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Gauge field theoretic solution of a uniformly moving screw dislocation and admissibility of supersonic speeds

P. Sharma *, X. Zhang

Department of Mechanical Engineering, University of Houston, Houston, TX 77204-4006, USA

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Abstract

The failure of classical elasticity to address dislocation behavior spatially close to its core and (in Lorentz-type fashion) near the speed of sound is well known. In gauge field theory of defects, the latter are not postulated a priori in an ad hoc fashion rather defects such as dislocations arise naturally as a consequence of broken translational symmetry exhibiting solutions that are physically meaningful (e.g., removal of divergence of stress and the natural emergence of a core making redundant the artificial cut-off radius). In the present work we present the gauge field theoretic solution to the problem of a uniformly moving screw dislocation. Apart from the formal derivations, we show that stress divergence at the core of the dislocation is removed at all time and (consistent with atomistic simulations), supersonic states are found to be admissible.

1. Introduction

In the past two decades topological defects such as dislocations have also been brought under the ambit of gauge field theories [1–4] where one thinks of them as a consequence of broken translational symmetry—although (relatively speaking), progress in this area still remains at its infancy with several open issues. Therein, defects such as dislocations arise naturally as a consequence of broken translational symmetry and their existence is not required to be postulated a priori. Thus simply by invoking local gauge invariance (which is now universally accepted as a fundamental physical law), without recourse to ad hoc postulates, the gauge field theory of defects allows dislocations to emerge naturally and further provides solutions that are physically meaningful (e.g., removal of divergence of stress and the natural emergence of a core making redundant the artificial cut-off radius). In this work we derive, for the first time, a formal gauge field theoretic solution to the problem of a moving screw dislocation. A salient characteristic of our gauge solution is that spatial singularity (of stresses, strains and energies) at the core of the dislocation is removed and supersonic

* Corresponding author.
E-mail address: psharma@uh.edu (P. Sharma).

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states are found to be admissible. While the inadequacy of classical elasticity to tackle admissibility of dislocations exceeding shear speeds may be partly mitigated by phenomenological approaches, one is loath to admit that there is not a fundamental physical principle which when brought to bear on this problem will rectify this inconsistency (between classical elastic prediction and the "reality")—presumably without any artificial ad hoc assumptions. We believe that such a principle is the principle of local gauge invariance which has been the basis for explaining much of the fundamental interactions in physics [5].

In so far as supersonic dislocations are concerned, while a wealth of evidence has begun to emerge that dislocations can indeed, contrary to conventional wisdom, break the (shear wave) sonic barrier [6–8], a convincing mechanistic and/or field theoretic *proof* for the *admissibility* of such moving defects is lacking. Taking the example of a screw dislocation moving with a velocity "v", say in the x-direction, classic elasticity yields the stress and energy per unit length as [9]

$$\sigma_{rz} = \frac{\mu b}{2\pi \sqrt{\frac{(x-vt)^2}{1-v^2/c^2} + y^2}}, \tag{1a}$$

$$W = \frac{1}{\sqrt{1-v^2/c^2}} W_0 = \frac{1}{\sqrt{1-v^2/c^2}} \left(\frac{\mu b^2}{4\pi} \ln \frac{R}{r_0} \right). \tag{1b}$$

Where c is the shear speed of sound, W_0 is the static strain energy, R is the system size, b is the magnitude of burger's vector and r_0 is the artificially introduced dislocation core cutoff radius. Obviously, in close analogy to special relativity, $v \geqslant c$ is prohibited. However, recent atomistic simulations have indeed shown the feasibility of this classically forbidden and non-intuitive phenomenon [6–8]. They show that dislocations can exceed the shear wave speed provided they are created ad initium as such, at strong stress concentration sites and are supplied high energy through large magnitudes of stress. We also note here a rather peculiar and well-known *classical elasticity* based prediction of Eshelby [10], that the $v = \sqrt{2}c > c$ state for a gliding edge dislocation in an isotropic linear elastic solid does not engender radiation emission. Gumbsch and Gao [7] as well as Rosakis [11], attempt to explain transonic and supersonic dislocations observed in atomistic simulations [6–8] by invoking the underlying discreteness of the lattice, nonlinear effects and nonlocal effects. Their focus is on clarifying the relation between applied stress and the velocity of the moving dislocation. Needless to say the failure of classical elasticity (spatially, close to the dislocation core and dynamically, when they move closer to sonic speeds) is patent. The chief motivation for the present work is that while the aforementioned works and other contributions (including the classics by Eshelby Refs. [10,12]) have provided valuable insights into this problem, the question of *admissibility* of supersonic states has never been rigorously addressed, in particular, from a field theoretic standpoint.[1] The present work, predicated on gauge field theory, provides an alternative perspective on this problem.

2. Formulation

A basic framework of gauge theory of defects in solid continua has already been well formulated by Kadić–Edelen–Lagoudas [1,2] and extended by various researchers [3–5]. The classical elastic Lagrangian (for an isotropic linear material) is

$$L_0 = \frac{1}{2}\rho_0 u_{i,4} u_{i,4} - \frac{1}{2}\lambda(\varepsilon_{kk})^2 - \mu\varepsilon_{ij}\varepsilon_{ij}. \tag{2}$$

Here $\mathbf{u}$ is the displacement and, $\boldsymbol{\varepsilon} = \frac{1}{2}[\nabla \otimes u + (\nabla \otimes u)^T]$. λ and μ are the usual Lame constants while $\boldsymbol{\varepsilon}$ is the infinitesimal strain tensor. ρ_0 is the material density. Cartesian framework is assumed and spatial coordinates run from 1–3, while the time coordinate is designated by "4". The classical elastic Lagrangian in Eq. (2) is invariant under a uniform continuous global gauge group of transformations (the three-dimensional Euclidean group): $G = \mathcal{SO}(3) \triangleright \mathcal{T}(3)$, i.e., the semi-direct product of the non-Abelian special rotation group, $\mathcal{SO}(3)$, and the Abelian group of translations, $\mathcal{T}(3)$. Consider the translation group only.[2] Making the gauge group local (i.e., dependent

[1] In the present work, we are not interested in the relation between applied stress and speed of the dislocation which was the focus of Refs. [6–8]. Our emphasis is on a rigorous field theory which allows such classical forbidden phenomena to be admissible without artificial assumptions and phenomenological maneuvers.

[2] In the Edelen–Kadić–Lagoudas theory, breaking of the rotational symmetry, i.e., $\mathcal{SO}(3)$ group results in formation of disclinations. Only dislocations are of concern here and thus solely the Abelian $\mathcal{T}(3)$ group is considered. See also Ref. [13].

on space–time) spoils this global gauge invariance. Eq. (3) shows that if the translations ($\mathbf{T}$) are inhomogeneous, the invariance of the elastic Lagrangian (Eq. (2)) is lost. The Lagrangian can be once again made invariant under the action of this group by introducing compensating fields (the so-called gauge fields, $\boldsymbol{\varphi}$) and defining the so-called gauge covariant derivative (superscript G)

$$\overset{G}{\nabla}\otimes\mathbf{u}\to\nabla\otimes\mathbf{u}+\boldsymbol{\varphi}, \tag{3a}$$

$$\boldsymbol{\varphi}'\to\boldsymbol{\varphi}-\nabla\otimes\mathbf{T}(\mathbf{x}). \tag{3b}$$

Thus, in the spirit of Yang–Mills minimal coupling type approach [5], espoused by Edelen–Kadić–Lagoudas [1,2], the definitions, $\boldsymbol{\varepsilon}\to\mathbf{E}$ and $B_{i4}=u_{i,4}+\phi_{i4}$ where, $\mathbf{E}=\frac{1}{2}[\nabla\otimes\mathbf{u}+(\nabla\otimes\mathbf{u})^T+\boldsymbol{\varphi}+\boldsymbol{\varphi}^T]$ in Eq. (4) lead to restored invariance under the inhomogeneous action of the translational group.

$$\mathcal{L}_{\text{total}}=\frac{1}{2}\rho_0B_{i4}B_{i4}-\frac{1}{2}\lambda(E_{kk})^2-\mu E_{ij}E_{ij}+\mathcal{L}_{\mathcal{G}}. \tag{4}$$

The term $\mathcal{L}_{\mathcal{G}}$ is appended in Eq. (4) to indicate that the newly introduced gauge fields (which are now incorporated in the new definition of “strain”, $\mathbf{E}$ to restore translational invariance), by themselves must also contribute to the total Lagrangian. This new term must only be a function of the gauge fields and additionally be constructed by using scalar functions that are invariant under the *local* translational group [3], i.e.,

$$\{\mathcal{L}_{\mathcal{G}}\mid G(\mathbf{x})\mathcal{L}_{\mathcal{G}}\to\mathcal{L}_{\mathcal{G}}\}. \tag{5}$$

This requirement lends naturally to the following construction

$$\mathcal{L}_{\mathcal{G}}=-\frac{1}{2}s_1F^i_{ab}F^i_{ab}+\frac{1}{2}s_2J^i_aJ^i_a, \tag{6a}$$

$$F^k_{ij}=\phi_{kj,i}-\phi_{ki,j},\qquad J^i_j=\phi_{i4,j}-\phi_{ij,4}. \tag{6b}$$

Here s_1 and s_2 are two coupling constants which respectively correspond to the static and dynamic gauge Lagrangian. In absence of these coupling constants, gauge fields play no role and we revert to classical elastodynamics.

A null Lagrangian may always be added to the total $\mathcal{L}_{\text{total}}$ in Eq. (4). Such an operation does not alter the field equations (i.e., the Euler–Lagrange equations) but allows one to correctly incorporate the boundary conditions [2]. We write the null Lagrangian as

$$\mathcal{L}_{\mathcal{N}}=\sigma^0_{ij}B_{ij}-P^4_iB_{i4}. \tag{7}$$

Where, σ^0_{ij} is classical stress and P^4_i is classical momentum $=\rho\delta_{ij}u_{j,4}$ while $B_{i4}=u_{i,4}+\phi_{i4}$, and $B_{ij}=u_{i,j}+\phi_{ij}+\delta_{ij}$. Following Kadić and Edelen [1], we select the pseudo-Lorentz gauge condition, $\phi_{ij,j}=\frac{s_2}{2s_1}\phi_{i4,4}$. Further now, an appeal to the Euler–Lagrange equations or a variational argument provides the following governing equations:

$$\left(\nabla^2-\frac{s_2}{2s_1}\partial_4^2\right)\phi_{ij}=\kappa^2\left(\phi_{ij}+\phi_{ji}+\frac{\lambda}{\mu}\phi_{kk}\delta_{ij}\right), \tag{8a}$$

$$\mu u_{i,jj}+(\mu+\lambda)u_{j,ji}+\left(\mu-\rho\frac{s_1}{2s_2}\right)\phi_{ij,j}+\mu\phi_{ji,j}+\lambda\phi_{kk,i}=\rho u_{i,44}, \tag{8b}$$

$$\phi_{i4}-\frac{s_2}{\rho_0}\left(\nabla^2-\frac{s_2}{2s_1}\partial_4^2\right)\phi_{i4}=0. \tag{8c}$$

The difference between (8a)–(8c) and the governing equations given by [1] and [2] are that the latter do not incorporate the null Lagrangian that is specific to the current problem. In subsequent work, Edelen has corrected and clarified this [14].

We now proceed to specialize the general equations indicated above for a moving screw dislocation. The symmetry of the screw dislocation problem indicates the following constraints on the displacement and gauge fields:

$$\mathbf{u}=u(r)\mathbf{e}_3, \tag{9a}$$

$$\boldsymbol{\varphi}=\varphi_{31}\mathbf{e}_3\otimes\mathbf{e}_1+\varphi_{32}\mathbf{e}_3\otimes\mathbf{e}_2, \tag{9b}$$

$\{\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3\}$ is the Cartesian basis. Given these symmetry constraints, we obtain

$$\left(\nabla^2-\frac{s_2}{2s_1}\partial_4\partial_4\right)\phi_{31}=\kappa^2\phi_{31}, \tag{10a}$$

$$\left(\nabla^2-\frac{s_2}{2s_1}\partial_4\partial_4\right)\phi_{32}=\kappa^2\phi_{32}, \tag{10b}$$

$$\phi_{34}-\frac{s_2}{\rho_0}\left(\nabla^2-\frac{s_2}{2s_1}\partial_4^2\right)\phi_{34}=0, \tag{10c}$$

$$\mu\phi_{31}=\sigma_{31}-\sigma^0_{31}, \tag{10d}$$

$$\mu\phi_{32}=\sigma_{32}-\sigma^0_{32}. \tag{10e}$$

To solve this system of equations, we set, $\varsigma=2s_1/s_2$ and invoke the Lorentz transformation, i.e., adopt a frame of reference which is moving along with the dislocation with identical speed, v:

$$x'=(x-vt)\beta, \tag{11a}$$

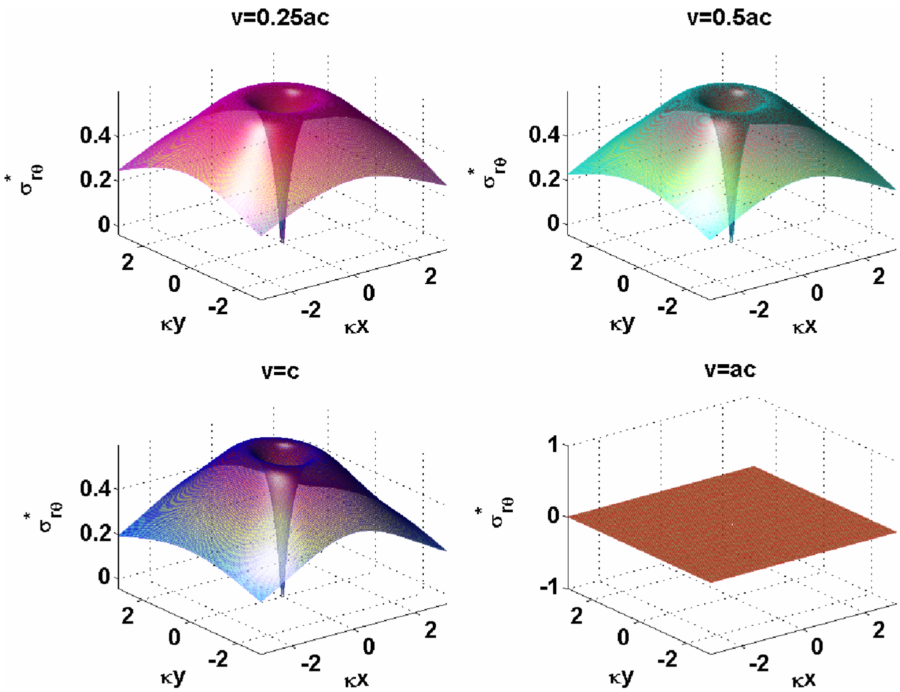

Fig. 1. Three-dimensional plot of the stress fields of a moving screw dislocation for various velocities based on our results predicated on gauge field theory. The snapshots are for instance $t = 0$. The spatial coordinates are normalized by κ while the stress $\sigma_{rz}^{*} = \sigma_{rz}/\sigma_{rz}^{0}$ is normalized with respect to the classical stress.

$$t' = (t - vx/\varsigma)\beta, \tag{11b}$$

$$y' = y, \tag{11c}$$

$$\beta = \frac{1}{\sqrt{1 - v^2/\varsigma}}. \tag{11d}$$

All variables referred to in the moving frame will be identified by an apostrophe, e.g., ϕ'_{31} or ∇'. With this notation, we have

$$\nabla'^2\phi'_{31} = \kappa^2\phi'_{31}, \tag{12a}$$

$$\nabla'^2\phi'_{32} = \kappa^2\phi'_{32}, \tag{12b}$$

$$\nabla'^2\phi'_{34} = \kappa_d^2\phi'_{34}. \tag{12c}$$

Here, κ^2 is $2\mu/s_1$ and κ_d^2 is $\frac{\rho_0}{s_2}$, which have units of reciprocal lengths squared while κ_d^2 defines a length scale relating to dynamic properties. Using a fairly standard argument, we note that the dislocation field is static with respect to the moving frame. Thus, the classical stresses satisfy [9]: $\nabla'^2\sigma'^0_{32} = \nabla'^2\sigma'^0_{31} = 0$. Transforming to cylindrical polar coordinates, we obtain finally

$$\left(1 - \kappa^{-2}\nabla'^2\right)\sigma'_{r\theta} = \sigma'^0_{r\theta}. \tag{13}$$

The solution to Eq. (13) is straightforward and we omit further details for the sake of brevity. We obtain (after transformation back to the natural frame of reference)

$$\sigma_{r\theta} = \frac{\mu b}{2\pi r'}\left[1 - \kappa r' K_1(\kappa r')\right],$$
$$(r')^2 = \frac{(x - vt)^2}{1 - v^2/\varsigma} + y^2. \tag{14}$$

Here K_1 is modified Bessel's function of second kind of order 1. Integration of the stress fields and the derived strains yields the following expression for energy per unit length

$$W = \frac{\mu b^2}{4\pi}\left\{-\frac{1}{2} + C + \frac{1}{2}\kappa^2(r')^2K_1(\kappa r')^2 + K_0(\kappa r') \times\left[2 - \frac{1}{2}\kappa^2(r')^2K_2(\kappa r')\right] + \ln\left(\frac{\kappa r'}{2}\right)\right\}. \tag{15}$$

Here, C is the Euler constant.

The dynamic gauge field ϕ'_{34} of (12c) can be solved similarly and gives

$$\phi'_{34} = CK_0(\kappa_d r'). \tag{16}$$

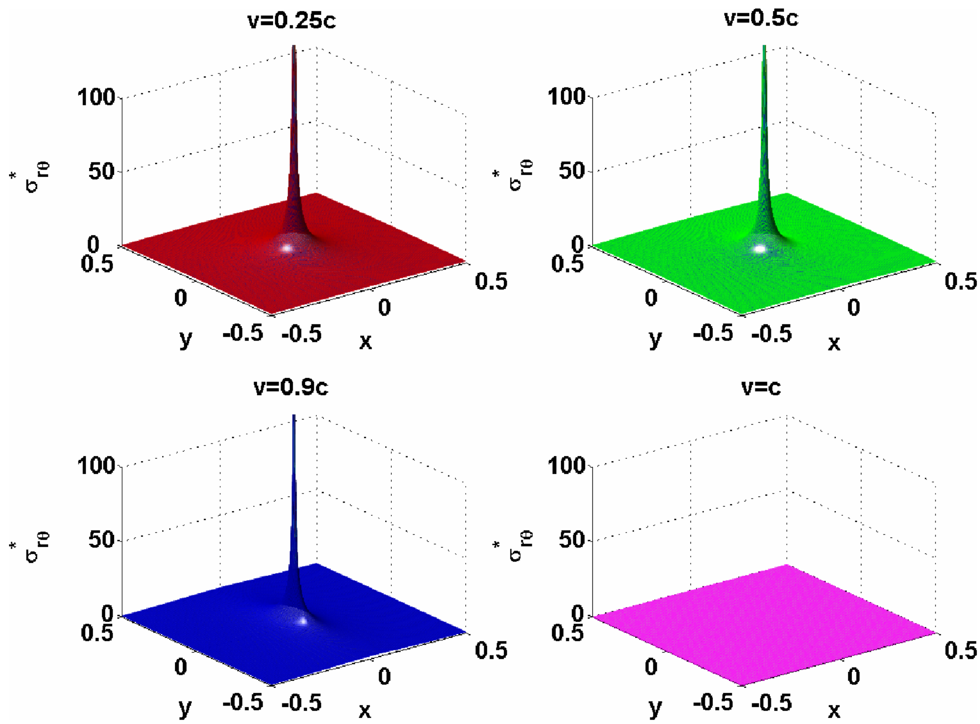

Fig. 2. Three-dimensional plot of the stress fields of a moving screw dislocations for various velocities as predicted by classical elasticity. The snapshots are for instance $t = 0$. The spatial coordinates are normalized by κ while the stress $\sigma^*_{rz} = \sigma_{rz}/\sigma^0_{rz}$ is normalized with respect to the classical stress.

We should keep in mind the assumption that the dislocation field is static with respect to the moving frame. Hence, momentum of dislocation should be 0, which implies $B'^4_i = P'^4_i = 0$ and thus $C = 0$ becomes the only physically reasonable option for Eq. (16).

3. Results and discussion

While the conclusions of our mathematical results are manifestly clear from Figs. 1–3, upon setting, $\varsigma = a^2c^2$ (where a is a constant), a cursory glance at Eqs. (14) and (15) indicates that transonic and supersonic states will be admissible provided $a > 1$. This factor a also arises in the context of dispersion curves (of the gauge field of defects) and has already been shown to be >1 by Kadić–Edelen–Lagoudas [1,2]. Their work implies that a is a material constant.

Fig. 1 clearly illustrates the lack of any singularities at $v = c$ while stress field completely vanishes at $v = ac$. The contrast with classical elasticity (Fig. 2) is striking which exhibits divergences both temporally and spatially.

The energy of the moving dislocation is also plotted (in Fig. 3) and compared with the classical prediction clearly indicating the admissibility of transonic and supersonic dislocations on energetic grounds. For illustrative purposes we have chosen $a = 1.5$ although the precise numerical choice (considering the intent of this Letter) is irrelevant as long as $a > 1$.

Some aspects of our results and their interpretation warrant further discussion. We emphasize here that, using a gauge field theoretic approach and consequently without any adoption of unnecessary postulates (that are not already accepted in fundamental physics), we have shown that speeds greater than c are not forbidden.

These results, however, by no means provide any insights into the relation between applied stress and the velocity of the dislocations. Indeed, such an issue can only be addressed by incorporating both the effect of underlying lattice and nonlinearities. Within

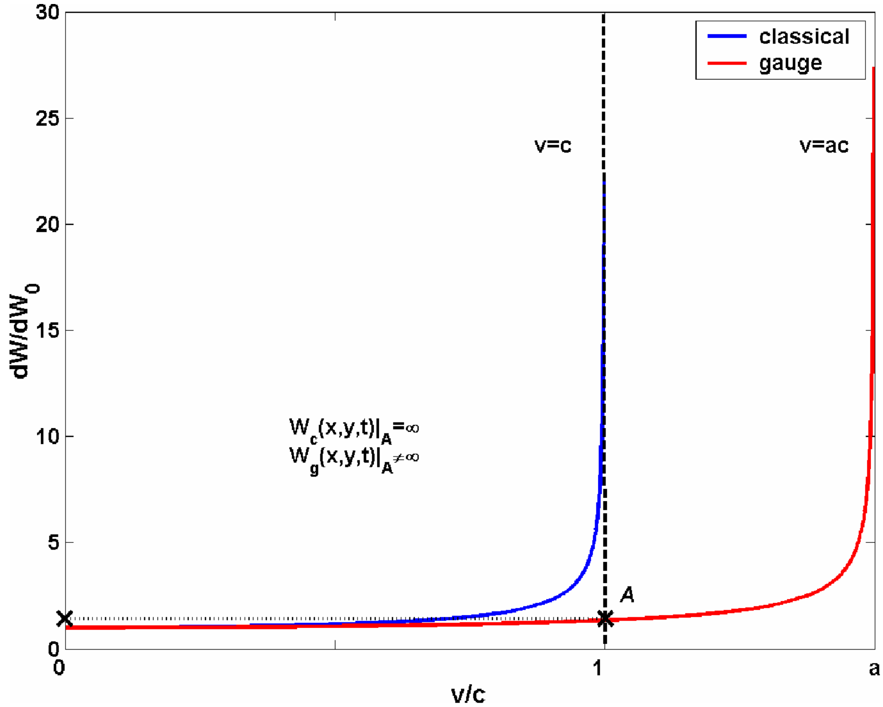

Fig. 3. Normalized energy versus normalized velocity. Our gauge solution and the classical predictions are contrasted.

a classical field theoretic standpoint, these were addressed by Gumbsch and Gao [7] and Rosakis [11]. Obviously, the incorporation of such effects in the gauge field approach outlined in the present work is the logical future step. In closing, we note here that the gauge field theory naturally incorporates nonlocal effects. In fact, Eq. (13) is reminiscent of the so-called phenomenological nonlocal elasticity theories [15,16]. However, we hasten to point out that it is unclear to the present authors whether the use of the actual phenomenological nonlocal elastodynamical theory [16] for the present problem will lead to the result shown here [17]. As already alluded to earlier, given the purpose of the present work, the actual value of the constant a is immaterial as long as one acknowledges the result of Edelen–Kadić–Lagoudas [1,2] that it must be >1. Their context was dispersion curves of gauge elastic continuum, while we have solved the specific problem of a moving screw dislocation to prove that $a > 1$ implies that transonic and supersonic states are admissible (which is not the same as “probable”) and the theoretical maximum speed is ac. The material parameter a is analogous to the characteristic length scale that appears in both phenomenological nonlocal elasticity theories and gauge field theory (i.e., $1/\kappa$) in the static case. Both these theories introduce a length scale parameter in the static solutions of mechanical deformation which is rightfully acknowledged to be a material level constant (and is currently the subject of much experimental and atomistic determination, see Refs. [16,17] and references therein). In the present case, which is a dynamical problem, the material constant a plays a similar role and “renormalizes” the shear speed of sound.

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