Physics Letters A 378 (2014) 597–601

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

The solid angle and the Burgers formula in the theory of gradient elasticity: Line integral representation

Markus Lazar [a,*], Giacomo Po [b]

[a] Heisenberg Research Group, Department of Physics, Darmstadt University of Technology, Hochschulstr. 6, D-64289 Darmstadt, Germany
[b] Mechanical and Aerospace Engineering, University of California, Los Angeles, Los Angeles, CA 90095, USA

ARTICLE INFO

Article history:
Received 20 May 2013
Received in revised form 19 November 2013
Accepted 10 December 2013
Available online 12 December 2013
Communicated by A.R. Bishop

Keywords:
Dislocation loops
Gradient elasticity
Burgers formula
Solid angle
Dirac monopole

ABSTRACT

A representation of the solid angle and the Burgers formula as line integral is derived in the framework of the theory of gradient elasticity of Helmholtz type. The gradient version of the Eshelby–deWit representation of the Burgers formula of a closed dislocation loop is given. Such a form is suitable for the numerical implementation in 3D dislocation dynamics (DD).

1. Introduction

The Burgers formula and the solid angle play an important role in the dislocation theory (e.g., [1–5]) and in the simulation of dislocation dynamics (e.g., [6–8]). The original formulas are given in the form of surface integrals. The transformation of the surface integrals into line integrals was proposed by deWit [9] and Eshelby [10] adopting Dirac's theory of magnetic monopoles [11–13]. In particular, it turned out that the representation as line integral is more appropriate for numerical implementation of these equations into the dislocation dynamics. The classical expressions for the Burgers formula and for the solid angle are singular at the line of the dislocation loop. Moreover, the Burgers formula is discontinuous on the slip surface.

Non-singular expressions for the Burgers formula and the solid angle have been recently found by Lazar [14,15] using the theory of gradient elasticity of Helmholtz type. The theory of gradient elasticity of Helmholtz type is a special version of Mindlin's gradient elasticity theory [16] (see also [17,15]) with only one characteristic length parameter. Lazar and Maugin [18] have shown that, for straight dislocations, the gradient parameter leads to a smoothing of the displacement profile, in contrast to the jump occurring in the classical solution. Lazar [14,15] has given the generalized solid angle and the corresponding part of the Burgers formula in the form of surface integrals. In this letter, we recast the Burgers formula and the solid angle of gradient elasticity in compact form as line integrals over the closed dislocation loop. The results have a direct application to the numerical implementation and the computer simulation of non-singular dislocations within the so-called (discrete) dislocation dynamics. In Section 2, we discuss and point out the basics of the line integral form of the solid angle and of the associated vector potential in the framework of classical elasticity and their relation to Dirac's solution of a magnetic monopole. In Section 3, we derive the corresponding expressions in the framework of gradient elasticity.

2. Classical elasticity

In the theory of classical elasticity, the solid angle is given as a surface integral (see, e.g., [1])

$$\Omega^0(\boldsymbol{r}) = \int_S v_i^0(\boldsymbol{R})\,\mathrm{d}S_i' = \int_V v_i^0(\boldsymbol{R})\delta_i\big(S'\big)\,\mathrm{d}V' = v_i^0(\boldsymbol{r}) * \delta_i(S), \tag{1}$$

where the vector field v_i^0 is

$$v_i^0 = -\frac{1}{2}\Delta\partial_i R = -\partial_i\frac{1}{R} = \frac{R_i}{R^3}, \tag{2}$$

while the Dirac δ-function on a surface S [19,20] is defined as

$$\delta_i(S) \equiv \int_S \delta(\boldsymbol{R})\,\mathrm{d}S_i'. \tag{3}$$

* Corresponding author. Tel.: +49(0)6151/163686; fax: +49(0)6151/163681.
E-mail address: lazar@fkp.tu-darmstadt.de (M. Lazar).

0375-9601/$ – see front matter
http://dx.doi.org/10.1016/j.physleta.2013.12.018

The relative radius vector $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}'$ connects a source point $\boldsymbol{r}'$ on the loop to a field point $\boldsymbol{r}$ and $R = |\boldsymbol{R}|$ denotes the norm of $\boldsymbol{R}$. Here S denotes an arbitrary smooth surface enclosed by the loop L, $\mathrm{d}S_i'$ is an oriented surface element, $\Omega^0(\boldsymbol{r})$ is the solid angle under which the loop L is seen from the point $\boldsymbol{r}$, and $*$ denotes the spatial convolution. The vector field (2) is analogous to the magnetic field of a magnetic monopole fixed at the origin (e.g., [12,13]). The divergence of the vector field (2) yields

$$\partial_i v_i^0 = -\frac{1}{2}\Delta\Delta R = 4\pi\delta(\boldsymbol{R}), \tag{4}$$

since

$$\Delta\Delta R = -8\pi\delta(\boldsymbol{R}). \tag{5}$$

The solid angle Ω^0 is a multi-valued quantity with the residue 4π. Thus, the solid angle Ω^0 changes by 4π when the field point crosses the surface S. In particular, this happens for a Burgers circuit that encircles L. In other words, S represents the surface of discontinuity. Notice that, in classical elasticity, the plastic distortion caused by a dislocation loop is concentrated at the surface S. From a physical viewpoint, S represents the area swept by the loop L during its motion and may be called the slip surface. Thus, the surface S is what determines the history of the plastic distortion of a dislocation loop (see, e.g., [1,19]).

We may use the Stokes theorem to arrive at a line integral over L for the solid angle. To do so, it is necessary to express v_i^0 as the curl of a "vector potential" A_k^0. However, Eq. (4) shows that the divergence of the vector field v_i^0 is not identically zero, and therefore it becomes impossible to write v_i^0 everywhere as the curl of a vector potential. Nevertheless, introducing a so-called fictitious vector field $v_i^{(f)0}$, which is sometimes called "string of singularity", (see, e.g., [12,13]) having the property

$$\partial_i v_i^{(f)0} = -\partial_i v_i^0, \tag{6}$$

a vector potential A_k^0 may be introduced for the divergenceless sum $v_i^0 + v_i^{(f)0}$:

$$v_i^0 + v_i^{(f)0} = \epsilon_{ijk}\partial_j A_k^0. \tag{7}$$

Subtraction of the fictitious vector field in Eq. (7) leads to the physical vector field v_i^0 given by

$$v_i^0 = \epsilon_{ijk}\partial_j A_k^0 - v_i^{(f)0}. \tag{8}$$

Taking the curl of Eq. (7) and imposing the "Coulomb gauge" $\partial_k A_k^0 = 0$, we find an inhomogeneous Laplace equation for the vector potential

$$\Delta A_k^0 = -\epsilon_{klm}\partial_l v_m^{(f)0}, \tag{9}$$

where the fictitious vector field $v_m^{(f)0}$ is the source term of the vector potential. Using the 3D Green function of the Laplace equation, $-1/(4\pi R)$, the solution of Eq. (9) reads

$$\begin{aligned} A_k^0(\boldsymbol{r}) &= \frac{1}{4\pi}\epsilon_{klm}\int_V \partial_l \frac{1}{R} v_m^{(f)0}(\boldsymbol{r}')\,\mathrm{d}V' \\ &= -\frac{1}{4\pi}\epsilon_{klm}\int_V v_l^0(\boldsymbol{R}) v_m^{(f)0}(\boldsymbol{r}')\,\mathrm{d}V'. \end{aligned} \tag{10}$$

The fictitious singular vector field $v_i^{(f)0}$ can be taken as [13,20]

$$\begin{aligned} v_i^{(f)0}(\boldsymbol{r}) &= \int_C v_{k,k}^0(\boldsymbol{r}-\boldsymbol{s})\,\mathrm{d}s_i \\ &= 4\pi\int_C \delta(\boldsymbol{r}-\boldsymbol{s})\,\mathrm{d}s_i \equiv 4\pi\delta_i(C), \end{aligned} \tag{11}$$

where C is a curve, called the "Dirac string", starting at $-\infty$ and ending at the origin and $\delta_i(C)$ is the δ-function along the Dirac string. The divergence of this field is concentrated at the endpoint of the string:

$$\partial_i v_i^{(f)0}(\boldsymbol{r}) = -4\pi\delta(\boldsymbol{r}) = -\partial_i v_i^0(\boldsymbol{r}). \tag{12}$$

Then the vector potential of the monopole (10) is given as a line integral along the path C (see, e.g., [12]):

$$A_k^0(\boldsymbol{r}) = \epsilon_{klm}\int_C v_m^0(\boldsymbol{r}-\boldsymbol{s})\,\mathrm{d}s_l = -\epsilon_{klm}\int_C \partial_m \frac{1}{|\boldsymbol{r}-\boldsymbol{s}|}\,\mathrm{d}s_l. \tag{13}$$

The fictitious vector field $v_m^{(f)0}$ is a singular field which vanishes everywhere except along the Dirac string C.

If we choose for the path C a straight line in the direction of a constant unit vector n_i, the fictitious vector field reads

$$v_i^{(f)0}(\boldsymbol{r}) = 4\pi n_i \int_{-\infty}^{0} \delta(\boldsymbol{r}-\boldsymbol{n}s)\,\mathrm{d}s, \tag{14}$$

and the vector potential of the "magnetic monopole" reduces to

$$A_k^0(\boldsymbol{r}) = \epsilon_{klm}\frac{n_l r_m}{r(r + r_i n_i)}. \tag{15}$$

Eq. (15) has the original form of the vector potential of Dirac's magnetic monopole (see, e.g., [11,12]) which was adopted by deWit [9] and Eshelby [10] for the representation of the solid angle as a line integral.

Substituting Eqs. (8) and (11) into (1) and using the Stokes theorem, we find

$$\begin{aligned} \Omega^0(\boldsymbol{r}) &= v_i^0(\boldsymbol{r}) * \delta_i(S) = \epsilon_{ijk}\partial_j A_k^0(\boldsymbol{r}) * \delta_i(S) - v_i^{(f)0}(\boldsymbol{r}) * \delta_i(S) \\ &= A_k^0(\boldsymbol{r}) * \epsilon_{kji}\partial_j\delta_i(S) - 4\pi\delta_i(C) * \delta_i(S) \\ &= A_k^0(\boldsymbol{r}) * \delta_k(L) - 4\pi\delta_i(C) * \delta_i(S), \end{aligned} \tag{16}$$

where

$$A_k^0(\boldsymbol{r}) * \delta_k(L) = \int_V A_k^0(\boldsymbol{R})\delta_k(L')\,\mathrm{d}V' = \oint_L A_k^0(\boldsymbol{R})\,\mathrm{d}L_k', \tag{17}$$

the δ-function on a closed line L [19,20]

$$\delta_i(L) \equiv \int_L \delta(\boldsymbol{R})\,\mathrm{d}L_i', \tag{18}$$

and $\epsilon_{kji}\partial_j\delta_i(S) = \delta_k(L)$. Here $\mathrm{d}L_i'$ denotes the line element at $\boldsymbol{r}'$. For the contribution of the fictitious vector field we used the formula [19,21]

$$\begin{aligned} \delta_i(L) * \delta_i(S) &= \int_S\int_L \delta(\boldsymbol{r}-\boldsymbol{r}')\,\mathrm{d}L_i'\,\mathrm{d}S_i \\ &= \begin{cases} 1, & \text{if } L \text{ crosses } S \text{ positively}, \\ 0, & \text{if } L \text{ does not cross } S, \\ -1, & \text{if } L \text{ crosses } S \text{ negatively}. \end{cases} \end{aligned} \tag{19}$$

Finally, the solid angle reduces to a line integral of the monopole vector potential (13) or (15) and a constant

$$\begin{aligned} \Omega^0(\boldsymbol{r}) &= \oint_L A_k^0(\boldsymbol{R})\,\mathrm{d}L_k' \\ &\quad - 4\pi \begin{cases} 1, & \text{if } C \text{ crosses } S \text{ positively}, \\ 0, & \text{if } C \text{ does not cross } S, \\ -1, & \text{if } C \text{ crosses } S \text{ negatively}. \end{cases} \end{aligned} \tag{20}$$