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Gauge theory of defects in elastic continua- II

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An overview of gauge theory of defects in an elastic continuum is given in this presentation. It is shown that the gauge theory based on the inhomogeneous action of the translation group $T(3)$ provides a physically meaningful description of the structure of topologically stable defects like dislocations and disclinations, as well as non-topological defects like the point defects.

To our dear Anantha

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1. Introduction

There is as yet no microscopic theory of plasticity that incorporates production, annihilation, and interaction of all the structural defects in a comprehensive and natural manner. Continuum elasticity theory is often used [1, 2] to model material response at large distances from the defects. Inability of continuum theory to correctly describe phenomena at short distances from the defects is well known. For example, in continuum elasticity theory, the stress and strain fields are singular along the dislocation lines, and hence the interaction between them is poorly represented at short distances between them. Given the current interest in miniaturisation of devices, we note that the length scales associated with nanodevices are too small for continuum models to be applicable. Continuum theory of dislocations, and the other defects, cannot be readily used to model mechanical properties of miniaturized devices.

The preeminent role of topological defects, like the dislocations, in plasticity of materials in three dimensions is well known. The change in the topology that arises as a consequence of the presence of topological defects can also affect the other physical properties of materials. For instance, enhanced scattering, and existence of infinite number of bound states for electrons was demonstrated in presence of dislocations [3 – 5]; electrons in dislocated crystals can undergo localization [6]; electrons can show modified Aharonov-Bohm type interference effects while getting scattered from dislocations [7]. Clearly, the details and significance of these effects would depend on the details of the structure of the defects, especially when the size of the material is small.

Topologically nontrivial objects arise in various physical contexts that includes gravity, particle physics and condensed matter physics and they have all been studied using appropriate *gauge theories* [8 – 10]. The aim of the present talk is to an overview of the gauge theoretic description of defects in an elastic continuum. After a brief introduction to gauge theory in section 2, we shall describe the gauge theoretic formulation of defects in an elastic continuum by Edelen and coworkers [11, 12] in section 3. They incorporated nonintegrable deformations by demanding invariance of the elastic Lagrangian under the local action of the Euclidean group SO(3)$\triangleright$T(3). Kadic and Edelen argued [11] that dislocations arise from the inhomogeneous action of the group of translations, T(3), while the disclinations owe their origin to action of the rotation group, SO(3). In spite of the mathematical beauty of the theory, their solution (of the linearized gauge field equations) for the stress field due to a screw dislocation was singular along the dislocation line, and worse, it did not agree with the solution of classical elasticity theory at large distances, which it should have.

We shall then discuss our [13] axially symmetric solutions of the gauge field equations that are analogous to screw dislocations and wedge disclinations. We showed that the gauge field equations indeed allowed for a solution that is devoid of both of these deficiencies. Later, Edelen [14] also obtained the same solution. We also argued [13] that the disclination cannot arise from the action of SO(3), which seems to be the currently accepted point of view [15]. Subsequently, we calculated [16] the interaction between two parallel screw dislocations and showed that the stress fields of screw dislocations, and interaction between them, can be obtained by multiplying the corresponding expressions in classical elasticity with a universal function [1-$\kappa r K_1(\kappa r)$], where r is the distance of the field point from the dislocation line, κ^{-1} is a characteristic length ($\sim$ core radius). and $K_1(\kappa r)$ is the modified Bessel function of order one. The correct solution of the gauge field equations that correspond to the edge dislocations was not available till recently. Very recently, Lazar [17] was able to obtain an appropriate solution for the edge dislocation by considering a more general form for gauge field Lagrangian [18, 19].

Presuming that the gauge theory of Kadic and Edelen [11] describes only the topologically stable defects, Kroner [20] made an observation that this theory is not closed, and he suggested that a unified gauge theory that incorporates separate gauge fields of dislocations and point defects would be necessary. In section 4, we show that in addition to the topological defects, nontopological defects like the point defects also can be described by the *same* gauge theory- there is no need to introduce extra gauge fields. The problem of dislocation pileup is taken up in section 5. We considered the problem of pileup of parallel screw dislocations along a line and showed [21] that this ensemble is unstable if the density of dislocations exceeds a limiting value. Finally the conclusions are brought out, and a list of open problems are discussed in section 6.

2. Introduction to Gauge Theory

At the fundamental level, Physics is study of symmetry aided by a variational principle. In the field theoretic approach, we are concerned with the space-time evolution of a set of fields $\{\psi_\alpha(x)\}$. The analysis proceeds by setting up a *Lagrangian* $L_0(\{\psi_\alpha(x)\},\{\partial_A\psi_\alpha(x)\})$, on the basis of symmetry considerations. Here x^A denotes the space-time coordinates (x, y, z, t), A =1,...,4 and $\partial_A = \partial/\partial x^A$. The space-time evolution of the fields is obtained by demanding that the *action* $S = \int d^4x L_0(\{\psi_\alpha(x)\},\{\partial_A\psi_\alpha(x)\})$ is an extremum. Using the *summation over repeated indices* convention, the resultant Euler-Lagrange equations can be written as

$$\frac{\delta S}{\delta\psi_\alpha} = \frac{\partial L_0}{\partial\psi_\alpha} - \partial_A\frac{\partial L_0}{\partial(\partial_A\psi_\alpha)} = 0 \tag{2.1}$$

We now explore the consequences of symmetry. Yang-Mill's type of gauge theories are based on transformation properties of the $\{\psi_\alpha(x)\}$ fields with the space-time unaltered, whereas gravity type of gauge theories are based on space-time symmetries. We are concerned with Yang-Mill's type of gauge theories. Let g be an element of a continuous group of transformations G that depends on a set of parameters. Consider a global transformation (the group parameters are independent of the space-time coordinates) $\psi_\alpha \to \psi'_\alpha = g\psi_\alpha$. This is a *symmetry* transformation if and only if the change δL_0 in the Lagrangian is a four-divergence so that the action S is invariant:

$$\delta L_0 = L_0\left(\{\psi'_\alpha\},\{\partial_A\psi'_\alpha\}\right) - L_0\left(\{\psi_\alpha\},\{\partial_A\psi_\alpha\}\right) = \partial_A\chi^A \tag{2.2}$$

The above condition corresponds to existence of a conserved current $J^A = \chi^A - \frac{\partial L_0}{\partial(\partial_A\psi_\alpha)}\delta\psi_\alpha$.

In gauge theories, the above mentioned global gauge invariance is promoted to local gauge invariance. That, is the the group parameters are made functions of space-time coordinates. It is clear that the action will no longer be invariant in view of the fact that $\partial_A g \neq 0$. The idea is best illustrated with the help of a simple example. Consider a set of complex scalar fields ψ and $\psi^\star$ ($\alpha = 1,2$) described by the Lagrangian

$$L_0\left(\{\psi_\alpha\},\{\partial_A\psi_\alpha\}\right) = (\partial_A\psi)(\partial^A\psi)^\star - V\left(\psi^\star\psi\right). \tag{2.3}$$

It is easy to see that the transformation $\psi' = g\psi = exp(iq\theta)\psi$ is a symmetry transformation. The set of transformations comprise the gauge group $U(1)$ and $J^A = iq\theta\left[\psi^\star(\partial^A\psi) - \psi(\partial^A\psi)^\star\right]$ is the conserved current. Now let us consider the *local* action $\psi' = exp(iq\theta(x))\psi$ of $U(1)$. The above is not a symmetry transformation if $\partial_A\theta \neq 0$. The reason for the lack of invariance is the fact that $\partial_A\psi$ does not transform like ψ. Symmetry can be restored by replacing the ordinary derivatives ∂_A by the covariant derivatives D_A defined as $\partial_A \to D_A = \partial_A - iqA_A$ so that $(D_A\psi)' = g(D_A\psi)$. This procedure, known as *minimal coupling*, involves introduction of a new set of fields $\{A_A\}$ which transforms in accordance with the rule $\psi \to \psi' = exp(iq\theta(x))\psi \Rightarrow A_A \to A'_A = A_A + \partial_A\theta$. Dynamics of these gauge potentials also have to be incorporated to make the theory complete. We need to add a gauge field Lagrangian L_g to the original Lagrangian L_0 and apply the variational principle to determine the gauge potentials self consistently. It can be seen that the gauge fields $F_{AB} = \partial_A A_B - \partial_B A_A$ are gauge invariant. This suggests that L_g can be written down in terms of invariants that can be constructed from the gauge fields F_{AB}. For example, $L_g = -\frac{1}{4}F_{AB}F^{AB}$ for electrodynamics.

In the above example, the gauge group is abelian. The analysis becomes a bit more involved if the gauge group is non-abelian. Let G is non-abelian with its generators $\{\gamma_a\}$ satisfying the Lie algebra $[\gamma_a, \gamma_b] = C^c_{ab}\gamma_c$. Then the covariant derivatives are defined through the relation

$$\partial_A\vec{\psi} \to D_A\vec{\psi} = \partial_A\vec{\psi} + \gamma_a W^a_A\vec{\psi}, \tag{2.4}$$

where $\{W^a_A\}$ are the gauge potentials. The gauge fields $F^a_{\mu\nu}$ are given by the relation

$$[D_A, D_B] = F^a_{AB}\gamma_a, \;\; F^a_{AB} = \partial_A W^a_B - \partial_B W^a_A + C^a_{bc}W^b_A W^c_B \tag{2.5}$$

The gauge field Lagrangian L_g can now be expressed in terms of the invariants that can be constructed out of $\{F^a_{AB}\}$. It can be seen that the gauge field $\{F^a_{AB}\}$ is nonlinear in the gauge potential $\{W^a_A\}$. This implies that the equations of motion of the gauge potentials will, in general, be nonlinear.

3. Gauge Theory of Elastic Continuum

Let a material point in the reference configuration of an isotropic elastic continuum be represented by the space-fixed position vector $\vec{x}$, and upon deformation, let it move to a new point $\vec{\eta} = \vec{x} + \vec{u}$, where $\vec{u}$ is the displacement. In the field theoretic study of the elastic response, one starts with the Lagrangian

$$L_0 = \frac{1}{2}\rho\delta_{ij}\frac{du^i}{dt}\frac{du^j}{dt} - \frac{1}{2}\left[\lambda(Tr(e))^2 + 2\mu Tr(e^2)\right] \tag{3.1}$$

The Strain tensor e_{ij} is given by

$$e_{ij} = \frac{1}{2}\left(\delta_{ik}u^k{}_{,j} + \delta_{jk}u^k{}_{,i} + \delta_{kl}u^k{}_{,i}u^l{}_{,j}\right) \tag{3.2}$$

It can be seen that the action is invariant under the rigid body motion $\vec{\eta} \to \vec{\eta}' = g\vec{\eta}$, where g is any element of the Euclidean group $E(3)$ in three dimensions. Note that $E(3)$ is the semidirect product $SO(3) \triangleright T(3)$ of the rotation group $SO(3)$ with the translation group $T(3)$.

3.1 Local Action of T(3)

It is now well established [13, 15] that both dislocations and disclinations can be described in the gauge theory by the inhomogeneous action of $T(3)$. The consequences of gauging $SO(3)$ are still not understood. However, that is beyond the scope of the present paper. For simplicity, we shall restrict ourselves to linear strain. This implies that the distinction between contra- and co-variant indices can be glossed over. We shall also consider only statics. The action (see Eq. 3.1) is invariant under the global transformation $\eta_j \rightarrow \eta_i' = \eta_i + b_i$, where b_i is a constant translation. Invariance under the local transformation $\eta_i \rightarrow \eta_i' = \eta_i + b_i(x)$. necessitates introduction of the covariant derivative

$$D_j u_i = \partial_j u_i + \phi_{ij} \tag{3.3}$$

where ϕ_{ij} are the gauge potentials. When $\eta_i \rightarrow \eta_i' = \eta_i + b_i$, the gauge potentials transform according to the rule $\phi_{ij} \rightarrow \phi_{ij}' = \phi_{ij} - \partial_j b_i$. $\partial_i u_j$ and ϕ_{ij} can be interpreted as the elastic and plastic distortions. We can now construct the gauge invariant strain E_{ij} and gauge field T_{ijk}

$$E_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i} + \phi_{ij} + \phi_{ji}\right) \tag{3.4}$$

$$T_{ijk} = \partial_k \phi_{ij} - \partial_j \phi_{ik} \tag{3.5}$$

3.2 Simplest Lagrangian and the field equations

The simplest gauge field Lagrangian L_g that Kadic and Edelen proposed [11] is $-\frac{s}{2} T_{ijk} T_{ijk}$. As mentioned in the introduction, there is a need to consider a more general L_g to describe edge dislocations. We shall return to this point in section 3.3.3. The total Lagrangian then becomes

$$L = -\frac{1}{2}\left[\lambda (E_{ii})^2 + 2\mu E_{ij} E_{ij}\right] - \frac{s}{2} T_{ijk} T_{ijk} \tag{3.6}$$

The corresponding Euler-Lagrange equations are given by [11]

$$u_{i,kk} + (L+1) u_{k,ki} = -\left[\phi_{ki,k} + \phi_{ik,k} + L\phi_{kk,i}\right] \tag{3.7}$$

$$\phi_{ik,ll} - \phi_{il,lk} - \kappa^2 \left[\phi_{ik} + \phi_{ki} + L\phi_{ll}\delta_{ik}\right] = \kappa^2 \left[u_{i,k} + u_{k,i} + L u_{l,l}\delta_{ik}\right] \tag{3.8}$$

Here $\kappa^2 = \mu/s$ ans $L = \lambda/\mu$. The expressions for the dislocation density tensor $\{\alpha_{ij}\}$, Burgers vector $\{b_i\}$, incompatibility tensor $\{\Theta_{ij}\}$ and Frank vector $\{\Omega_i\}$ (for disclinations) are then given by

$$\alpha_{ij} = \varepsilon_{ikl} \phi_{jl,k}, \; b_i = \oint_S \alpha_{ij} dS_j \tag{3.9}$$

$$\theta_{ij} = -\varepsilon_{ikm} \varepsilon_{jln} \frac{1}{2}\left(\phi_{kl} + \phi_{lk}\right)_{,mn}, \; \Omega_i = \oint_S \theta_{ij} dS_j \tag{3.10}$$

3.3 Solutions of the gauge field equations

Kadic and Edelen [11] took the view that dislocations and disclinations arise respectively from breaking of $T(3)$ and $SO(3)$ invariance.

3.3.1 Screw dislocation

The Burger's vector $b_3(\rho)$ (at a distance ρ from the dislocation) that they obtained from their solution of the gauge field equations for a screw dislocation along $\hat{z}$ reads as [11]

$$b_3(\rho) = b\kappa\rho K_1(\kappa\rho) \tag{3.11}$$

It can be seen that $b_3(\rho) \to b$ for $\kappa\rho << 1$, and $b\sqrt{\frac{\kappa\rho}{2}}e^{-\kappa\rho}$ for $\kappa\rho >> 1$. Clearly, this does not agree with the continuum elasticity solution for $\kappa\rho >> 1$. The near field ($\kappa'\rho << 1$) solution matches continuum elasticity results, whereas the far field solution doesn't! Their solution for the stress fields also show similar unphysical limiting behaviour. Kadic and Edelen's suggestion that the near field solution be continued to $\kappa'\rho >> 1$ using lattice periodicity is not tenable.

We were able to show [13] that the very same gauge field equations (Eq. 3.7 and 3.8) yield solutions analogous to the screw dislocations and wedge disclinations of classical elasticity. That is, gauging of $T(3)$ is sufficient for obtaining both dislocations and disclinations in an isotropic elastic continuum. For screw dislocation along $\hat{z}$, we obtained [13]

$$b_j(\rho) = \delta_{j3} b\,[1 - \kappa\rho K_1(\kappa\rho)] \tag{3.12}$$

$$\sigma_{ij}(\rho) = \sigma_{ij}^{classical}\,[1 - \kappa\rho K_1(\kappa\rho)] \tag{3.13}$$

Edelen gave the same solution in 1996 [14]. It can be seen that the stress and strain are finite along the dislocation. The solution matches continuum elasticity solution for $\kappa\rho >> 1$, as it should. We also note that the self energy $\sim \frac{\mu b^2}{4\pi}\,[1 - \kappa\rho K_1(\kappa\rho)]^2\, ln(\kappa\rho)$, and that too does not have any divergence.

3.3.2 Wedge disclination

Let us consider a wedge disclination along $\hat{z}$. In continuum elasticity, $\theta_{ij} = \delta_{i3}\delta_{j3}\Omega\delta(\vec{\rho})$, and the nonvanishing components of the stress tensor are given by

$$\sigma_{11} = -\frac{\mu\Omega}{2\pi(1-\nu)}\left(ln(\rho) + \frac{x_2^2}{\rho^2} + \frac{1}{2}\right),\ \sigma_{22} = -\frac{\mu\Omega}{2\pi(1-\nu)}\left(ln(\rho) + \frac{x_1^2}{\rho^2} + \frac{1}{2}\right) \tag{3.14}$$

$$\sigma_{12} = \frac{\mu\Omega}{2\pi(1-\nu)}\frac{x_1 x_2}{\rho^2},\ \sigma_{33} = \nu\,(\sigma_{11} + \sigma_{22}) \tag{3.15}$$

In gauge theory, we get [13]

$$\theta_{ij} = \delta_{i3}\delta_{j3}\frac{\Omega}{2\pi}K_0(\kappa\rho) \tag{3.16}$$

$$\Omega_j(\rho) = \delta_{j3}\Omega\,[1 - \kappa\rho K_1(\kappa\rho)] \tag{3.17}$$

$$\sigma_{ij}(\rho) = \sigma_{ij}^{classical}\,[1 - \kappa\rho K_1(\kappa\rho)] \tag{3.18}$$

Like in the case of the solution for screw dislocation, we find that σ_{ij} are bounded along the disclination line.

3.3.3 Edge dislocation

For the case of the edge dislocation, it is easy to prove that no solution of the form $\phi_{ij} = f(\rho)\phi_{ij}^{classical}$ exists for the gauge field equations 3.7 and 3.8. One of the reasons for nonexistence of a solution of the gauge field equations that resembles an edge dislocation could be that the gauge field Lagrangian proposed by Kadic and Edelen is too restrictive. There have been efforts to try other forms of L_g. Drawing analogy with gravity, Malyshev [18] used the curvature scalar as L_g (Hilbert-Einstein form). However, his 'edge dislocation' solution does not agree with continuum elasticity solution for large ρ. Lazar [17] used the expression $T_{ijk}\left(a_1^{(1)}T_{ijk} + a_2^{(2)}T_{ijk} + a_3^{(3)}T_{ijk}\right)$ in place of $sT_{ijk}T_{ijk}$ with appropriate choice of the coefficients $\{a_i\}$ to get a solution that agrees with continuum elasticity solution for large ρ. The solution for the screw dislocation and wedge dislocation, discussed earlier, remain unaltered for this choice of L_g as well. To be specific,

$$^{(1)}T_{ijk} = T_{ijk} -^{(2)} T_{ijk} -^{(3)} T_{ijk}, \ ^{(2)}T_{ijk} = \frac{1}{2}\left(\delta_{ij}T_{llk} + \delta_{ik}T_{ljl}\right), \ ^{(3)}T_{ijk} = \frac{1}{3}\left(T_{ijk} + T_{jki} + T_{kij}\right) \quad (3.19)$$

The components of the stress tensor are given by

$$\sigma_{11} = \partial_2^2 f, \ \sigma_{12} = -\partial_1\partial_2 f, \ \sigma_{22} = \partial_1^2 f, \text{etc.} \quad (3.20)$$

where f is stress function

$$f = -\frac{\mu b}{2\pi(1-\nu)}x_2\left[ln(\rho) + \frac{2}{\kappa^2\rho^2}(1-\kappa\rho K_1(\kappa\rho))\right] \quad (3.21)$$

σ_{ij} is bounded as $\kappa\rho \to 0$, and agrees with continuum elasticity solution when $\kappa\rho >> 1$

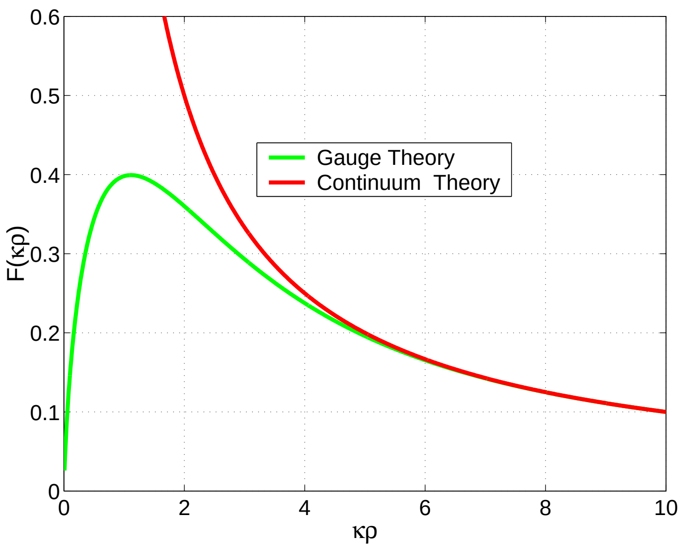

Figure 1: Magnitude of the force between two parallel dislocations as a function of the dimensionless distance $\kappa\rho$ between them. The force diverges at $\kappa\rho$ =0 in continuum theory, whereas it vanishes in gauge theory.

3.4 Interaction between Dislocations

Force between two screw dislocations with Burger's vectors $\vec{b}_1$ and $\vec{b}_2$ parallel to $\hat{z}$ and separated by $\vec{R}$ is given by [16]

$$\vec{F}_{12}(\vec{R}) = \frac{\mu b_1 b_2}{2\pi R}\left[1-\kappa R K_1(\kappa R)\right]\hat{R} \tag{3.22}$$

We have already seen that in the gauge theory, the stress σ_{ij} at a distance R from a screw dislocation is $[1-\kappa R K_1(\kappa R)]$ times the corresponding expression in continuum elasticity theory. It is interesting to note that the force between the dislocations in the gauge theory is $[1-\kappa R K_1(\kappa R)]$ times the force given by continuum theory, and *not* $[1-\kappa R K_1(\kappa R)]^2$ times as one would have naively expected. As can be seen from Fig. 1, the force between the dislocations tend to the continuum elasticity solution when $\kappa\rho > 1$. More importantly, the force vanishes when the two dislocations approach each other, regardless of the sign of the Burger's vectors.

4. Spherically symmetric solutions- I

We found that there exist axially symmetric solutions of the gauge field equations that are in one-to-one correspondence with the well known linear defects of the elastic continuum. These solutions agree with the corresponding continuum elasticity solutions for large distances. However, the gauge field solutions are well behaved along the defect lines. In other words, dislocations and disclinations are line singularities in continuum elasticity theory, whereas these defects are extended objects with a core in the gauge theory. In this section, we shall examine spherically symmetric solutions of the gauge field equations, and compare these solutions with the well known continuum elasticity solutions for point defects.

Before discussing the most general solution, we shall first consider the *ansatz*

$$u_i(\vec{r}) = x_i V(r), \phi_{ij}(\vec{r}) = \delta_{ij} h(r) \tag{4.1}$$

Our aim is to look for solutions such that the magnitude of the displacement $rV(r)$ and the plastic strain $h(r)$ are bounded every where. One of the ways to proceed further would be to substitute Eq. 4.1 in the the gauge field equations (Eq. 3.7 and 3.8), and then obtain the equations to be satisfied by $V(r)$ and $h(r)$. We find that the two functions $V(r)$ and $h(r)$ satisfy *three* equations, which can be simplified to two. Another method proceeds by first obtaining the Lagrangian with the above definition for the matter field $u_i(\vec{r})$ and gauge potentials $\phi_{ij}(\vec{r})$, and then obtaining the field equations satisfied by $V(r)$ and $h(r)$. Both the methods lead to the same equations. In what follows, we describe the latter method. The minimally coupled strain tensor is given by

$$E_{ij} = \delta_{ij}(V+h) + \frac{x_i x_j}{r} V \tag{4.2}$$

and the minimally coupled Lagrangian L_0 reads as

$$L_0 = -(3\lambda+2\mu)\left\{\frac{3}{2}(V+h)^2 + r(V+h)V'\right\} - \frac{1}{2}(\lambda+2\mu)r^2 V'^2 \tag{4.3}$$

The gauge fields are given by

$$T_{ijk} = \phi_{ij,k} - \phi_{ik,j} = (\delta_{ij}x_k - \delta_{ik}x_j)\frac{1}{r}h' \quad {}^{(1)}T_{ijk} = 0, \quad {}^{(2)}T_{ijk} = T_{ijk}, \quad {}^{(3)}T_{ijk} = 0 \tag{4.4}$$

Since only ${}^{(2)}T_{ijk}$ is nonzero, the unique quadratic Lagrangian of the gauge fields is given by

$$L_g = -\frac{s}{2} T_{ijk} T_{ijk} = -2sh'^2 \tag{4.5}$$

In the above equations, V' corresponds to differentiation of V with respect to r, and so on. The field equations are obtained by extremizing the action $S[V,h] = \int \; dr \; r^2 L(V, V', h, h')$. More explicitly, $\frac{\partial}{\partial V}(r^2 L) - \frac{d}{dr}\frac{\partial}{\partial V'}(r^2 L) = 0$, *etc.*

$$rV'' + 4V' + \left(\frac{3L+2}{L+2}\right) h' = 0, \; L = \frac{\lambda}{\mu} \tag{4.6}$$

$$h'' + \frac{2}{r} h' - \frac{L+2}{4} \kappa^2 \left[rV' + 3V + 3h \right] = 0, \; \kappa^2 = \left(\frac{\mu}{s}\right) \left(\frac{3L+2}{L+2}\right) \tag{4.7}$$

Most general solution of Eqs. 4.6 and 4.7 can be shown to be

$$h = \frac{A}{\xi} \exp(\xi) + \frac{B}{\xi} \exp(-\xi) + C, \;\; \xi = \kappa r \tag{4.8}$$

$$V = \left(\frac{3L+2}{L+2}\right) \left[\frac{B}{\xi^3}(\xi+1)\exp(-\xi) - \frac{A}{\xi^3}(\xi-1)\exp(\xi) \right] + \frac{D}{\xi^3} - C \tag{4.9}$$

C is irrelevant and can be set to zero. Notice presence of the classical solution of point defects D/ξ^3 in Eq. 4.9.

4.1 Boundary conditions

It can be seen that no global solution exists with ξV and h bounded for all ξ. Therefore we try a piecewise solution

$$\begin{aligned} h &= \frac{A_1}{\xi} \exp(\xi) + \frac{B_1}{\xi} \exp(-\xi) \\ V &= \left(\frac{3L+2}{L+2}\right) \left[\frac{B_1}{\xi^3}(\xi+1)\exp(-\xi) - \frac{A_1}{\xi^3}(\xi-1)\exp(\xi) \right] + \frac{D_1}{\xi^3} \end{aligned}$$

for $\xi \leq \xi_\star$, and

$$\begin{aligned} h &= \frac{A_2}{\xi} \exp(\xi) + \frac{B_2}{\xi} \exp(-\xi) \\ V &= \left(\frac{3L+2}{L+2}\right) \left[\frac{B_2}{\xi^3}(\xi+1)\exp(-\xi) - \frac{A_2}{\xi^3}(\xi-1)\exp(\xi) \right] + \frac{D_2}{\xi^3} \end{aligned}$$

for $\xi > \xi_\star$. The aim is to determine the constants A_1, A_2, B_1, B_2, D_1, D_2 and $\xi_\star$ by demanding continuity of V and h, and if possible, their derivatives, at $\xi = \xi_\star$. It turns out that continuity of V and h can be enforced, but, not of their derivatives. It is interesting to note that the value of $\xi_\star$ can be uniquely determined to be unity. The final solution is given by

$$V = \left(\frac{a}{e}\right) \frac{\xi \cosh(\xi) - \sinh(\xi)}{\xi^3}, \;\; h = -\left(\frac{a}{e}\right) \left(\frac{L+2}{3L+2}\right) \frac{\sinh(\xi)}{\xi}, \tag{4.10}$$

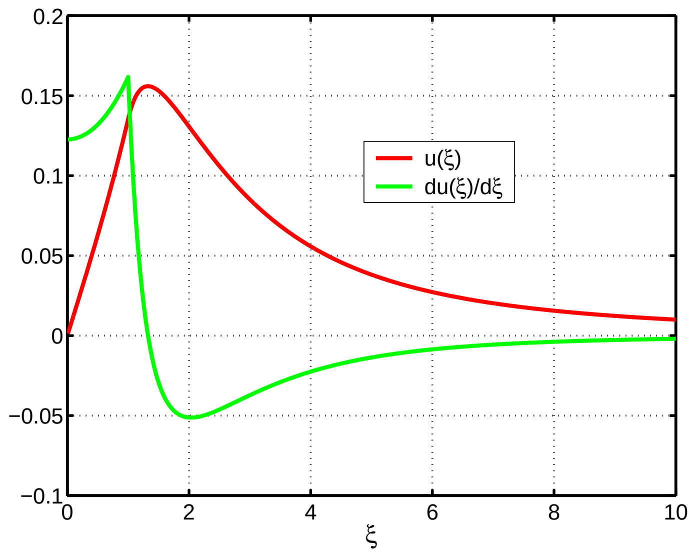

Figure 2: The displacement u and its derivative as a function of the dimensionless distance $\xi = \kappa r$. u is continuous and vanishes at the origin. It's derivative is singular at ξ =1.

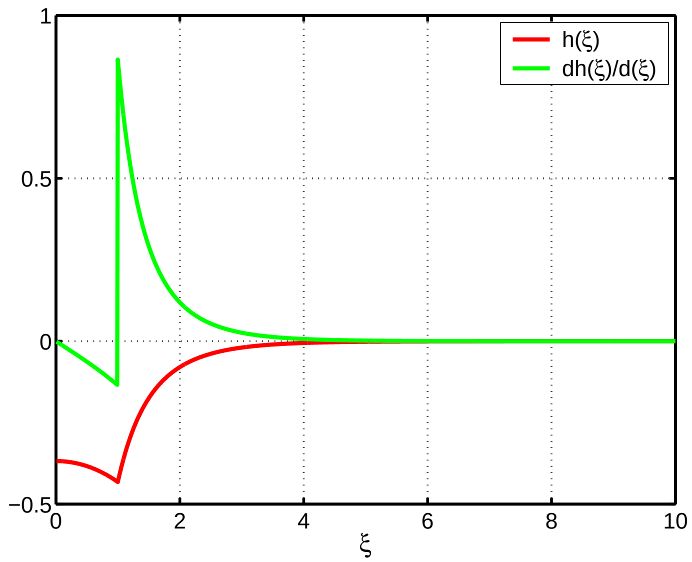

Figure 3: The gauge potential h and its derivative as a function of the dimensionless distance $\xi = \kappa r$. h is continuous every where. It's derivative is discontinuous at ξ =1

for $\xi < 1$, and

$$V = \left(\frac{a}{\xi^3}\right)[1-\sinh(1)(1+\xi)\exp(-\xi)], \quad h = -a\, sinh(1)\left(\frac{L+2}{3L+2}\right)\frac{\exp(-\xi)}{\xi}, \tag{4.11}$$

for $\xi > 1$. a is a parameter that decides the strength of the defect.

As in the case of dislocations and disclinations, the point defects are also extended objects in the gauge theory. There is a core for the point defect with its radius $\sim 1/\kappa$. For large ξ, the present solution matches the classical solution. We find that the displacement, strain, stress and the self energy are all bounded.

4.2 Spherically symmetric solutions- II

In the previous section, we found a spherically symmetric solution of the gauge field equations that correspond to point defects. The displacement and the gauge fields were continuous every where; however, the derivatives were discontinuous at ξ =1. We now consider the most general solution of the gauge field equations with the aim of discovering solutions with better characteristics.

Following Parthasarathy *et al* [22], the most general *ansatz* for the spherically symmetric static solution of the field equations can be written as

$$u_i(\vec{r}) = x_i V(r) = \frac{x_i}{r} u(r) \tag{4.12}$$

$$\phi_{ij}(\vec{r}) = \varepsilon_{ijn} x_n f(r) + x_i x_j \left[\frac{h'}{r} + g(r)\right] + \delta_{ij} h(r) \tag{4.13}$$

There is no loss of generality in writing the function that multiplies $x_i x_j$ as $[h'r + g(r)]$. We have written it in that particular form in view of the simplicity of the resultant equations of motion. We note that the displacement, gauge potentials and hence the stress fields are bounded if $rV(r)$, $rf(r)$, $r^2 g(r)$ and $h(r)$ are bounded. The minimally coupled strain E_{ij} and rotational strain ω_{ij} are given by

$$E_{ij} = \delta_{ij}(V+h) + \frac{x_i x_j}{r}\left(V' + h'\right) + x_i x_j g(r) \tag{4.14}$$

$$\omega_{ij} = \varepsilon_{ijn} x_n f(r) \tag{4.15}$$

The minimally coupled Lagrangian then reads as

$$L_0 = -(3\lambda + 2\mu)\left[\frac{3}{2}\tilde{V}^2 + r\tilde{V}(\tilde{V}' + rg)\right] - \frac{1}{2}(\lambda + 2\mu) r^2 \left(\tilde{V}' + rg\right)^2 \tag{4.16}$$

Notice that the function $f(r)$ appears only in ω_{ij}. That is, nonvanishing f corresponds to nonzero rotational plastic strain, and it is relevant only in media with nonzero rotational elastic constants. We also note that the functions V and h appear only in the combination $\tilde{V} = (V + h)$ in the expression for the strain E_{ij} and the Lagrangian L_0. The gauge fields $T_{ijk} = \phi_{ij,k} - \phi_{ik,j}$ are given by

$$T_{ijk} = 2\varepsilon_{ijk} f + (\varepsilon_{ijn} x_k - \varepsilon_{ikn} x_j)\frac{x_n}{r} f' + (\delta_{ik} x_j - \delta_{ij} x_k)\, g \tag{4.17}$$

We see that the gauge fields depend only on f and g. The simplest gauge field Lagrangian is given by

$$L_g = -\frac{s}{2} T_{ijk} T_{ijk} = -2sr^2 g^2 - 2s\left[6f^2 + 4rff' + r^2 f'^2\right], \tag{4.18}$$

In the gauge field Lagrangian also f is decoupled from the other fields. For the isotropic elastic continuum that we have been considering, we thus find that f is irrelevant; V and h occur in the combination $\tilde{V} = (V + h)$; hence h can be gauged away. Thus we arrive at the Lagrangian

$$L = -(3\lambda + 2\mu)\left[\frac{3}{2}V^2 + rV(V' + rg)\right] - \frac{1}{2}(\lambda + 2\mu) r^2 \left(V' + rg\right)^2 - 2sr^2 g^2 \tag{4.19}$$

It is interesting to note that derivative of g is absent in L.

The field equations obtained by extremizing the action $S[V,g] = \int drr^2 L(V,V',g)$ are

$$V'' + \frac{4}{r}V' + rg' + 2\left(\frac{L+4}{L+2}\right)g = 0 \tag{4.20}$$

$$V' + \left(\frac{3L+2}{L+2}\right)\frac{V}{r} + (r + \frac{c}{r})g = 0,\ c = \frac{4s}{\mu(L+2)} \tag{4.21}$$

Using the above equations, it is possible to express the function V in terms of g. Substituting that expression for V, we get

$$g'' + \frac{4}{r}g' - \kappa^2 g = 0 \tag{4.22}$$

$$V = -\frac{1}{\kappa^2}\left[rg' + \left(\frac{4}{L+2}\right)g\right] \tag{4.23}$$

4.3 Solution of the field equations

The most general solution of the above equations can be written in terms of the two linearly independent solutions $g_1(\xi)$ and $g_2(\xi)$ of Eq. 4.22 which are given by

$$g_1(\xi) = \frac{1+\xi}{\xi^3}e^{-\xi},\ g_2(\xi) = \frac{1-\xi}{\xi^3}e^{\xi} \tag{4.24}$$

Thus the general solution for V is given by

$$V(\xi) = AV_1(\xi) + BV_2(\xi);\ V_i(\xi) = -\frac{1}{\kappa^2}\left[\xi g_i(\xi)' + \frac{4}{L+2}g_i(\xi)\right] \tag{4.25}$$

A and B are the same in the expressions for both g and V. It can be seen that ξV_i and $\xi^2 g_i$ are unbounded as $\xi \to 0$. However, we can obtain a solution bounded at $\xi = 0$ by choosing B = -A. g_1 and V_1 are well behaved as $\xi \to \infty$, whereas g_2 and, hence, V_2 are not. Hence the solution obtained by demanding boundedness of ξV_i and $\xi^2 g_i$ at the origin cannot be continued for all ξ. Thus no global solution exists such that ξV and $\xi^2 g$ are nonsingular as $\xi \to \infty$ as well as $\xi \to 0$. Hence we now look for a *piecewise solution*

$$V(\xi) = AV_1(\xi) + BV_2(\xi),\ g(\xi) = Ag_1(\xi) + Bg_2(\xi),\ \text{for } \xi < \xi_\star \tag{4.26}$$

$$V(\xi) = CV_1(\xi),\ g(\xi) = Cg_1(\xi),\ \text{for } \xi > \xi_\star \tag{4.27}$$

Demanding continuity of ξV and $\xi^2 g$ at $\xi = \xi_\star$ implies that the Wronskian$(g_1(\xi), g_2(\xi)) = 0$ at $\xi = \xi_\star$, which is impossible for any $\xi_\star > 0$. Hence we conclude that the ansatz considered here does not lead to a continuous valued solution for the displacement and the gauge potentials.

Given the fact that the second *ansatz* (Eq. 4.13) is more general than the first one (Eq. 4.1), the failure of the second ansatz to produce a physically meaningful solution is surprising. The reasons for the failure is currently under investigation- We have seen that the derivative of h is discontinuous in the final solution obtained by the first *ansatz*. The calculation of the gauge fields T_{ijk} in the second *ansatz* assumed existence of second derivatives of h, which, in retrospect, seems to be untenable.

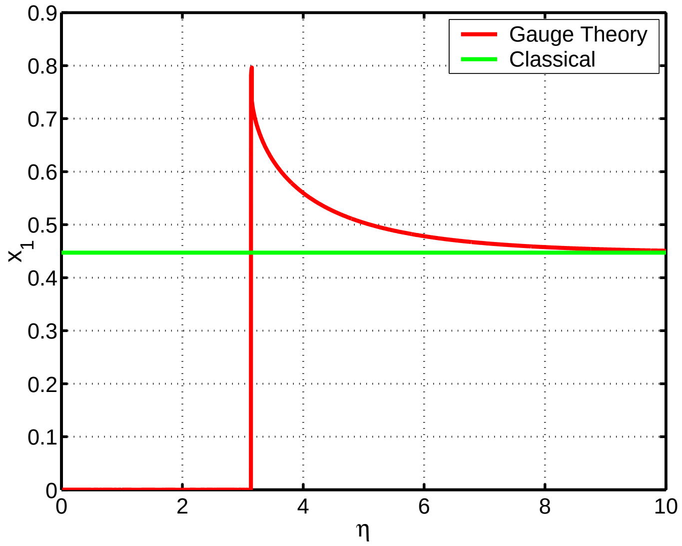

Figure 4: Solution of the force balance equation for dislocation pileup as function of η for $N = 2$. There is no solution if $\eta < \eta_c(2) \sim 3.14$. Also shown is the continuum elasticity solution.

5. Dislocation Pileup

We now turn to gauge theoretic analysis of the dislocation pileup problem [1, 23, 24]. Consider $N+2$ identical screw dislocations of parallel to $\hat{z}$ and lying between $X = \pm l$ with the end members fixed, and the others free. Our aim is to determine the positions X_j ($j = 1, ..., N$) of the free dislocations. Using the fact that the force on the j^{th} free dislocation must be equal to zero, we get

$$\sum_{k \neq j} f(x_j - x_k) + f(x_j + 1) + f(x_j - 1) = 0, \tag{5.1}$$

where $x_j = X_j/l$, and $f(x)$ is the force between two parallel screw dislocations at a distance lx from each other.

$$f(x) = \frac{1 - \eta|x|K_1(\eta|x|)}{x}, \tag{5.2}$$

where $\eta = \kappa l$. In the continuum elasticity case ($\eta \to \infty$), $\{x_j\}$ are given by the zeros of $\frac{d}{dx}P_{N+1}(x)$ [23], where $P_N(x)$ is the Legendre polynomial of order N. Our analysis [21] shows that only the degenerate solution $\delta_{x_j,0}$ is possible in gauge theory if η is less than a critical value $\eta_c(N)$. Consider the case $N = 2$. In view of the symmetry, we can assume x_2 = -x_1. Figure 4 shows the solution of Eq. 5.2 as function of η. It is clear that there is no solution if $\eta < \eta_c(2) \sim 3.14$. That is, the system becomes unstable when the number of dislocations in between the obstacles exceeds a critical value. This implies that the dynamics of dislocations should be should be nontrivial when $\eta < \eta_c(N)$.

5.1 Continuous distribution of dislocations:

When the number of dislocations is large, it may be expedient to have a description in terms of the *number* density $\rho(x)$ of the dislocations. Then the force balance equation becomes

$$\rho(x)\left(\left[\int_{-1}^{1} dy\rho(y)f(x-y)\right]+f(x+1)+f(x-1)\right)=0 \tag{5.3}$$

In the classical limit ($\eta \to \infty$), one gets the well known solution

$$\rho(x)=\frac{1}{\pi}\frac{N}{\sqrt{1-x^2}}+\frac{1}{\pi^2}\left[\int_{-1}^{1} dy\sqrt{\frac{1-y^2}{1-x^2}}\;\frac{f(y+1)+f(y-1)}{x-y}\right] \tag{5.4}$$

It is obvious that the degenerate solution $\rho(x)=N\delta(x)$ exists for any η in the gauge theory. It can be shown [21] that a continuous, non-negative and normalizable solution does not exist for any finite η in the gauge theory. This implies that the correct way to describe an ensemble of dislocations should be in terms of the dislocation density tensor and not in terms of the number density.

6. Summary, Conclusions and Outlook

Many investigators have already shown that a gauge theory based on the inhomogeneous action of the translation group $T(3)$ can account for both dislocations and disclinations in an elastic continuum. The present work has shown that even a non-topolgical defect like the point defect also can be described the the same gauge theory. That is, there is no need to have separate gauge fields for dislocations and point defects. Gauge theory provides a physically meaningful description of the structure of dislocations, disclinations and point defects. All these defects have got a core, and the stress fields produced by them are bounded every where. We have seen that the force between two dislocations vanishes when they approach each other regardless of the sign of the Burger's vector of the two dislocations. Through the study of the dislocation pileup problem, we infer that the dynamics of dislocations should be nontrivial when their number exceeds a limiting value. We have also seen that it is necessary to describe an ensemble of dislocations in terms of the consolidated dislocation density tensor, and not the number density.

Interaction between point defects, point defects and dislocations, as well as mixed dislocations remain to be done. The consequences of breaking $SO(3)$ symmetry is yet to be explored. Gauge theoretic study of media with anisotropy or nonzero rotational elastic constants would be interesting. The gauge theoretic solutions are expected to be more appropriate for the study of mechanical and electronic properties of small systems. In particular, it would be interesting to study the changes in electronic and magnetic properties of small systems with dislocations. It is important to know how the presence of the underlying lattice would modify the results of the gauge theory. Description of production (and annihilation) as well as incorporation of dissipative forces are the other unfinished tasks.

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