

Gauge-field-theory solution of the elastic state of a screw dislocation in a dispersive (non-local) crystalline solid

By P. Sharma¹ and S. Ganti²

¹Department of Mechanical Engineering, University of Houston, Houston, TX 77204, USA (psharma@uh.edu) ²General Electric Corporate Research and Development, Schenectady,

NY 12309, USA

The relaxed state of a type of topological defect (screw dislocation) located in a dispersive (non-local) elastic solid is discussed from a viewpoint of gauge field theory. The starting point of this work is the non-local elastic Lagrangian, that is, like its classic elastic counterpart, globally gauge invariant under the Euclidean group of transformations $SO(3) \triangleright \mathcal{T}(3)$. When compared with gauge solutions of the same problem predicated on the classical elastic Lagrangian, the present solution sheds some interesting insights into the nature of non-locality-gauge field interactions. Both the $\mathcal{T}(3)$ gauge theory of dislocations (predicated on breaking of the translational symmetry) and the phenomenological non-local elasticity introduce their own respective characteristic length-scale parameters in the elastic equilibrium of dislocations while removing unphysical singularities. In the present work we show that, surprisingly, attempts to elucidate gauge interactions in a dispersive or non-local medium lead to functionally the same solution as in the gauge theory based on local elasticity, albeit, the gauge lengthscale must be replaced by an effective length-scale measure. In particular, the non-local and the gauge length-scale combine in a nonlinear fashion to yield the aforementioned effective length-scale. Our results allow one to immediately write the solution of most screw dislocation problems in the gauge non-local theory of defects, provided the counterpart gauge solution based on classical elasticity is known.

Keywords: gauge field theory; non-local elasticity; strain gradient elasticity; dislocations; defects

1. Introduction

While the application of gauge theories to explain fundamental interactions in much of physics (e.g. quantum field theory, relativity, particle physics) is well known (Moriyasu 1983; O'Raifeartaigh 1997), their application in the study of defects in crystalline solids is relatively recent (Kadić & Edelen 1983) and, with the exception of a comparatively sparse literature, it is largely unexplored. As motivated by Valsakumar & Sahoo (1988), in classical continuum mechanics of crystalline solids, topological defects are typically introduced in an *ad hoc* fashion (see as an example the seminal paper by Eshelby (1956)). The stresses are found

to be unphysically singular at the eye of defects such as dislocations. In the gauge theory of defects in crystalline solids, topological defects can be seen to arise naturally based on group theoretic symmetry arguments (Kadić & Edelen 1983; Valsakumar & Sahoo 1988; Edelen & Lagoudas 1988). Unphysical singularities are removed in the gauge analysis of defects while the mathematical framework appears to provide a natural and aesthetic formalism to account for various field interactions.

In this work, we present a gauge field theoretic solution of a screw dislocation located in a non-local or dispersive media. Both non-local elasticity and the gauge theory of defects independently introduce a characteristic length-scale, rendering the continuum field description of defects *size-dependent* as opposed to the well-known size-independency of classical continuum mechanics or elasticity. As shall be discussed in the next section, currently, gauge solutions for a screw dislocation have been found only for a classically elastic medium (Valsakumar & Sahoo 1988; Edelen 1996). The question of how the gauge fields of defects interact in a dispersive media has not yet been addressed. In particular it is of interest to see how the two length-scales in each respective theory combine; the answer to this forms one of the major outcomes of the present work.

In the following section (§ 2), we will first briefly review the relevant literature on this topic. Our motivation for the present study is also clarified. Subsequently, in § 3, the general gauge formalism for defects in solids is discussed. Our point of departure from existing works arises in this section, where we adopt a non-local material behaviour as a starting point before applying the gauge theory. The new field equations are derived. In § 4, the field equations are solved in closed-form for the specific case of a screw dislocation. The results and implications of the present work are discussed in § 5. In particular, the gauge solution to the force between two screw dislocations in an infinite non-local medium is also addressed. Closing remarks are provided in § 6.

2. Background and motivation

The first paper on the use of gauge theory in the study of defects in crystalline solids appears to be Golebiewska-Lasota (1979). Although other contributions appeared around the same time (e.g. Gairola 1981; Edelen 1982; Golebiewska-Lasota & Edelen 1979), the work of Kadić & Edelen (1983) can be credited for setting the gauge theory of defects on a rigorous footing. Subsequently, their work was enhanced in numerous articles (Lagoudas & Edelen 1989; Edelen 1989a,b; Edelen & Lagoudas 1999), and a monograph by Edelen & Lagoudas (1988) that is seen to cover most of the formal foundation concepts of this theory. We will largely follow the gauge theory of defects as established by Edelen, Kadić and Lagoudas, and in recognition of their pioneering work will refer to it as simply the EKL theory. Several other works have appeared in the literature on the gauge theory of defects, but these are of limited interest in the present context. They are not mentioned for the sake of brevity. Further literature that is appropriate to the problem at hand will be discussed contextually.

Continuum elasticity is subject to invariance under the three-dimensional Euclidean group, $SO(3) \triangleright \mathcal{T}(3)$, that is, the semi-direct product of the non-Abelian

special rotation group, SO(3), and the Abelian group of translations, $\mathcal{T}(3)$. In the EKL theory, breaking of either the translational or rotational symmetry leads to defects in the material continuum. The EKL gauge theory of defects essentially consists of the following ingredients (some formal aspects of which will become apparent in the next section in the course of our derivations): (i) adopting an admissible Lagrangian which is invariant under a global gauge group, that is, the Euclidean group in the elasticity; (ii) making the gauge group inhomogeneous in space-time spoils the invariance of the Lagrangian; (iii) using a Yang–Mills type construct (minimal coupling) the standard derivative is replaced by a 'gauge covariant' derivative and 'compensating gauge fields' are introduced to restore the 'spoiled invariance' of the Lagrangian; and (iv) the original Lagrangian is now modified by an additional contribution from the compensating gauge fields. The new field equations are obtained as customary, via appeal to the Euler-Lagrange equations, and are supplemented by an appropriate choice of gauge to render a unique solution. There are both deeper and wider implications, often philosophical, of the EKL gauge theory of defects. Brevity considerations preclude a discussion of some finer points of their theory, as is evident from the brief preceding paragraph, which purports to summarize it. The reader is, of course, encouraged to consult the original reference (Edelen & Lagoudas 1988) for a complete understanding of this theory.

Kadić & Edelen (1983), based on the classical elastic Lagrangian, presented a solution to the EKL field equations that was claimed to represent the gauge field solution of a screw dislocation. This was subsequently criticized (Valsakumar & Sahoo 1988), since, in the far field, the Kadić–Edelen screw dislocation solution did not asymptotically match the classical one (as it should). This was independently corrected by Valsakumar & Sahoo (1988) and Edelen himself (1996). The work of Valsakumar & Sahoo (1988) is worth noting, since, in addition to presenting the correct gauge solution of screw dislocation, they also derived a solution of a disclination arising out of the breaking of the translational invariance – in contrast to the belief until then that local symmetry breaking of the group leads to disclinations (see Edelen & Lagoudas 1988). This notion that the $\tau(3)$ group, as for dislocations, is also the correct gauge group for disclinations persists in the modern literature (see, for example, Lazar 2003a,b), and indeed it has been a misconception with the present authors also. Recently, in a private communication (2004), D. G. B. Edelen clarified this matter to the first author. He conclusively shows that the existing disclination solutions based on the $\tau(3)$ theory (Valsakumar & Sahoo 1988; Lazar 2003a,b) are incorrect, and in fact, disclinations arising in such theories can be 'gauged' away! Not withstanding this confusion and controversy regarding disclinations, we note that Lazar (2003c), in a recent work, has provided the first (correct) gauge solution for an edge dislocation.

The aforementioned works are all predicated on the classical elastic Lagrangian. As is well known, the classical elastic media is non-dispersive in contrast to real crystals, which are essentially non-local (to a lesser or greater degree). By now extensive literature has appeared on non-local elasticity, a review of which is beyond the scope of this paper. Recently, Eringen (2002) reviewed most of the literature in this area to which the reader is referred. Briefly, in non-local elasticity, the algebraic constitutive equations are replaced

by integral equations whereby the stress or strain at a point depends not only on the strain or stress at that point but also on all neighbouring points in the material. Under certain conditions, an approximation to the true non-local material behaviour can be made by the so-called strain gradient elasticity where strain gradients with suitable coupling constants are added to the classical elastic Lagrangian. The reader is referred to the extensive reviews by Gutkin (2000) and Aifantis (2003) in this area. Non-local strain gradient elastic solutions to dislocations problems (and other defects) have been addressed exhaustively by Aifantis and co-workers, for example, in Gutkin & Aifantis (1996).

The interest of the present authors in combining gauge theory, and the strain gradient elasticity, arose because of the following observation. The gauge solution of a screw dislocation (based on the classical local Lagrangian) is functionally identical to that obtained via both the integral formulation of nonlocal elasticity as well as the strain gradient elasticity. This is a fact noted and remarked with considerable interest by several researchers (e.g. Edelen 1996). Obviously, in a natural manner the gauge theory induces some non-local effects owing to the presence of defects. In hindsight, this even appears intuitive. However, the correct gauge solution of the screw dislocation was constructed based on classical *local* elasticity. That itself is an approximation. A true crystal is dispersive or *non-local* even without defects. That is, a characteristic lengthscale exists in an elastic solid even without defects, while on the other hand. correct accounting for gauge interactions leads to an introduction of another length-scale (owing to the defects). Thus, one may ask what the interactions between gauge fields and non-local elastic fields are. More pertinently, one can ask how the two length-scales combine.

Further interest in this problem was generated by the recent work of Valsakumar & Sahoo (1996), who attempted to evaluate the interactions between two screw dislocations. They compared gauge results of screw dislocation interactions with classical elasticity and a particular non-local theory (Vörös & Kovács 1993). The classical elastic stress solution is (as is well known) singular when dislocations approach infinitesimally close to each other. Both the Vörös & Kovács (1993) solution and that of Valsakumar & Sahoo (1996) removed such singularities, although their respective solutions differed in other aspects. Valsakumar & Sahoo's (1996) speculation in closure of their work, on how the non-local-gauge fields might interact in the 'two-screw dislocation interaction problem', forms the second motivation for the present work.

3. $\mathcal{T}(3)$ gauge formalism for non-local elasticity and field equations

Cartesian tensors are employed throughout unless otherwise noted. Isotropic material behaviour is assumed. Let \mathcal{L} be an admissible Lagrangian in the static limit. For now, u can be considered to be any field, although we will later identify it with the displacement vector of a material point. The Lagrangian is assumed to be invariant under a continuous global gauge group of transformations (G):

$$\mathcal{L} = \mathcal{L}(\boldsymbol{u}, \nabla \otimes \boldsymbol{u}, \nabla \otimes \nabla \otimes \boldsymbol{u}, \ldots), \tag{3.1a}$$

$$u' \to Gu,$$
 (3.1b)

$$\mathcal{L}' \to \mathcal{L}. \tag{3.1c}$$

Making the gauge group local (i.e. dependent on space-time) spoils this invariance:

$$\boldsymbol{u}' \to G(\boldsymbol{x}) \boldsymbol{u} \Rightarrow \mathcal{L}' \to \mathcal{L}.$$
 (3.2)

Equation (3.3) shows as an illustration that if the translations (\mathbf{t}) , which are a sub-group of the Euclidean group, are inhomogeneous, then the invariance of the elastic Lagrangian is generally lost. In this paper, we shall exclusively deal with the Abelian gauge group of translations,

$$u' \to u + t(x) \Longrightarrow \mathcal{L}' \to \mathcal{L}.$$
 (3.3)

The Lagrangian can be made invariant again by introducing compensating fields (gauge fields, $\boldsymbol{\varphi}$) and defining the so-called gauge covariant derivative (super-script G),

$$\stackrel{G}{\nabla} \otimes \boldsymbol{u} \to \nabla \otimes \boldsymbol{u} + \boldsymbol{\varrho}, \qquad (3.4a)$$

$$\underline{\varphi}' \to \underline{\varphi} - \nabla \otimes t(x).$$
 (3.4b)

In this fashion a new Lagrangian is formed that also includes the compensating gauge fields together with a coupling constant, s:

$$\mathcal{L} = \mathcal{L}(\boldsymbol{u}', \overset{G}{\nabla} \otimes \boldsymbol{u}', \overset{G}{\nabla} \otimes \overset{G}{\nabla} \otimes \boldsymbol{u}', \ldots) + s\mathcal{L}_{\mathcal{G}}(\boldsymbol{\phi}, \nabla \otimes \boldsymbol{\phi}, \nabla \otimes \nabla \otimes \boldsymbol{\phi}, \ldots)$$

$$\{\mathcal{L}_{\mathcal{G}} | G(\boldsymbol{x})\mathcal{L}_{\mathcal{G}} \to \mathcal{L}_{\mathcal{G}} \}.$$

$$(3.5)$$

Consider now an admissible isotropic non-local elastic Lagrangian that includes strain gradient terms and thus a natural length-scale parameter, $l_{\rm N}$:

$$\mathcal{L} = -\frac{1}{2} \Big\{ \lambda (\operatorname{Tr} \boldsymbol{\varepsilon})^2 + 2\mu(\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon}) + l_{\mathrm{N}}^2 [\lambda(\nabla \otimes \operatorname{Tr} \boldsymbol{\varepsilon}) \cdot (\nabla \otimes \operatorname{Tr} \boldsymbol{\varepsilon}) + 2\mu(\nabla \otimes \boldsymbol{\varepsilon}) : (\nabla \otimes \boldsymbol{\varepsilon})] \Big\},$$
(3.6*a*)

$$\boldsymbol{\varepsilon} = \frac{1}{2} [\boldsymbol{\nabla} \otimes \boldsymbol{u} + (\boldsymbol{\nabla} \otimes \boldsymbol{u})^{\mathrm{T}}], \qquad (3.6b)$$

where λ and μ are the usual Lame constants, while $\boldsymbol{\varepsilon}$ is the infinitesimal strain tensor. Here we have chosen a particular non-local Lagrangian proposed by Atlan & Aifantis (1992; see also Aifantis 2003). Not much importance should be attached to this particular choice of non-local Lagrangian (among other variations). Non-local elastic theories that are based on gradients of strains are typically characterized by the presence of a modified Helmholtz operator, and as such, adoption of any of them should mathematically lead to similar results with

greater or less difficulty. The Lagrangian embodied in equation (3.6a) has some simple appealing features. As discussed by Aifantis (2003), the Lagrangian in equation (3.6a) implies (under typical boundary conditions of the kind considered in this work) that the gradient stress definition is the same as classical stress. This results in considerable simplification of both our equations, as well as purely strain gradient problems. In particular, results for dislocations in this particular theory are readily available for comparison (Gutkin 2000; Aifantis 2003).

Obviously, the Lagrangian in equation (3.6a) is invariant under both threedimensional homogeneous rotations and translations, as it should be. The Lagrangian in equation (3.6a) implies the following constitutive law:

$$\boldsymbol{\sigma} = \lambda(\operatorname{Tr}\boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon} - l_{\mathrm{N}}^{2}\nabla^{2}[\lambda(\operatorname{Tr}\boldsymbol{\varepsilon}) + 2\mu\boldsymbol{\varepsilon}].$$
(3.7)

Here, $\boldsymbol{\sigma}$ is the stress tensor. As mentioned earlier, breaking the translational internal symmetry leads to the formation of dislocations. Implementing equations (3.4a,b) and (3.6a,b) we obtain

$$\boldsymbol{\underline{E}} = \frac{1}{2} \Big[\boldsymbol{\nabla} \otimes \boldsymbol{u} + (\boldsymbol{\nabla} \otimes \boldsymbol{u})^{\mathrm{T}} + \boldsymbol{\varrho} + \boldsymbol{\varrho}^{\mathrm{T}} \Big], \qquad (3.8a)$$
$$\mathcal{L}_{\text{total}} = -\frac{1}{2} \Big\{ \lambda (\operatorname{Tr} \, \boldsymbol{\underline{E}})^2 + 2\mu (\boldsymbol{\underline{E}} \, : \, \boldsymbol{\underline{E}}) + l_{\mathrm{N}}^2 [\lambda (\boldsymbol{\nabla} \otimes \operatorname{Tr} \, \boldsymbol{\underline{E}}) \cdot (\boldsymbol{\nabla} \otimes \operatorname{Tr} \, \boldsymbol{\underline{E}}) + 2\mu (\boldsymbol{\nabla} \otimes \boldsymbol{\underline{E}}) \, : \, (\boldsymbol{\nabla} \otimes \boldsymbol{\underline{E}}) \Big] \Big\} + s \mathcal{L}_{\boldsymbol{\mathcal{G}}}, \qquad (3.8b)$$

where the gauge Lagrangian, $\mathcal{L}_{\mathcal{G}}$, is formed by a suitable contraction of the gauge fields:

$$\mathcal{L}_{\mathcal{G}} = -\frac{1}{2} \Big[\{ (\nabla \otimes \tilde{\boldsymbol{\varphi}})_{aji} - (\nabla \otimes \tilde{\boldsymbol{\varphi}})_{aij} \} : \{ (\nabla \otimes \tilde{\boldsymbol{\varphi}})_{aji} - (\nabla \otimes \tilde{\boldsymbol{\varphi}})_{aij} \} \Big].$$
(3.9)

The original Lagrangian is now modified in two ways. Firstly, the redefinition of $\boldsymbol{\varepsilon} \to \boldsymbol{E}$ leads to the presence of gauge fields in the classical scalar. Secondly, the new gauge fields introduce their own addition to the total Lagrangian, \mathcal{L}_{G} . Note that one of the conditions for forming the gauge Lagrangian is that it must also be invariant under the inhomogeneous gauge transformation. This condition, for example, excludes the possibility of the gauge fields themselves appearing in equation (3.9), and thus, only its gradients are employed to construct the gauge scalar (Moriyasu 1983). A key point to note here is that when we implement the minimal replacement construct and introduce the translational gauge field, the only effect on the non-local Lagrangian is through $\boldsymbol{\varepsilon} \to \boldsymbol{E}$. For example, we do not construct a replacement of the derivative of the strain by a gauge covariant type of derivative, similar to that which has been done to the displacement gradient. The rationale for this is that it is the displacement field that is being gauged (leading to, of course, defects) and not strain (which does not immediately present any known defect configuration, even if it is gauged).²

² Nevertheless, this point deserves further investigation. The first author thanks Professor Dimitris Lagoudas for pointing out this interesting possibility.

The modified EKL field equations for gauge theory predicated on a non-local Lagrangian can be generated via an appeal to the Euler–Lagrange equations,

$$\frac{\partial \mathcal{L}_{\mathcal{F}}}{\partial \psi} - \nabla_k \frac{\partial \mathcal{L}_{\mathcal{F}}}{\partial (\nabla_k \otimes \psi)} + \nabla_k \otimes \nabla_l : \frac{\partial \mathcal{L}_{\mathcal{F}}}{\partial (\nabla_k \otimes \nabla_l \otimes \psi)} - \cdots,$$

$$\psi = \boldsymbol{u} \text{ or } \boldsymbol{\varphi}.$$
(3.10)

In the present case, these are a set of 12 field equations in terms of displacement and gauge fields.

4. Gauge solution of a screw dislocation in a non-local media

The challenge of obtaining a general solution to the coupled gauge-non-local elasticity field equations as represented by equations (3.10), while possible, is tedious at best. The symmetries of the screw dislocation problem, however, make a closed-form solution tractable. The displacement and gauge fields must satisfy the following symmetry requirements:

$$\boldsymbol{u} = u(r)\boldsymbol{e}_3,\tag{4.1a}$$

$$\boldsymbol{\varphi} = \varphi_1 \boldsymbol{e}_3 \otimes \boldsymbol{e}_1 + \varphi_2 \boldsymbol{e}_3 \otimes \boldsymbol{e}_2. \tag{4.1b}$$

As per Kröner (1981), the dislocation density tensor, which we will have occasion to use, is simply

$$\boldsymbol{\alpha} = \operatorname{curl} \boldsymbol{\varphi} = (\varphi_2 - \varphi_1) \boldsymbol{e}_3 \otimes \boldsymbol{e}_3. \tag{4.2}$$

Note that the use of the Pseudo-Lorentz gauge is implicit. From the 12 general field equations in the previous section (equation (3.10)), we need retain only three for our particular problem,

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} = -\left(\frac{\partial \varphi_1}{\partial x_1} + \frac{\partial \varphi_2}{\partial x_2}\right) + l_{\rm N}^2 \left\{\frac{\partial^4 u}{\partial x_1^4} + \frac{\partial^4 u}{\partial x_2^4} + 2\frac{\partial^4 u}{\partial x_1^2 \partial x_2^2} + \frac{\partial^3 \varphi_1}{\partial x_1^3} + \frac{\partial^3 \varphi_2}{\partial x_2^3} + \frac{\partial^3 \varphi_1}{\partial x_1 \partial x_2^2} + \frac{\partial^3 \varphi_2}{\partial x_2 \partial x_1^2}\right\},$$

$$(4.3a)$$

$$\kappa^2 \frac{\partial u}{\partial x_1} = -\kappa^2 \varphi_1 + \kappa^2 l_{\rm N}^2 \left\{ \frac{\partial^3 u}{\partial x_1^3} + \frac{\partial^3 u}{\partial x_2^2 \partial x_1} + \frac{\partial^2 \varphi_1}{\partial x_1^2} + \frac{\partial^2 \varphi_1}{\partial x_2^2} \right\} + \frac{\partial^2 \varphi_2}{\partial x_1 \partial x_2} - \frac{\partial^2 \varphi_1}{\partial x_2^2}, \quad (4.3b)$$

$$\kappa^2 \frac{\partial u}{\partial x_2} = -\kappa^2 \varphi_2 + \kappa^2 l_{\rm N}^2 \left\{ \frac{\partial^3 u}{\partial x_2^3} + \frac{\partial^3 u}{\partial x_2 \partial x_1^2} + \frac{\partial^2 \varphi_2}{\partial x_1^2} + \frac{\partial^2 \varphi_2}{\partial x_2^2} \right\} + \frac{\partial^2 \varphi_1}{\partial x_1 \partial x_2} - \frac{\partial^2 \varphi_2}{\partial x_1^2}, \quad (4.3c)$$

where κ^2 is $2\mu/s$ and has units of inverse length square. The underbracketed terms are the additional terms induced by non-local interactions absent from previous works based on the classical elastic Lagrangian. It is worth noting that, as is customary in theories of such complexity, linearized equations have been considered. Full nonlinear equations can of course be setup, however, for the moment that would be but a digression. For a detailed discussion of scaling and approximation issues to the nonlinear EKL field equations, see Edelen & Lagoudas (1988).

Differentiating equation (4.3b) with respect to x_2 and equation (4.3c) with respect to x_1 (and subtracting) we obtain the following:

$$(1 - \kappa^2 l_{\rm N}^2) \left(\frac{\partial^2 \alpha}{\partial x_1^2} + \frac{\partial^2 \alpha}{\partial x_2^2} \right) - \kappa^2 \alpha = 0.$$
(4.4)

The cylindrically symmetric solution to this equation is well known. We must distinguish between two scenarios depending upon the relative magnitude of $\kappa^2 l_N^2$ as compared with unity. Accordingly,

Case I
$$(\kappa^2 l_N^2 < 1)$$
 : $\alpha = C_1 K_0 \left(\frac{\kappa r}{\sqrt{1 - \kappa^2 l_N^2}} \right) = C_1 K_0 \left(\frac{r}{l_G \sqrt{1 - (l_N/l_G)^2}} \right),$ (4.5*a*)

Case II
$$(\kappa^2 l_N^2 > 1)$$
 : $\alpha = C_1 K_0 \left(\frac{\kappa r}{\sqrt{\kappa^2 l_N^2 - 1}}\right) = C_1 K_0 \left(\frac{r}{l_G \sqrt{(l_N/l_G)^2 - 1}}\right).$ (4.5b)

Here, we have identified the gauge length-scale parameter, $l_{\rm G} = 1/\kappa$. K_0 is the modified Bessel function of order zero, while r represents the radial distance in cylindrical polar coordinates (i.e. $r = \sqrt{(x_1^2 + x_2^2)}$). Based on our results, we can now easily define an effective length to be:

Case I
$$(\kappa^2 l_n^2 < 1)$$
 : $l_{eff} = l_G \sqrt{1 - (l_N/l_G)^2}$, (4.6*a*)

Case II
$$(\kappa^2 l_n^2 > 1)$$
 : $l_{eff} = l_G \sqrt{(l_N/l_G)^2 - 1}$. (4.6b)

The constant, C_1 , is evaluated based on the asymptotic far-field value of Burger's vector that must coincide with the classical solution, that is, we must set

$$\lim_{r \to \infty} b^{\text{gauge}}(r) = \lim_{r \to \infty} \int \alpha(r) dr = b$$
(4.7*a*)

$$\Rightarrow C_1 = \frac{b}{2\pi l_{\text{eff}}^2}.$$
(4.7b)

To solve the remaining equations, we take a cue from Valsakumar & Sahoo (1988) and make the following definitions:

$$\hat{\varphi}_1 = \frac{\partial u}{\partial x_1} + \varphi_1; \quad \hat{\varphi}_2 = \frac{\partial u}{\partial x_2} + \varphi_2,$$

$$(4.8a)$$

$$\left\{ \hat{\varphi}_1 = \frac{\partial g}{\partial x_1} - \frac{\partial h}{\partial x_2}; \quad \hat{\varphi}_2 = \frac{\partial g}{\partial x_2} + \frac{\partial h}{\partial x_1} \middle| \operatorname{div}(\nabla \otimes g) = 0, \quad \operatorname{curl}(\nabla \otimes h) = 0 \right\}.$$
(4.8b)

Here, the newly defined $\hat{\varphi}$ variables have been written in terms of divergence free and curl free vectors (g and h) to decouple the remaining field equations.

The two uncoupled equations in terms of the variables g and h are

$$\frac{\partial^2 h}{\partial x_1^2} + \frac{\partial^2 h}{\partial x_2^2} = C_1 K_0 \left(\frac{r}{l_{\text{eff}}}\right), \tag{4.9a}$$

$$\frac{\partial^2 g}{\partial x_1^2} + \frac{\partial^2 g}{\partial x_2^2} = l_{\rm N}^2 \left(\frac{\partial^4 g}{\partial x_1^4} + \frac{\partial^4 g}{\partial x_2^4} + 2 \frac{\partial^4 g}{\partial x_1^2 \partial x_2^2} \right). \tag{4.9b}$$

The first equation, equation (4.9a), is easy to solve and is precisely the same equation that occurs in previous works (Valsakumar & Sahoo 1988), save for the important difference that $l_{\rm G}$ is replaced with $l_{\rm eff}$:

$$\frac{\partial h}{\partial x_i} = \frac{x_i}{r^2} \left(C_2 - C_1 r l_{\text{eff}} K_1 \left(\frac{r}{l_{\text{eff}}} \right) \right), \tag{4.10}$$

where a new constant C_2 is introduced. The second equation, equation (4.9b), is simplified by making the substitution

$$z = \frac{\partial^2 g}{\partial x_1^2} + \frac{\partial^2 g}{\partial x_2^2} = l_{\rm N}^2 \left(\frac{\partial^4 g}{\partial x_1^4} + \frac{\partial^4 g}{\partial x_2^4} + 2 \frac{\partial^4 g}{\partial x_1^2 \partial x_2^2} \right) \tag{4.11a}$$

$$\Rightarrow \frac{\partial^2 z}{\partial x_1^2} + \frac{\partial^2 z}{\partial x_2^2} = \frac{z}{l_N^2}.$$
(4.11b)

One then easily obtains

$$\frac{\partial^2 g}{\partial x_1^2} + \frac{\partial^2 g}{\partial x_2^2} = C_3 K_0 \left(\frac{r}{l_N}\right). \tag{4.12}$$

Analogous to the solution of h we have

$$\frac{\partial g}{\partial x_i} = \frac{x_i}{r^2} \left(C_4 - C_3 r l_N K_1 \left(\frac{r}{l_N}\right) \right). \tag{4.13}$$

To compute the stresses we need only derivatives of g and h. For example,

$$\sigma_{31} = \mu \hat{\varphi}_1 = -\frac{\mu x_2}{r^2} \left(C_2 - C_1 r l_{\text{eff}} K_1 \left(\frac{r}{l_{\text{eff}}} \right) \right) + \frac{\mu x_1}{r^2} \left(C_4 - C_3 r l_N K_1 \left(\frac{r}{l_N} \right) \right).$$
(4.14)

At this point the various unknown constants C_2 to C_4 need to be determined. Their evaluation turns out to be rather trivial, however. Consider equation (4.14). The far-field of the σ_{31} component of the stress field in the classical theory (which has been confirmed innumerably via experiments) is well known to be independent of the x_1 coordinate. Thus, we must set C_3 and C_4 to zero. Further, requiring the solution to behave regularly (vanish) at origin determines C_2 . In cylindrical coordinates we can then finally write

$$\sigma_{rz} = \frac{\mu b}{2\pi r} \left(1 - \frac{r}{l_{\text{eff}}} K_1 \left(\frac{r}{l_{\text{eff}}} \right) \right). \tag{4.15}$$

The solution in equation (4.15) is *functionally* identical to that obtained by Valsakumar & Sahoo (1988) and Edelen (1996) for a screw dislocation via gauge theory predicated on the classical elasticity Lagrangian. The important distinction, of course, is that in their solution, instead of l_{eff} the term l_{G} appears.

Thus, the gauge solution to screw dislocation problem based on non-local elasticity can be obtained by the mere substitution: $l_{\rm G} \rightarrow l_{\rm eff}$, where $l_{\rm eff}$ is defined by equation (4.6*a*,*b*). This answers the two questions raised in the motivating sections. We now know that, insofar as the screw dislocation is concerned, non-local elastic-gauge interactions result in no *functional* change, however, the characteristic length-scale does alter. Further, it is clear that the non-local and gauge length-scales combine in a nonlinear fashion. Related results and implications are discussed in the next section.

5. Further results, implications and discussion

The variation of the effective length-scale as a function of the two non-local and gauge length-scales is graphically represented in figure 1.

As is obvious from both equation (4.6a, b) and figure 1, in the limit when $l_{\rm G} \rightarrow 0$, the effective length reverts to $l_{\rm eff} \rightarrow l_{\rm N}$, and conversely, when $l_{\rm N} \rightarrow 0$, one obtains $l_{\rm eff} \rightarrow l_{\rm G}$. As depicted in figure 1, in the intermediate range of length-scales, the interactions are more complex. Interestingly, when these two length-scales coincide, we obtain a zero effective length signifying that classical elasticity is a special case where gauge effects and non-local effects are exactly equal. While this is intuitively and mathematically true for the case when both $l_{\rm G} \rightarrow 0$ $l_{\rm N} \rightarrow 0$, the implications of why this 'cancellation' of effects should persist even at finite non-local and gauge length-scales (provided they are equal) is somewhat puzzling. Nevertheless, we provide below a brief discussion of our interpretation of these results.

While both gauge field theory and non-local elasticity end up removing divergence of field quantities representing the defects (stresses, energies) in a mathematically similar manner, they seem to do so in completely different directions and through different means. In non-local elasticity formalism, the (phenomenological) gradient terms act as penalty functions to smoothen the singularity; in gauge theory, the smoothening occurs through compensating fields that force local translational invariance of the total Lagrangian (which, incidentally, arise naturally rather than being postulated phenomenologically). The non-local effect and the gauge effect seem to act in opposite directions as shown by the character of the effective length (equation (4.6a, b), figure 1). This unexpected smoothening effect in two completely different directions gives rise to the non-trivial solution where the fields owing to gauge and non-local effects cancel each other, as is given by the current formulation at $l_{\rm N} = l_{\rm G}$. Here, one must keep in mind that although, coincidentally, each theory alone gives similar mathematical results, the physical cause or nature of the length-scale appearing



Figure 1. Effective length as a function of the ratio of the non-local length-scale and gauge length-scale. The effective length is normalized with the gauge length-scale.

in each theory is different. Their physical origins are completely different. As a consequence, the length-scale that appears in each formulation is also different (i.e. $l_N \neq l_G$). In reality, there is no physical situation where $l_N=0$. All solids are non-local to a greater or lesser extent. The length-scale, l_N , is finite even in the complete absence of defects, while l_G strictly arises owing to the presence of the defects. Since the effective length is a combination of the two length sales, numerically, our results will always lie between the gauge solution and the gradient solution. Given that (in reality) the case, $l_N=0$ does not exist, what is the definition of classical elasticity in the context of defects? According to our work, a natural definition of classical elasticity for defects is consequently when $l_N=l_G$, that is, when non-local effects persist only up to the core radius of the dislocation. This appears to be both reasonable and intuitive. Despite this simple interpretation, there appear to be philosophical implications of this work (which must await further work) that are yet to be fully clarified.

In any case, a major consequence of our results is that by merely replacing the gauge length with the effective length, most known gauge solutions (based on classical elasticity) involving screw dislocations can be converted to gauge solutions based on non-local elasticity. Thus, we can now address Valsakumar & Sahoo's (1996) speculation on how the force between two screw dislocations might change if non-local elasticity is combined with the gauge theory. Based on their work, we can now directly write the force between two parallel screw dislocations (extending along the x_3 direction) in the gauge-non-local theory as

$$\boldsymbol{F}(R) = \frac{\mu b_1 b_2}{2\pi R} \left(1 - \frac{R}{l_{\text{eff}}} K_1\left(\frac{R}{l_{\text{eff}}}\right) \right) \hat{\boldsymbol{e}}_r.$$
(5.1)

Here, R is the separation distance between the dislocations. While the results can be plotted parametrically, some simple estimates of the various length-scales can



Figure 2. Variation of the normalized force between two parallel screw dislocations with respect to normalized separation. (a) Classical elasticity results (b) Present work. Gauge solution predicated on the non-local Lagrangian (c) Results of Valsakumar & Sahoo (1996). Gauge solution predicated on the classical elasticity Lagrangian. The force is normalized with a factor of $2\pi l_G/\mu b_1 b_2$, while the separation is normalized by $1/l_G$. Consistent with the typical values quoted in the text, a ratio of $l_N/l_G = 1/\sqrt{2}$ is chosen.

be used to provide a more concrete picture. The gauge length-scale can be identified with the dislocation core radius. A typical dislocation core radius can be taken to be approximately equal to b (Hirth & Lothe 1982), while b itself is $a/\sqrt{2}$ (for an ideal face-centred cubic (FCC) material), where a is the lattice parameter. Thus, we set $l_{\rm G} \sim a/\sqrt{2}$. The non-local length-scale is a measure of the materials dispersivity and is highly dependent upon the material under consideration. Experimentally, it can be determined by measuring the phonon spectra. For example, in the case of lanthanum, this value is as small as 0.1 nm, but is as large as 3.4 nm for graphite (Reid & Gooding 1992). Of course, experimental values will invariably reflect effects of existing dislocation and other defects. A theoretical estimate (via the simple Born–Karman model) is that $l_{\rm N} \sim a/2$ (Eringen 2002). The results for the force between two parallel screw dislocations are plotted in figure 2. For comparison, the classical elastic and the gauge theory solution based on classical elasticity are also shown. For the given length-scale ratio adopted, a peak force difference of as much as 100% is predicted. The location of the peak force is also weakly shifted.

Clearly, the peak force between dislocations is highly sensitive to the gauge length-non-local length ratio. In the limit when the length-scale ratio approaches one (i.e. the classical elasticity case), the peak force location is shifted towards the origin while exhibiting a singularity. This high sensitivity in the peak force could be possibly used to experimentally verify the presence of gauge-non-local interactions. Unfortunately, however, experimental distinction between the length-scale effects is fraught with challenges. It would be crucial to first obtain the non-local length-scale without interference from other effects such as defects and surface energies (see, for example, Sharma *et al.* 2003; Sharma & Ganti 2004 for a discussion on surface effects). The gauge length-scale must also be then separated out and determined precisely. Perhaps, a combination of experimental and numerical work may be more appropriate.

6. Closing remarks

In the present work, the relaxed elastic state of a screw dislocation in a non-local medium was investigated from the viewpoint of gauge field theory of defects in solids. We find that, while the elastic state description is functionally the same across the gauge theory based on classical elasticity and the present non-local elasticity based gauge solution, a new effective length measure needs to be introduced. In particular, the material parameters of non-local elasticity and the gauge theory combine in a nonlinear fashion to yield an effective length-scale. One of the implications of this result, is that several known (or easily obtained) gauge theory solutions, for screw dislocation problems based on classical elastic medium, can now be converted over to a non-local medium with a mere change in the characteristic length-scale. As an example, the force between two screw dislocations located in a non-local medium was evaluated. Using typical lengthscale parameters, the authors find a significant difference in the peak force estimation, depending upon whether the gauge theory is predicated on a classical medium or a non-local one. This observation could be used for experimental verification of the predicted interactions.

There are several limitations of the present work which need to be highlighted. Firstly, a linearized version of the Edelen-Kadić-Lagoudas theory was employed. It would be instructive to see, whether, a nonlinear theory engenders any significant qualitative shift. Second, couple stresses were ignored. While granted that the dual of the dislocation density is a moment stress, such a term should be inserted *a priori* in the elastic Lagrangian also. The present strain gradient Lagrangian suffers from the advantage (or disadvantage, depending upon one's perspective) that the resulting stress definition is the same as that of classical elasticity, and higher order stresses (such as moments stresses) do not appear (Ru & Aifantis 1993). For that purpose, perhaps, a mixture of Eringen's micropolar constitutive law (Eringen 2002) together with the present gradient Lagrangian can be used. The latter can be of importance in certain lattices which allow for easy rotational accommodation (e.g. KNO₃). Finally, while we suspect that our results are general, and might hold true for defects other than just the screw dislocation, we can by no means pretend to make such a strong statement. Further investigation is clearly required to verify the universal character (or the lack thereof) of the present results.

Helpful comments and suggestions from Professor Dimitris Lagoudas (Texas A&M University) and Rajdeep Sharma (Massachusetts Institute of Technology) are gratefully acknowledged. In particular, Professor Lagoudas alerted the first author to the possibility of higher order minimal replacement for the derivative of strain, which we expect to pursue in future works.

References

- Aifantis, E. C. 2003 Update on a class of gradient theories. Mech. Mater. 35, 259-280.
- Altan, B. & Aifantis, E. C. 1992 On the structure of the mode III crack-tip in gradient elasticity. Scripta Met. Mater. 26, 319–324.
- Edelen, D. G. B. 1982 Effective stress in the gauge theory of dislocations. Int. J. Eng. Sci. 20, 1049.
- Edelen, D. G. B. & Lagoudas, D. C. 1988 *Gauge theory and defects in solids*. Amsterdam: North-Holland.
- Edelen, D. G. B. 1989a Material and spatial gauge theories of solids—II. Problems with given material dislocation densities. Int. J. Eng. Sci. 27, 641–652.
- Edelen, D. G. B. 1989b Material and spatial gauge theories of solids—III. Dynamics of disclination free states. Int. J. Eng. Sci. 27, 653–666.
- Edelen, D. G. B. 1996 A correct, globally defined solution of a screw dislocation problem in the gauge theory of defects. Int. J. Eng. Sci. 34, 81–86.
- Edelen, D. G. B. & Lagoudas, D. C. 1999 Matching the inner and outer solutions in the continuum theory of dislocations. Int. J. Eng. Sci. 37, 59–73.
- Eringen, A. C. 2002 Nonlocal continuum field theories. New York: Springer.
- Eshelby, J. D. 1956 Solid state physics (ed. F. Seitz & D. Turnbull), vol. 3, pp. 79–141. New York: Academic Press.
- Gairola, B. K. D. 1981 Gauge invariant formulation of continuum theory of defects. In Proc. 4th Int. Symp. Continuum Models and Discrete Systems (ed. O. Brulin & R. K. T. Hsieh), p. 55. Amsterdam: North-Holland.
- Golebiewska-Lasota, A. A. 1979 Dislocations and gauge invariance. Int. J. Eng. Sci. 17, 329.
- Golebiewska-Lasota, A. A. & Edelen, D. G. B. 1979 On the gauge transformations admitted by the equations of defect dynamics. Int. J. Eng. Sci. 17, 335–339.
- Gutkin, M. Y. 2000 Nanoscopics of dislocation and disclinations in gradient elasticity. Rev. Adv. Mater. Sci. 1, 27–60.
- Gutkin, M. Y. & Aifantis, E. C. 1996 Screw dislocation in gradient elasticity. Scripta Mater. 35, 1353.
- Hirth, J. P. & Lothe, J. 1982 Theory of dislocations. New York: John Wiley.
- Kadić, A. & Edelen, D. G. B. 1983 A gauge theory of dislocations and disclinations. Berlin: Springer.
- Kröner, E. 1981 Continuum theory of defects. In Physics of defects (Les Houches, Session 35) (ed. R. Balian et al.), p. 215. Amsterdam: North-Holland.
- Lagoudas, D. C. & Edelen, D. G. B. 1989 Material and spatial gauge theories of solids—I. Gauge constructs, geometry and kinematics. Int. J. Eng. Sci. 27, 411–431.
- Lazar, M. 2003a Twist disclination in the field theory of elastoplasticity. J. Phys.: Condens. Matter 15, 6781–6800.
- Lazar, M. 2003b Wedge disclination in the field theory of elastoplasticity. Phys. Lett. A 311, 416–425.
- Lazar, M. 2003c A nonsingular solution of the edge dislocation in the gauge theory of dislocations. J. Phys. A: Math. Gen. 36, 1415–1437.
- Moriyasu, K. 1983 An elementary primer for gauge theory. Singapore: World Scientific.
- O'Raifeartaigh, L. 1997 The dawning of gauge theory. Princeton: Princeton University Press.
- Reid, A. C. E. & Gooding, R. J. 1992 Inclusion problem in a two-dimensional nonlocal elastic solid. *Phy. Rev. B.* 46, 6045.
- Ru, C. Q. & Aifantis, E. C. 1993 A simple approach to solve boundary-value problems in gradient elasticity. Acta Mech. 101, 59–68.
- Sharma, P. & Ganti, S. 2004 Size-dependent Eshelby's tensor for embedded nano-inclusions incorporating surface/interface energies. J. Appl. Mech. 71, 663.
- Sharma, P., Ganti, S. & Bhate, N. 2003 Effect of surfaces on the size-dependent elastic state of nano-inhomogeneities. Appl. Phys. Lett. 82, 535–537.

- Valsakumar, M. C. & Sahoo, D. 1988 Gauge theory of defects in the elastic continuum. Bull. Mater. Sci. 10, 3.
- Valsakumar, M. C. & Sahoo, D. 1996 Force between two parallel screw dislocations—gauge theory result. *Phys. Lett.* **215A**, 305–308.
- Vörös, G. & Kovács, I. 1993 Static lattice defects in a quasi-continuum. Phys. Status Solidi B. 178, 99.