\,\frac{\hat{u}'(\theta)}{r} = C\,(r)\ , \tag{4.4}$$

the constant of integration C possibly being a function of r. In (4.3) and (4.4) we have

$$|\nabla\hat{u}|^2 = \frac{1}{r^2}\,\hat{u}'^2(\theta). \tag{4.5}$$

Recall the definition of the material shear response $\tau\ (\kappa)$

$$\tau\ (\kappa) \equiv 2\,\kappa\,\hat{W}'(3 + \kappa^2), \quad -\infty < \kappa < \infty\ , \tag{4.6}$$

so that equation (4.4) then reduces to

$$\tau\ \left(\frac{\hat{u}'(\theta)}{r}\right) = C\ (r)\ . \tag{4.7}$$

Recall (from section 2.4) that the shear response function $\tau(\kappa)$ is invertible. Let $\kappa(\tau)$ be the inverse of $\tau\ (\kappa)$. Equation (4.7) thus leads to

$$\frac{\hat{u}'(\theta)}{r} = \kappa\ (C\ (r)\ ) \tag{4.8}$$

Since $\hat{U}'(\theta)$ can only be a function of θ, it follows that,

$$r\,\kappa\ (C\ (r)\ ) = K_2\ , \tag{4.9}$$

where K_2 is constant. From (4.8), (4.9)

$$\hat{u}(\theta) = K_2\theta + K_3 \quad \text{on } D_o\,; \tag{4.10}$$

K_3 is now a pure constant of integration. Finally, by applying the boundary conditions in (4.3), K_2 is evaluated, leading to the final solution

$$\hat{u}(\theta) = \frac{b}{2\pi}\theta \quad \text{on } D_o\,. \tag{4.11}$$

(Note that K_3 refers to a rigid translation in the x_3-direction and so has been taken to be zero). Equation (4.11) satisfies the second of the boundary conditions $u_{,\alpha} \to O(\frac{1}{r})$, as $r \to \infty$. It also happens to be the same solution as in the linear elastic solution derived in Chapter 3.

We now obtain the stresses from equation (2.40), they are given in polar coordinates as

$$\tau_{\theta 3} = \frac{b}{\pi}\hat{W}'(I_1)\frac{1}{r}\,,$$

$$\tau_{r3} = 0\,, \tag{4.12}$$

$$\tau_{33} = \frac{b^2}{\pi^2}\hat{W}'(I_1)\frac{1}{r^2}\,, \qquad I_1 = 3 + \frac{b^2}{4\pi^2 r^2}\,.$$

all others being zero; in cartesian coordinates,

$$\tau_{31} = \frac{-b}{\pi} \hat{W}'(I_1) \frac{\sin\theta}{r} ,$$

$$\tau_{32} = \frac{b}{\pi} \hat{W}'(I_1) \frac{\cos\theta}{r} , \tag{4.13}$$

$$\tau_{33} = \frac{b^2}{\pi^2} \hat{W}'(I_1) \frac{1}{r^2} , \qquad I_1 = 3 + \frac{b^2}{4\pi^2 r^2} .$$

This concludes the solution of a screw dislocation in a nonlinearly elastic material. One can readily see that the stresses in the finite elastic formulations equation (4.12) - (4.13) are different than those in the linear solution, equation (3.4) - (3.5). They depend on the form of $\hat{W}$, the strain energy density; however, the displacement $\hat{u}$ is the same as before. Note that for a Neo-Hookean material, $W = \mu(I_1-3)$, the stresses τ_{31}, τ_{32} in (4-13) coincide with the corresponding stresses in the linearized problem. On the other hand $\tau_{33} \neq 0$ here, while it is zero in the linearized problem.

It can again be readily argued that the force on the screw dislocation is zero for the same physical reasons as in Chapter 3. This can, of course, be mathematically proven by calculating the J-integral on a contour taken around the screw dislocation: the value of J becomes zero.

4.2 Two Dislocations

Now consider two dislocations in an infinite region R made of a homogeneous isotropic incompressible elastic material. The two dislocations are located in the reference configuration at $(\ell, 0)$ and $(-\ell, 0)$ on the x_1 axis, each has the same Burgers vector $b\underset{\sim}{e}_3$. We set up polar coordinate systems (r, θ) $(r>0$ and $-\pi<\theta\leq\pi)$ centered at the dislocation at $(-\ell, 0)$ and (ξ, ϕ), $(\xi>0, 0<\phi\leq 2\pi)$ centered at the dislocation at $(\ell, 0)$ Figure 4.1. The notation here is different from that used in the linearized problem. The equilibrium equation (2.41) for $u(r, \theta)$ is given as

$$\frac{\partial}{\partial r}\left(2\hat{W}'\frac{\partial u}{\partial r}\right)+\frac{2\hat{W}'}{r}\frac{\partial u}{\partial r}+\frac{1}{r^2}\frac{\partial}{\partial\theta}\left(2\hat{W}'\frac{\partial u}{\partial\theta}\right)=0 \qquad (4.14)$$

on D_o where D_o is D with the two line segments $x_2=0$, $x_1\geq\ell$ and $x_2=0$, $x_1\leq-\ell$ deleted. The boundary conditions are

$$u(r, \pi)-u(r, -\pi)=b \quad \text{for } r>\ell, \qquad (4.15)$$

(on the dislocation line emanating from $(-\ell, 0)$,) and

$$u(r, 0^+)-u(r, 0^-)=b \quad \text{for } r>2\ell, \qquad (4.16)$$

(on the dislocation line emanating from $(\ell, 0)$). We also require that the displacement gradient vanish at infinity. We further impose the continuity of tractions across the two dislocation lines:

$$u_{,\alpha} \to 0\left(\frac{1}{r}\right) \text{ as } r \to \infty ,$$

$$\sigma_{32}(r, \pi) - \sigma_{32}(r, -\pi) = 0 \quad \text{for } r > \ell , \tag{4.17}$$

$$\sigma_{32}(r, 0+) - \sigma_{32}(r, 0-) = 0 \quad \text{for } r > 2\ell .$$

In order to solve the boundary value problem (4.14) - (4.17), we employ the technique of small deformations superposed on large deformations. The general theory of this technique in finite elasticity is discussed in Green and Zerna [22] and Ogden [23]. The displacement field in the presence of the two screw dislocations is assumed to be approximately the same as the sum of the displacement of the single screw dislocation in the non-linear field found in section (4.1), plus some small perturbation $\tilde{u}(r, \theta)$ caused by the presence of the second screw dislocation. Accordingly, the displacement field $u(r, \theta)$ is now assumed to be of the form

$$u(r, \theta) = \frac{b}{2\pi}\theta + \tilde{u}(r, \theta) , \quad |\nabla \tilde{u}| << 1, \tag{4.18}$$

where the first term is the displacement field if there was only the single dislocation at $(-\ell, 0)$. Our aim is to substitute (4.18) into the boundary value problem (4.14) - (4.17) and linearize it based on $|\nabla\tilde{u}| << 1$. In order to do this we first linearize the various quantities involved in our problem. From (4.18) we have

$$\frac{\partial u}{\partial r} = \frac{\partial \tilde{u}}{\partial r},$$
$$\frac{\partial u}{\partial \theta} = \frac{b}{2\pi} + \frac{\partial \tilde{u}}{\partial \theta} \quad \text{on } D. \tag{4.19}$$

The first principal scalar invariant I_1, is calculated to leading order from equation (2.23)

$$I_1 = 3 + |\nabla u|^2 = I_o + \tilde{I}, \tag{4.20}$$

where I_o and $\tilde{I}$ are defined as

$$I_o = 3 + \frac{b^2}{4\pi^2 r^2},$$
$$\tilde{I} = \frac{2b}{2\pi r^2} \frac{\partial \tilde{u}}{\partial \theta}. \tag{4.21}$$

The strain energy density $\hat{W}(I_1)$ and its derivatives with respect to I_1, are now represented by a series expansion about I_o.

$$\hat{W}(I_1) = \hat{W}(I_o + \tilde{I}) = \hat{W}(I_o) + \hat{W}'(I_o)\,\tilde{I}\,,$$

$$\hat{W}'(I_1) = \hat{W}'(I_o) + \hat{W}''(I_o)\,\tilde{I}\,, \tag{4.22}$$

$$\hat{W}''(I_1) = \hat{W}''(I_o) + \hat{W}'''(I_o)\,\tilde{I}\,.$$

We can show by substituting (4.20) - (4.22) into equation (4.14) and retaining the leading order terms, that the governing differential equation (4.14) takes the form

$$2\hat{W}'\frac{\partial^2\tilde{u}}{\partial r^2} + \left[\,2\,\frac{\hat{W}'}{r} - \frac{b^2}{2\pi r^3}\,2\,\hat{W}''\right]\frac{\partial\tilde{u}}{\partial r} + \left[\frac{2\hat{W}'}{r^2} + \frac{1}{r^2}\,\frac{2b^2}{4\pi^2 r^2}\,2\,\hat{W}''\right]\frac{\partial^2\tilde{u}}{\partial\theta^2} = 0 \tag{4.23}$$

where $\hat{W}'$ and $\hat{W}''$ are evaluated at I_o. This is a linear differential equation with variable coefficients depending on r. We define the secant shear modulus $M(\kappa)$ by

$$M(\kappa) = 2\,\hat{W}'(3+\kappa^2)\,. \tag{4.24}$$

Differentiating the material shear response function (2.44) with respect to κ, gives the tangent shear modulus $\tau'(\kappa)$ as

$$\tau'(\kappa) = 2\,\hat{W}' + 4\,\kappa^2\,\hat{W}''. \tag{4.25}$$

Solving for $\hat{W}'$ and $\hat{W}''$ in terms of $\tau'(\kappa)$ and $M(\kappa)$ from the above equations and then substituting them into the differential equation (4.23), leads to the simpler form,

$$M(\kappa)\frac{\partial^2\tilde{u}}{\partial r^2}+\left[2M(\kappa)-\tau'(\kappa)\right]\frac{1}{r}\frac{\partial\tilde{u}}{\partial r}+\tau'(\kappa)\frac{1}{r^2}\frac{\partial^2\tilde{u}}{\partial\theta^2}=0. \tag{4.26A}$$

Here we have

$$\kappa=\frac{b}{2\pi r} \tag{4.26B}$$

The linear differential equation (4.26A) for $\tilde{u}\,(r,\theta)$ has coefficients which depend on r. In the particular case of a pure power-law material $\tau(\kappa)= A\kappa^n$, this cancels out and (4.26A) becomes a re-scaled Laplace equation.

If we keep in mind the fact that our goal is simply to calculate the dislocation force J, and that to do this we will evaluate the J-integral on an infinitesimal contour surrounding the dislocation at $(\ell,0)$, it becomes clear that we are only interested in the value of $\tilde{u}$ near $(\ell,0)$. Therefore we now specialize the differential equation to the region near the second dislocation located at $(\ell,0)$. Letting $r=2\ell$ in (4.26B) gives

$$\kappa = \frac{b}{2\pi(2\ell)} = \kappa_o \quad (= \text{known constant}) \ , \tag{4.27}$$

and therefore the shear moduli, near $(\ell, 0)$, are

$$\tau'(\kappa) = \tau'(\kappa_o) \ , \tag{4.28}$$

$$M(\kappa) = M(\kappa_o) \ .$$

Thus, we replace (4.26) by

$$M(\kappa_o) \frac{\partial^2 \tilde{u}}{\partial r^2} + \Big[2M(\kappa_o) - \tau'(\kappa_o) \Big] \frac{1}{r} \frac{\partial \tilde{u}}{\partial r} + \tau'(\kappa_o) \frac{1}{r^2} \frac{\partial^2 \tilde{u}}{\partial \theta^2} = 0 \ , \tag{4.29}$$

in the vicinty of $(\ell, 0)$.

We now write this equation in terms of polar coordinates (ξ, ϕ), $(\xi > 0,\ 0 < \phi < 2\pi)$ centered at the second dislocation, i.e. at $(\ell, 0)$, Figure 4.2. We change the variables from (r, θ) to (ξ, ϕ) with the aid of the transformation equations,

$$\frac{\partial \xi}{\partial r} = \frac{\xi + \ell \cos\phi}{\sqrt{\xi^2 + \ell^2 + 2\ell\xi\cos\phi}} ,$$

$$\frac{\partial \phi}{\partial r} = -\frac{\ell \sin\phi}{\xi\sqrt{\xi^2 + \ell^2 + 2\ell\xi\cos\phi}} ,$$

$$\frac{\partial \xi}{\partial \theta} = \ell \sin\phi ,$$

$$\frac{\partial \phi}{\partial \theta} = \frac{\xi + \ell\cos\phi}{\xi} , \tag{4.30}$$

$$\frac{\partial^2 \xi}{\partial r^2} = \frac{\ell^2 \sin^2\phi}{\xi(\xi^2 + \ell^2 + 2\ell\xi\cos\phi)} ,$$

$$\frac{\partial^2 \phi}{\partial r^2} = \frac{2\ell\ (\xi\sin\phi + \ell\sin\phi\cos\phi)}{\xi^2(\xi^2 + \ell^2 + 2\ell\xi\cos\phi)} ,$$

$$\frac{\partial^2 \xi}{\partial \theta^2} = \ell\cos\phi \left(\frac{\xi + \ell\cos\phi}{\xi}\right) .$$

The partial derivatives of $\tilde{u}$ are then derived as

$$\frac{\partial}{\partial r}(r\,\tilde{u}_{,r}) = \left[\frac{(\xi+\ell\cos\phi)^2}{\sqrt{\xi^2+\ell^2+2\xi\ell\cos\phi}}\right]\tilde{u}_{,\xi\xi} - 2\left[\frac{\ell\sin\phi(\xi+\ell\cos\phi)}{\xi\sqrt{\xi^2+\ell^2+2\xi\ell\cos\phi}}\right]\tilde{u}_{,\xi\phi} +$$

$$\left[\frac{\ell^2\sin^2\phi}{\xi^2\sqrt{\xi^2+\ell^2+2\ell\xi\cos\phi}}\right]\tilde{u}_{,\phi\phi} + \left[\frac{\xi^2+\xi\ell\cos\phi+\ell^2\sin^2\phi}{\xi\sqrt{\xi^2+\ell^2+2\xi\ell\cos\phi}}\right]\tilde{u}_{,\xi} +$$

$$\left[\frac{\xi\ell\sin\phi+2\ell^2\sin\phi\cos\phi}{\xi^2\sqrt{\xi^2+\ell^2+2\xi\ell\cos\phi}}\right]\tilde{u}_{,\phi}, \tag{4.31}$$

$$\frac{\partial}{\partial\theta}\left(\frac{\tilde{u}_{,\theta}}{r}\right) = \left[\frac{\ell^2\sin^2\phi}{\sqrt{\xi^2+\ell^2+2\xi\ell\cos\phi}}\right]\tilde{u}_{,\xi\xi} + 2\left[\frac{\ell\sin\phi(\xi+\ell\cos\phi)}{\xi\sqrt{\xi^2+\ell^2+2\xi\ell\cos\phi}}\right]\tilde{u}_{,\xi\phi} +$$

$$\left[\frac{(\xi+\ell\cos\phi)^2}{\xi^2\sqrt{\xi^2+\ell^2+2\xi\ell\cos\phi}}\right]\tilde{u}_{,\phi\phi} + \left[\frac{\ell\cos\phi(\xi+\ell\cos\phi)}{\xi\sqrt{\xi^2+\ell^2+2\xi\ell\cos\phi}}\right]\tilde{u}_{,\xi} +$$

$$\left[\frac{-\ell\sin\phi(\xi+\ell\cos\phi)-\ell^2\sin\phi\cos\phi}{\xi^2\sqrt{\xi^2+\ell^2+2\xi\ell\cos\phi}}\right]\tilde{u}_{,\phi},$$

$$r\frac{\partial\tilde{u}}{\partial r} = \frac{\partial\tilde{u}}{\partial\xi}(\xi+\ell\cos\phi) - \frac{\partial\tilde{u}}{\partial\phi}\left(\frac{\ell\sin\phi}{\xi}\right).$$

Keeping in mind that ξ is small in the immediate vicinity of $(\ell, 0)$, the partial derivatives in (4.31) are, to the leading order,

$$\frac{\partial}{\partial r}(r\,\tilde{u}_{,r}) \sim \ell\cos^2\phi \quad \tilde{u}_{,\xi\xi} - \frac{2\ell\,\sin\phi\,\cos\phi}{\xi}\tilde{u}_{,\xi\phi} +$$

$$\frac{\ell\sin^2\phi}{\xi^2}\tilde{u}_{,\phi\phi} + \frac{\ell\sin^2\phi}{\xi}\tilde{u}_{,\xi} + \frac{2\ell\sin\phi\cos\phi}{\xi^2}\tilde{u}_{,\phi}\,,$$

$$\tilde{u}_{,r} \sim \cos\phi\,\tilde{u}_{,\xi} - \frac{\sin\phi}{\xi}\tilde{u}_{,\phi}\,, \tag{4.32}$$

$$\frac{\partial}{\partial\theta}\left(\frac{\tilde{u}_{,\theta}}{r}\right) \sim \ell\,\sin^2\phi\,\tilde{u}_{,\xi\xi} + \frac{2\ell\,\sin\phi\,\cos\phi}{\xi}\tilde{u}_{,\xi\phi} +$$

$$\frac{\ell\,\cos^2\phi}{\xi^2}\tilde{u}_{,\phi\phi} + \frac{\ell\,\cos^2\phi}{\xi}\tilde{u}_{,\xi} - \frac{2\ell\,\sin\phi\,\cos\phi}{\xi^2}\tilde{u}_{,\phi}\,,$$

$$\frac{\partial\tilde{u}}{\partial\theta} = \ell\,\sin\phi\,\tilde{u}_{,\xi} + \frac{\ell}{\xi}\cos\phi\,\tilde{u}_{,\phi}\,.$$

Incorporating equations (4.32) into the differential equation (4.29) and regrouping the terms, we get

$$\xi^2[M(\kappa_o)\cos^2\phi + \tau'(\kappa_o)\sin^2\phi]\tilde{u}_{,\xi\xi} + 2\xi[\tau'(\kappa_o)-M(\kappa_o)]$$

$$\sin\phi\,\cos\phi\;\tilde{u}_{,\xi\phi} + [\tau'(\kappa_o)\cos^2\phi + M(\kappa_o)\sin^2\phi]\,\tilde{u}_{,\phi\phi} + \qquad (4.33)$$

$$\xi[\tau'(\kappa_o)\cos^2\phi + M(\kappa_o)\sin^2\phi]\tilde{u}_{,\xi} + 2[M(\kappa_o) - \tau'(\kappa_o)]\sin\phi\,\cos\phi\;\tilde{u}_{,\phi} = 0.$$

Equation (4.33) is a second order linear partial differential equation with variable coefficients depending on both ξ and ϕ. Note that if we linearize the constitutive law by letting $M(\kappa_o) = \tau'(\kappa_o)$ we arrive at the Laplace's equation in polar coordinates.

We seek a solution to (4.33) in the form

$$\tilde{u}\,(\xi,\,\phi) = V\,(\phi)\,. \qquad (4.34)$$

Upon substituting equation (4.34) into (4.33), we find

$$(\tau'(\kappa_o)\cos^2\phi + M(\kappa_o)\sin^2\phi)\ddot{V} + 2(M(\kappa_o) - \tau'(\kappa_o))\sin\phi\cos\phi\dot{V} = 0\,, \qquad (4.35)$$

or,

$$\frac{d}{d\phi}\left[(\tau'(\kappa_o)\cos^2\phi + M(\kappa_o)\sin^2\phi)\,\dot{V}\right] = 0. \qquad (4.36)$$

Integrating this once gives

$$\dot{V} = \frac{2C}{(\tau'(\kappa_o) - M(\kappa_o))\cos 2\phi + \tau'(\kappa_o) + M(\kappa_o)} \; , \tag{4.37}$$

where C is a constant of integration. On integrating (4.37), (See Appendix A), we arrive at the solution,

$$V(\phi) = D + \frac{C}{\sqrt{M(\kappa_o)\tau'(\kappa_o)}} \tan^{-1}\left(\sqrt{\frac{M(\kappa_o)}{\tau'(\kappa_o)}}\tan\phi\right) + C\,\frac{p'\pi}{\sqrt{M(\kappa_o)\tau'(\kappa_o)}} \; , \tag{4.38A}$$

where p' is an integer to be chosen according to

$$(2p'-1)\frac{\pi}{2} < \phi \le (2p'+1)\frac{\pi}{2} \; , \tag{4.38B}$$

for $0 < \phi < 2\pi$.

We turn next to the boundary condition (4.16). In view of (4.18) we see that it requires

$$-\bar{u}(r, 0^+) + \bar{u}(r, 0^-) = b \quad \text{for } r>2l \; , \tag{4.39}$$

which in view of (4.34) requires

$$- V\ (0^+) + V\ (2\pi^-) = b. \tag{4.40}$$

(Recall that $-\pi<\theta<\pi$ and $0<\phi<2\pi$.) In order to impose (4.40) we need $V(0)$ and $V(2\pi)$, when $\phi = 0$ (4.38B) requires that we take $p' = 0$ and so (4.38A) gives

$$V\ (0^+) = D. \tag{4.40A}$$

When $\phi = 2\pi$, (4.38B) requires that we take $p' = 2$ and so,

$$V\ (2\pi -) = D + \frac{2\pi C}{\sqrt{M(\kappa_o)\ \tau'(\kappa_o)}} \tag{4.40B}$$

From equations (4.40A), (4.40B), (4.40), we obtain

$$C = \frac{b\sqrt{M(\kappa_o)\ \tau'(\kappa_o)}}{2\pi}\ . \tag{4.41}$$

Therefore, the solution $V(\phi)$ takes the form

$$V\ (\phi) = \frac{b}{2\pi}\tan^{-1}\left(\sqrt{\frac{M(\kappa_o)}{\tau'(\kappa_o)}}\tan\phi\right) + \frac{p'b}{2} + D, \tag{4.42}$$

or from equation (4.34)

$$\tilde{u}\,(\xi,\ \varphi) = \frac{b}{2\pi}\tan^{-1}\left(\sqrt{\frac{M(\kappa_o)}{\tau'(\kappa_o)}}\tan\phi\right) + \frac{p'b}{2} + D,$$

$$\begin{cases} p' = 0 \text{ for } 0 < \phi < \pi/2\ , \\ p' = 1 \text{ for } \frac{\pi}{2} < \phi < \frac{3\pi}{2}\ , \\ p' = 2 \text{ for } \frac{3\pi}{2} < \phi < 2\pi\ . \end{cases} \tag{4.43}$$

The traction continuity condition $(4.17)_3$ is automatically satisfied. Equation (4.43) represents the perturbation in the displacement field due to the presence of the second dislocation. Note that the value of the constant D cannot be found from this purely local calculation near the dislocation (ℓ, 0). However, D does not enter the results for the dislocation force J and so it is not of concern to us. We can now determine the force on the first dislocation using equation (4.43).

4.3 J-Integral Evaluation

In order to calculate J, a path of integration must be chosen. In this case a circular path is chosen to contain the second dislocation and it is centered at (ℓ, 0) the radius δ of the circle is taken to be infinitesimal. One can show that the linearized version of J is also path independent.

The J-integral of (2.52) is rewritten as

$$J = J_a + J_b + J_c$$

where

$$J_a = \int_0^{2\pi} \hat{W} \cos\phi \, \xi d\phi \quad ,$$

$$J_b = \int_0^{2\pi} - \cos\phi \sigma_{31} u_{,1} \xi d\phi \quad , \tag{4.44}$$

$$J_c = \int_0^{2\pi} -\sin\phi \sigma_{32} u_{,1} \xi d\phi \, .$$

Substituting from equation (4.22), one can readily show that the first term of the integral (4.44) is

$$J_a = \int_0^{2\pi} (\hat{W}(I_o) + \hat{W}'(I_o)\tilde{I})\cos\phi \; \xi d\phi = \int_0^{2\pi} \hat{W}'(I_o)\tilde{I}\cos\phi \; \xi d\phi. \tag{4.45}$$

(The first term in the left hand side of (4.45) vanishes). Substituting for $\tilde{I}$ from equation (4.19) gives

$$J_a = \hat{W}'(I_o) \int_0^{2\pi} \frac{b}{\pi r^2} \frac{\partial \tilde{u}}{\partial \theta} \cos\phi \; \xi d\phi \quad . \tag{4.46}$$

Next, we express $\partial\tilde{u}/\partial\theta$ in terms of polar coordinates (ξ, ϕ). By (4.30),

$$\frac{1}{r}\,\frac{\partial\tilde{u}}{\partial\theta} = \frac{\partial\tilde{u}}{\partial\xi}\left(\frac{2\ell\sin\phi}{\sqrt{\xi^2+4\ell^2+4\ell\xi\cos\phi}}\right) + \frac{\partial\tilde{u}}{\partial\phi}\left(\frac{\xi + 2\ell\cos\phi}{\xi\sqrt{\xi^2+4\ell^2+4\ell\xi\cos\phi}}\right). \tag{4.47}$$

As ξ tends to zero, equation (4.47) reduces, to leading order, to

$$\frac{\partial\tilde{u}}{\partial\theta} = 2\ell\,\sin\phi\;\tilde{u}_{,\xi} + \frac{2\ell}{\xi}\cos\phi\;\tilde{u}_{,\phi}\ . \tag{4.48}$$

Substituting (4.48) back into the integral (4.46) and incorporating the solution $\tilde{u}$ given in equation (4.43), the integral becomes

$$J_a = \frac{b^2}{4\pi^2\ell}\,\hat{W}'(I_o)\int_0^{2\pi}\cos^2\phi\,\frac{d}{d\phi}\,\tan^{-1}\left[\sqrt{\frac{M(\kappa_o)}{\tau'(\kappa_o)}}\,\tan\phi\right]\,d\phi\ . \tag{4.49}$$

The integral in (4.49) is evaluated in appendix A: the result is

$$J_a = \frac{b^2}{4\pi\ell}\,M(\kappa_o)\,\frac{\sqrt{M(\kappa_o)}}{\sqrt{M(\kappa_o)}+\sqrt{\tau'(\kappa_o)}}\ . \tag{4.50}$$

The second term in the integrand (4.44) can be similarly evaluated. It turns out to vanish identically. Finally we evaluate the third term in the integrand (4.44). J_c becomes

$$J_c = \frac{b^2 M(\kappa_o)}{4\pi\ell} - \frac{b^2}{4\pi\ell} M(\kappa_o) \frac{\sqrt{M(\kappa_o)}}{\sqrt{M(\kappa_o)} + \sqrt{\tau'(\kappa_o)}} . \tag{4.51}$$

Thus the <u>dislocation force</u> J is obtained by combining (4.50) and (4.51), to get

$$J = \frac{b^2 M(\kappa_o)}{4\pi\ell} , \tag{4.52}$$

where $\kappa_o = \dfrac{b}{4\pi\ell}$, and $M(\kappa_o)$ is the secant modulus of shear.

CHAPTER 5

SUMMARY AND DISCUSSION

In section 5.1 of this chapter, we linearize the nonlinear expression for J to recover what was derived in chapter 3, while in section 5.2 we discuss J for pure power law materials. Equation (4.52) is the final expression for the force on a screw dislocation of strength b due to a second screw dislocation, also of strength b, located at a distance 2ℓ. It is also the force on a screw dislocation of strength b placed at a distance ℓ from a traction-free boundary. The formula (4.52) for the dislocation-force is given in terms of the magnitude b of the Burger's vector, the distance ℓ and the secant shear modulus M. Finally we conclude our investigation in 5.3 of this chapter.

5.1 Linearized Elasticity

In the case of an infinitesimal deformation, we have

$$\hat{W}'(I_o) = \frac{\mu}{2} \quad , \tag{5.1}$$

where μ is the infinitesimal shear modulus for the material.

We also have,

$$M(\kappa_o) = \tau'(\kappa_o) = \mu \ . \tag{5.2}$$

By virtue of equations (4.25), (5.1), (5.2) and (4.52), it follows that

$$J = \frac{\mu b^2}{4\pi \ell}, \tag{5.3}$$

which is the result obtained using the two different techniques in the previous chapter.

5.2 Pure Power Law Materials

In this section we specialize the formula (4.52) for the dislocation-force to power law materials. Recall that for our purpose here, we can view the material as being completely characterized by its response in shear. The class of "pure power law materials" is characterized by the shear response

$$\frac{\tau(\kappa)}{\tau_*} = \left(\frac{\kappa}{\kappa_*}\right)^m, \tag{5.4}$$

where $\frac{\tau_*}{\kappa_*^m} > 0$ and $m > 0$ are constitutive parameters, Figure 5.1. An alternative class of power law materials is the one proposed by Knowles [11]. The second model has the advantage that it linearizes well about $\kappa=0$. On the other hand, for large values of κ, they are both of the same form.

For the pure power law materials described by the shear response (5.4), one can readily show that the secant shear modulus and the tangent shear modulus take the form

$$M(\kappa_o) = \frac{\tau_*}{\kappa_*^m} \kappa_o^{m-1} , \tag{5.5}$$

and

$$\tau'(\kappa_o) = \frac{\tau_*}{\kappa_*^m} m \kappa_o^{m-1} = m\, M(\kappa_o) , \tag{5.6}$$

where κ_o is described in (4.27) as $\kappa_o = b/4\pi\ell$.

The force on a dislocation in pure power law form of materials can now be calculated by substituting (5.5) in (4.52), it becomes

$$J = \frac{b^2 \tau_*}{4\pi\ell\kappa_*^m} \kappa_o^{m-1} . \tag{5.7}$$

In dimensionless form, (5.7) becomes

$$J_* = \frac{J}{\tau_* b} = \frac{b^m}{(4\pi\ell)^m \kappa_*^m} \; . \tag{5.8}$$

A graph of J_* vs ℓ is shown in Figure 5.2. Note that as ℓ increases the force on a dislocation decreases which is expected since the effect of the second dislocation is negligible when the separation is large. Since the results here would be more accurate for larger values of ℓ the range $\frac{\ell}{b} > 1$ is of primary interest here. We also note that for fixed separation ℓ, the force between the dislocations decreases with increasing hardening exponent m. In particular, this means that for softening materials ($m < 1$) the force is greater than that predicted by the linear theory; for hardening materials ($m > 1$) it is less.

5.3 Summary

This study was concerned with estimating the value of the force between two screw dislocations in an elastic solid. Since the linear theory of elasticity predicted unbounded strains at a dislocation, the results predicted by such a theory were suspect. The present study was carried out within the fully nonlinear theory of elasticity.

Since the force between two dislocations was defined as the rate of change of energy with respect to the separation between the dislocations, one way to calculate this force was to first calculate the total energy stored in the body. This was an almost impossible task to carry out exactly in a fully nonlinear theory. However, we observed that the value of the J-integral evaluated along a path surrounding one dislocation was precisely equal to the magnitude of this force. We exploited the path-independence of the J-integral in order to obtain accurate estimates of the force between two dislocations in the presence of nonlinearity.

APPENDIX A

In Chapter 4 we have integrated $\dot{V}(\phi)$ as follows: Recall that

$$\dot{V}(\phi) = \frac{C}{(\tau'+M)+(\tau'-M)\cos 2\phi}\,, \tag{A.1}$$

where C is a constant. By using trigonometry,

$$\dot{V}(\phi) = \frac{C}{2}\left(\frac{1-\frac{\tau'}{M}}{\tau'}\right)\frac{1}{1+\frac{M}{\tau'}\tan^2\phi} + \frac{C}{2M}\,. \tag{A.2}$$

Integrating (A.2) gives,

$$V(\phi)-V(0) = \int_0^{\phi} \dot{V}(s)ds = \frac{C}{2}\,\frac{1-\frac{\tau'}{M}}{\tau'}\int_0^{\phi}\frac{1}{1+\frac{M}{\tau'}\tan^2\phi}\,ds + \frac{C}{2M}\,\phi\,. \tag{A.3}$$

The principal value of the integral in (A.3) is

$$\frac{\sqrt{\frac{M}{\tau'}}}{\frac{M}{\tau'}-1}\tan^{-1}\left(\sqrt{\frac{M}{\tau'}}\tan\phi\right), \tag{A.4}$$

and therefore,

$$V(\phi)-V(0) = \frac{C}{2}\,\frac{1-\frac{\tau'}{M}}{\tau'}\left\{\frac{\sqrt{\frac{M}{\tau'}}}{\frac{M}{\tau'}-1}\tan^{-1}\left(\sqrt{\frac{M}{\tau'}}\tan\phi\right) - \frac{\phi}{\frac{M}{\tau'}-1} + \frac{p'\pi\tau'\sqrt{\frac{M}{\tau'}}}{M-\tau'}\right\} + \frac{C}{2M}\phi\,, \tag{A.5}$$

where the integer p' is to be chosen from

$$(2p'-1)\frac{\pi}{2} < \phi < (2p'+1)\frac{\pi}{2}\,. \tag{A.6}$$

Simplifying (A.5) shows that

$$V(\phi) = V(0) + \frac{C}{2}\frac{1}{\sqrt{M\tau'}}\tan^{-1}\left(\sqrt{\frac{M}{\tau'}}\tan\phi\right) + \frac{C}{2}\frac{p'\pi}{\sqrt{M\tau'}}\,. \tag{A.7}$$

We now can integrate,

$$\int_0^{2\pi}\cos^2\phi\,\frac{d}{d\phi}\tan^{-1}\left[\sqrt{\frac{M}{\tau'}}\tan\phi\right]d\phi = \int_0^{2\pi}\frac{\sqrt{\frac{M}{\tau'}}\,d\phi}{1+\frac{M}{\tau'}\tan^2\phi}\,. \tag{A.8}$$

Using (A.7), (A.8) becomes,

$$\frac{2\pi\sqrt{\tau'}}{\sqrt{M}+\sqrt{\tau'}}\,. \tag{A.9}$$

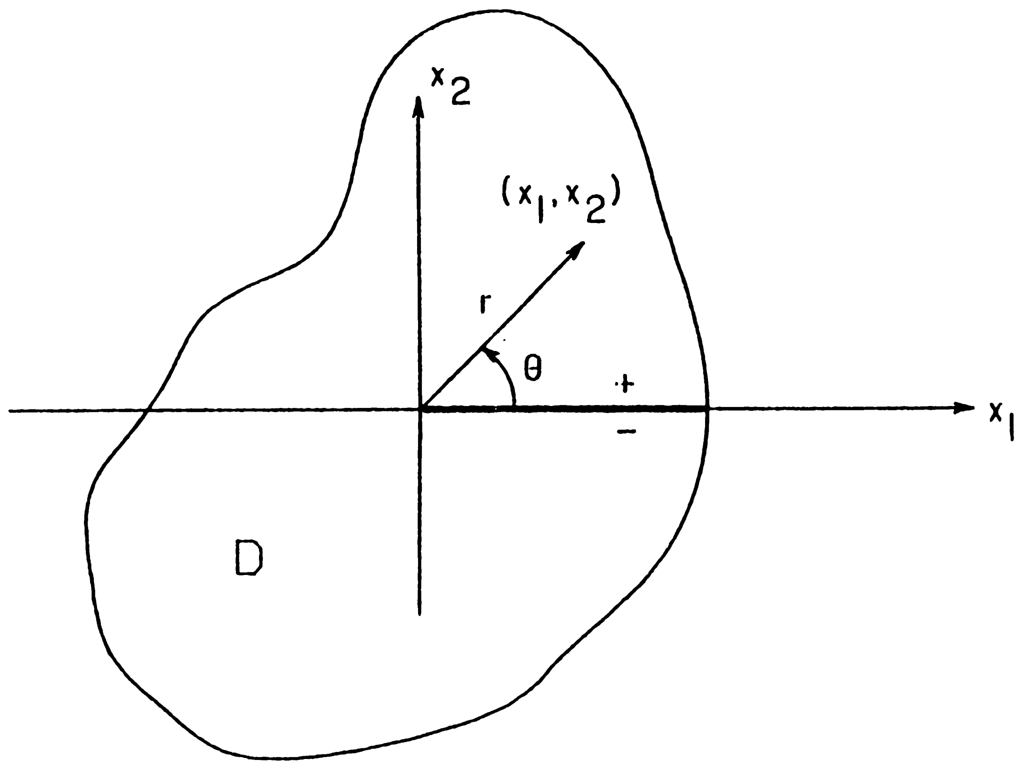

Figure 3.1. Cross section D of cylinder with dislocation on $x_2=0$, $x_1 \geq 0$

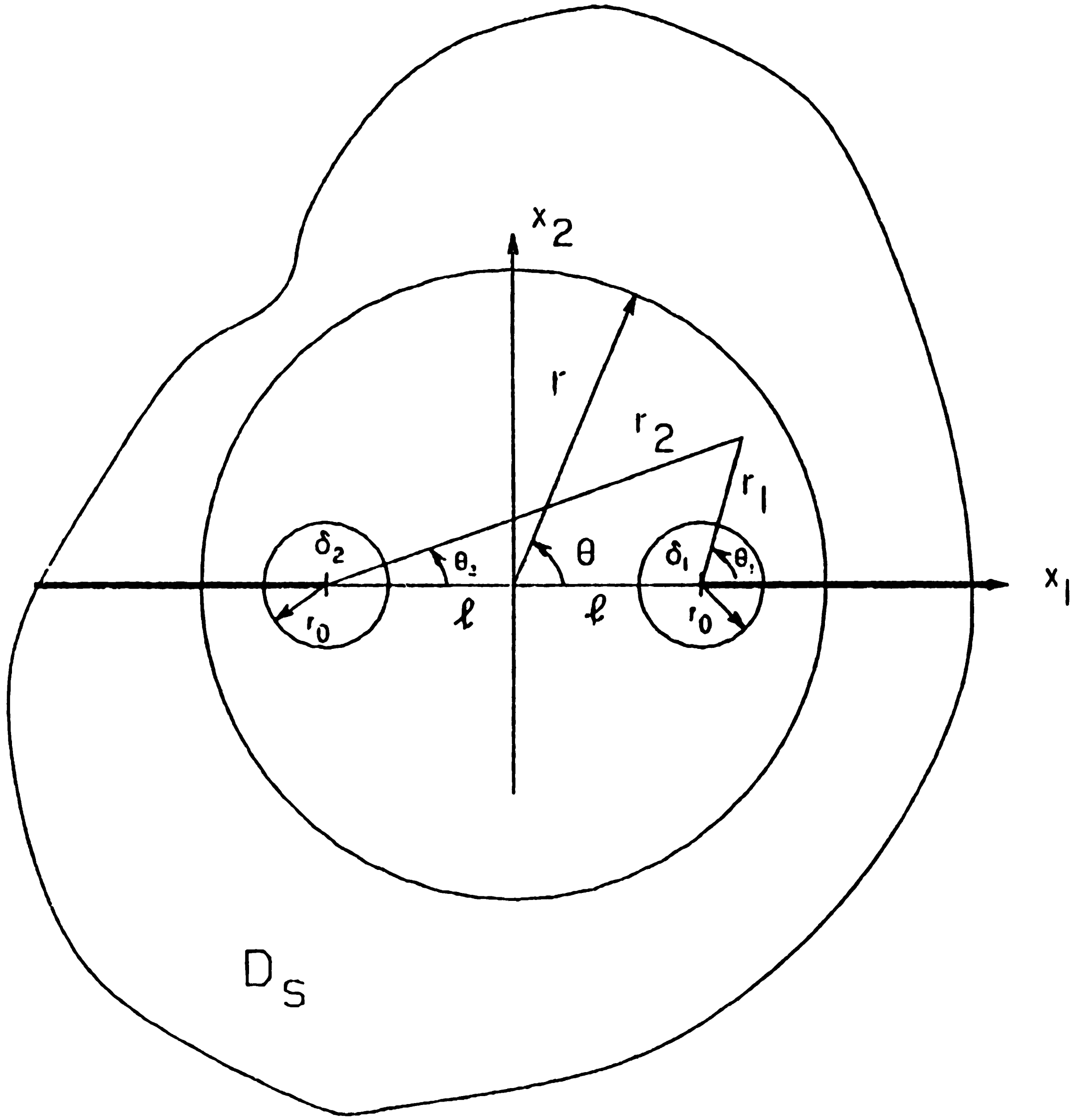

Figure 3.2. Dislocation cores in two dislocation regions D_s

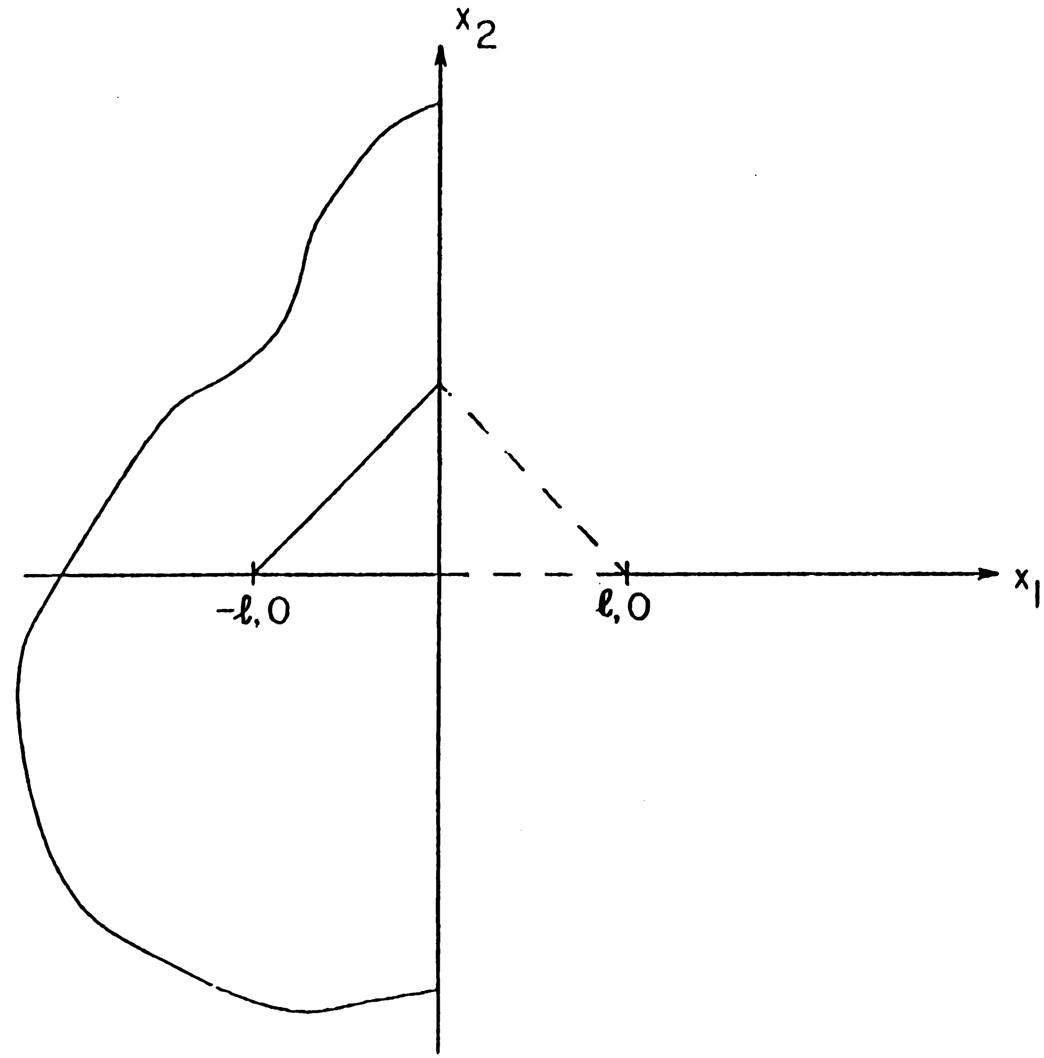

Figure 3.3. Dislocation in a traction free half-space

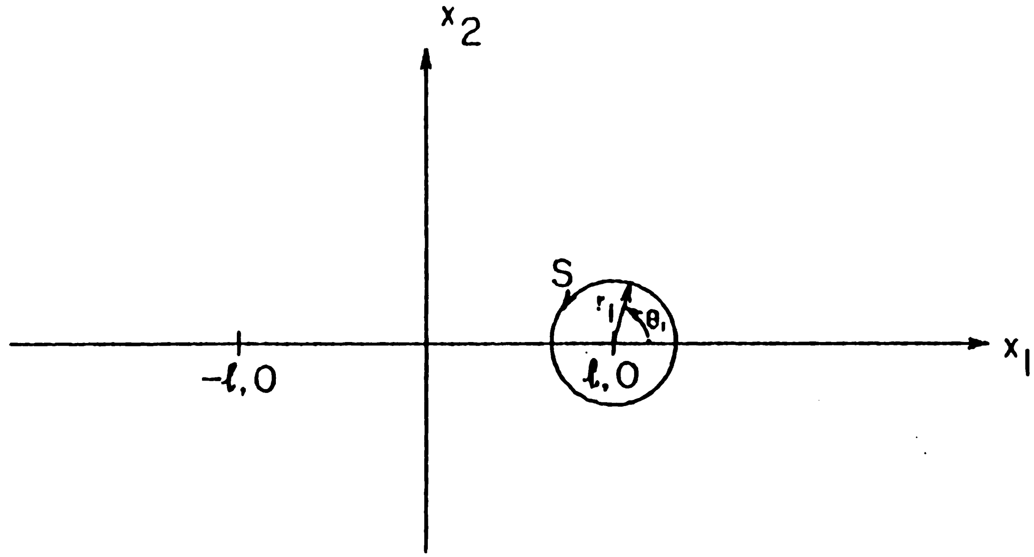

Figure 3.4. Two dislocations centered at $x_1=\ell$ and $x_1=-\ell$

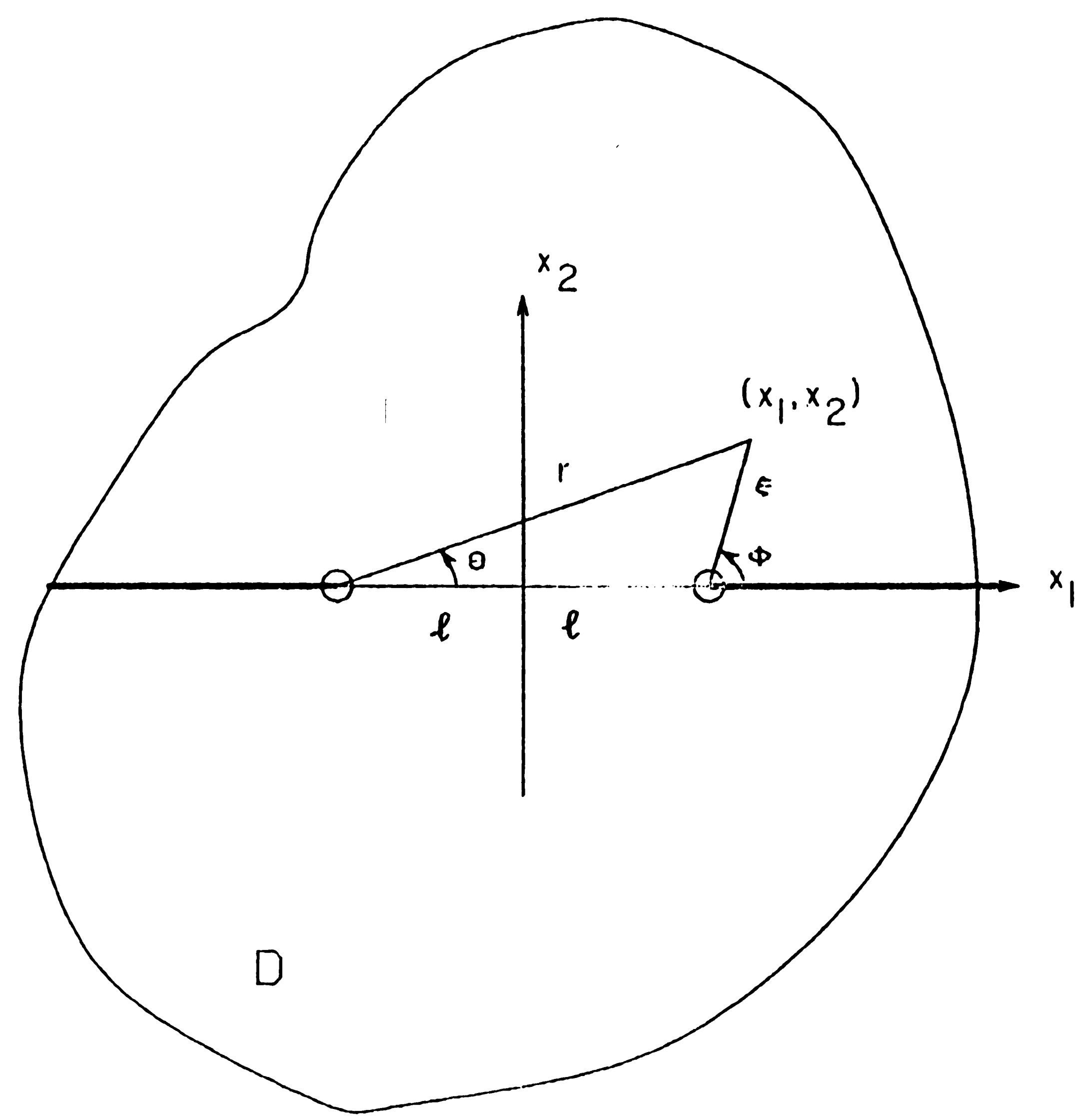

Figure 4.1. Two dislocations in a non-linear domain D

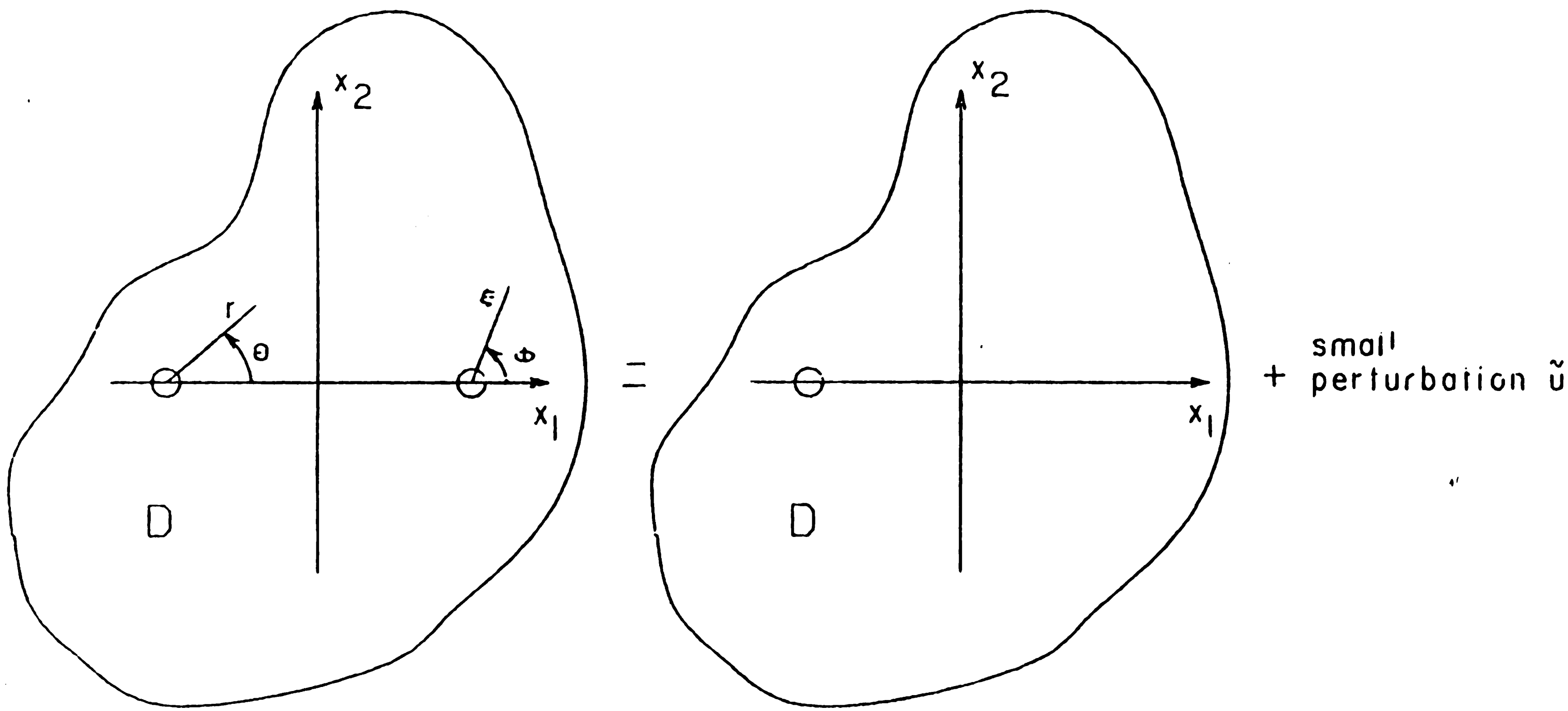

Figure 4.2. Representation of two dislocations with one and small perturbation $\tilde{u}$

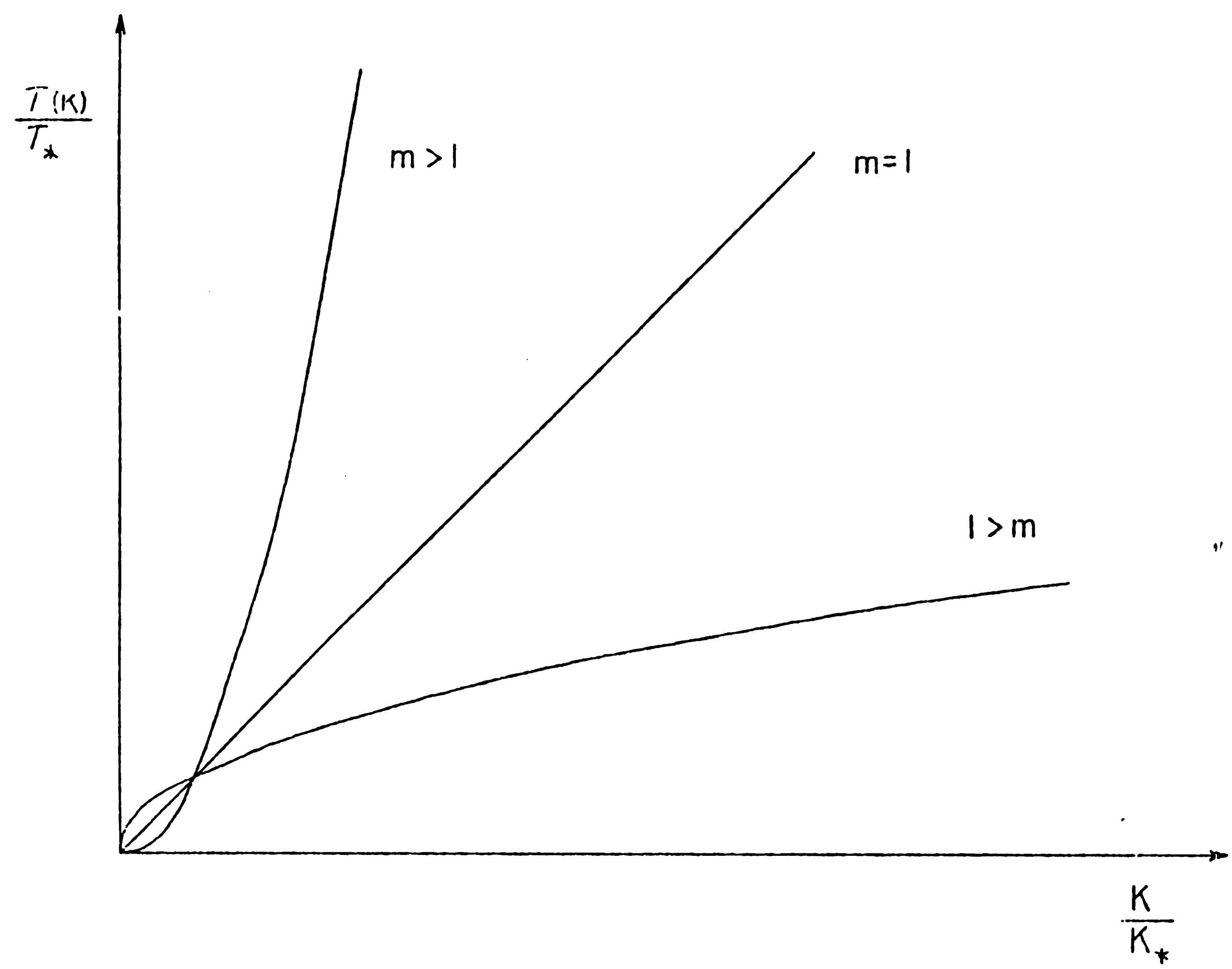

Figure 5.1. Shear response curves for pure power law materials

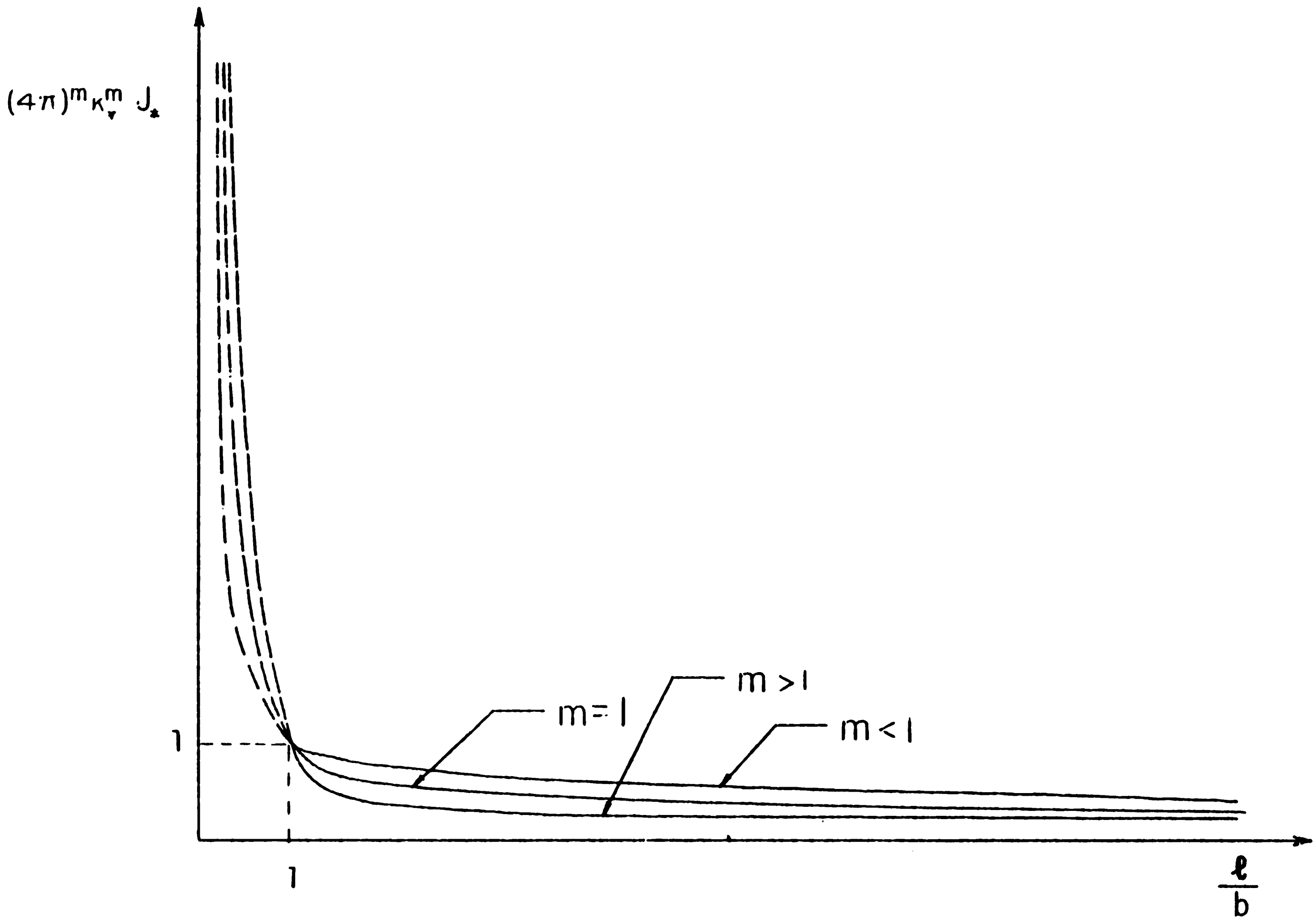

Figure 5.2. Variation of J_* with ℓ

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