Chapter 15

PEACH-KOEHLER FORCES WITHIN THE THEORY OF NONLOCAL ELASTICITY

Markus Lazar
Laboratoire de Modélisation en Mécanique,
Université Pierre et Marie Curie,
4 Place Jussieu, Case 162,
F-75252 Paris Cédex 05, France
lazar@lmm.jussieu.fr

Abstract We consider dislocations in the framework of Eringen's nonlocal elasticity. The fundamental field equations of nonlocal elasticity are presented. Using these equations, the nonlocal force stresses of a straight screw and a straight edge dislocation are given. By the help of these nonlocal stresses, we are able to calculate the interaction forces between dislocations (Peach-Koehler forces). All classical singularities of the Peach-Koehler forces are eliminated. The extremum values of the forces are found near the dislocation line.

Keywords: Nonlocal elasticity, material force, dislocation

1. INTRODUCTION

Traditional methods of classical elasticity break down at small distances from crystal defects and lead to singularities. This is unfortunate since the defect core is a very important region in the theory of defects. Moreover, such singularities are unphysical and an improved model of defects should eliminate them. In addition, classical elasticity is a scale-free continuum theory in which no characteristic length appears. Thus, classical elasticity cannot explain the phenomena near defects and at the atomic scale.

In recent decades, a theory of elastic continuum called nonlocal elasticity has been developed. The concept of nonlocal elasticity was originally proposed by Kröner and Datta [1, 2], Edelen and Eringen [3, 4, 5], Kunin [6] and some others. This theory considers the inner structures of materials and takes into account long-range (nonlocal) interactions.

It is important to note that the nonlocal elasticity may be related to other nonstandard continuum theories like gradient theory [7, 8] and gauge theory of defects [9, 10, 11]. In all these approaches characteristic inner lengths (gradient coefficient or nonlocality parameter), which describe size (or scale) effects, appear. One remarkable feature of solutions in nonlocal elasticity, gradient theory and gauge theory is that the stress singularities which appear in classical elasticity are eliminated. These solutions depend on the characteristic inner length, and they lead to finite stresses. Therefore, they are applicable up to the atomic scale.

In this paper, we investigate the nonlocal force due to dislocations (nonlocal Peach-Koehler force). We consider parallel screw and edge dislocations. The classical singularity of Peach-Koehler force is eliminated and a maximum/minimum is obtained.

2. FUNDAMENTAL FIELD EQUATIONS

The fundamental field equations for an isotropic, homogeneous, nonlocal and infinite extended medium with vanishing body force and static case have been given by the nonlocal theory [3, 4, 5]

$$\begin{aligned} &\partial_j \sigma_{ij} = 0, \\ &\sigma_{ij}(r) = \int_V \alpha(r - r')\, \overset{\circ}{\sigma}_{ij}(r')\, \mathrm{d}v(r'), \\ &\overset{\circ}{\sigma}_{ij} = 2\mu \left(\overset{\circ}{\epsilon}_{ij} + \frac{\nu}{1-2\nu}\, \delta_{ij} \overset{\circ}{\epsilon}_{kk} \right), \end{aligned} \tag{1}$$

where μ, ν are shear modulus and Poisson's ration, respectively. In addition, $\overset{\circ}{\epsilon}_{ij}$ is the classical strain tensor, $\overset{\circ}{\sigma}_{ij}$ and σ_{ij} are the classical and nonlocal stress tensors, respectively. The $\alpha(r)$ is a nonlocal kernel. The field equation in nonlocal elasticity of the stress in an isotropic medium is the following inhomogeneous Helmholtz equation

$$\Big(1 - \kappa^{-2}\Delta\Big)\sigma_{ij} = \overset{\circ}{\sigma}_{ij}, \tag{2}$$

where $\overset{\circ}{\sigma}_{ij}$ is the stress tensor obtained for the same traction boundary-value problem within the "classical" theory of dislocations. The factor κ^{-1} has the physical dimension of a length and it, therefore, defines an internal characteristic length. If we consider the two-dimensional problem and using Green's function of the two-dimensional Helmholtz equation (2), we may solve the field equation for every component of the stress field (2) by the help of the convolution integral and the two-dimensional Green function

$$\alpha(r-r') = \frac{\kappa^2}{2\pi} K_0\big(\kappa\sqrt{(x-x')^2+(y-y')^2}\big). \tag{3}$$

Here K_n is the modified Bessel function of the second kind and $n = 0, 1, \ldots$ denotes the order of this function. Thus,

$$\Big(1-\kappa^{-2}\Delta\Big)\alpha(r) = \delta(r), \tag{4}$$

where $\delta(r) := \delta(x)\delta(y)$ is the two-dimensional Dirac delta function. In this way, we deduce Eringen's so-called nonlocal constitutive relation for a linear homogeneous, isotropic solid with Green's function (3) as the nonlocal kernel. This kernel (3) has its maximum at $r = r'$ and describes the nonlocal interaction. Its two-dimensional volume-integral yields

$$\int_V \alpha(r-r')\,\mathrm{d}v(r) = 1, \tag{5}$$

which is the normalization condition of the nonlocal kernel. In the classical limit ($\kappa^{-1} \to 0$), it becomes the Dirac delta function

$$\lim_{\kappa^{-1}\to 0} \alpha(r-r') = \delta(r-r'). \tag{6}$$

In this limit, Eq. (1) gives the classical expressions. Note that Eringen [4, 5] found the two-dimensional kernel (3) by giving the best match with the Born-Kármán model of the atomic lattice dynamics and the atomistic dispersion curves. He used the choice $e_0 = 0.39$ for the length, $\kappa^{-1} = e_0\,a$, where a is an internal length (e.g. atomic lattice parameter) and e_0 is a material constant.

3. NONLOCAL STRESS FIELDS OF DISLOCATIONS

Let us first review the nonlocal stress fields of screw and edge dislocations in an infinitely extended body. The dislocation lines are along the z-axis. The nonlocal stress components of a straight screw dislocation with the Burgers vector $\mathbf{b} = (0, 0, b_z)$ is given by [4, 5, 7, 10]

$$\sigma_{xz} = -\frac{\mu b_z}{2\pi}\frac{y}{r^2}\Big\{1-\kappa r K_1(\kappa r)\Big\}, \quad \sigma_{yz} = \frac{\mu b_z}{2\pi}\frac{x}{r^2}\Big\{1-\kappa r K_1(\kappa r)\Big\}, \tag{7}$$

where $r = \sqrt{x^2 + y^2}$. The nonlocal stress of a straight edge dislocation with the Burgers vector $\mathbf{b} = (b_x, 0, 0)$ turns out to be [7, 11]

$$\sigma_{xx} = -\frac{\mu b_x}{2\pi(1-\nu)} \frac{y}{r^4}\Big\{ (y^2 + 3x^2) + \frac{4}{\kappa^2 r^2}(y^2 - 3x^2) - 2y^2 \kappa r K_1(\kappa r) - 2(y^2 - 3x^2) K_2(\kappa r)\Big\},$$

$$\sigma_{yy} = -\frac{\mu b_x}{2\pi(1-\nu)} \frac{y}{r^4}\Big\{ (y^2 - x^2) - \frac{4}{\kappa^2 r^2}(y^2 - 3x^2) - 2x^2 \kappa r K_1(\kappa r) + 2(y^2 - 3x^2) K_2(\kappa r)\Big\},$$

$$\sigma_{xy} = \frac{\mu b_x}{2\pi(1-\nu)} \frac{x}{r^4}\Big\{ (x^2 - y^2) - \frac{4}{\kappa^2 r^2}(x^2 - 3y^2) - 2y^2 \kappa r K_1(\kappa r) + 2(x^2 - 3y^2) K_2(\kappa r)\Big\},$$

$$\sigma_{zz} = -\frac{\mu b_x \nu}{\pi(1-\nu)} \frac{y}{r^2}\Big\{ 1 - \kappa r K_1(\kappa r)\Big\}. \tag{8}$$

It is obvious that there is no singularity in (7) and (8). For example, when r tends to zero, the stresses $\sigma_{ij} \to 0$. It also can be found that the far-field expression ($r > 12\kappa^{-1}$) of Eqs. (7) and (8) return to the stresses in classical elasticity. Of course, the stress fields (7) and (8) fulfill Eq. (2) and correspond to the nonlocal kernel (3).

4. PEACH-KOEHLER FORCES DUE TO DISLOCATIONS

The force between dislocations, according to Peach-Koehler formula in nonlocal elasticity [12], is given by

$$F_k = \varepsilon_{ijk}\sigma_{in} b'_n \xi_j, \tag{9}$$

where b'_n is the component of Burgers vector of the 2nd dislocation at the position r and ξ_j is the direction of the dislocation. Obviously, Eq. (9) is quite similar in the form as the classical expression of the Peach-Koehler force. Only the classical stress is replaced by the nonlocal one. Eq. (9) is particularly important for the interaction between dislocations.

4.1. PARALLEL SCREW DISLOCATIONS

We begin our considerations with the simple case of two parallel screw dislocations. For a screw dislocation with $\xi_z = 1$ we have in Cartesian

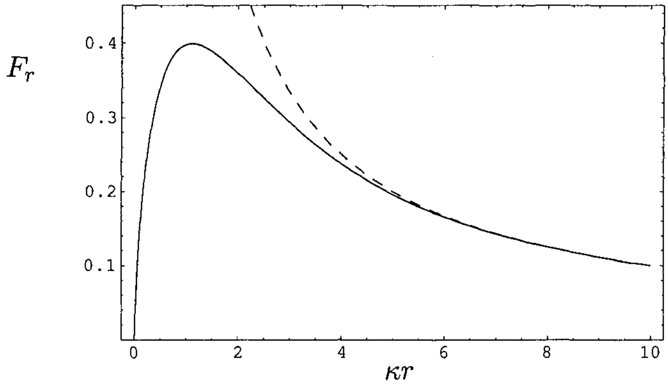

Figure 15.1. The Peach-Koehler force between screw dislocations is given in units of $\mu\kappa b_z b'_z/[2\pi]$. Nonlocal elasticity (solid) and classical elasticity (dashed).

coordinates

$$F_x = \sigma_{yz} b'_z = \frac{\mu b_z b'_z}{2\pi} \frac{x}{r^2} \Big\{1 - \kappa r K_1(\kappa r)\Big\},$$
$$F_y = -\sigma_{xz} b'_z = \frac{\mu b_z b'_z}{2\pi} \frac{y}{r^2} \Big\{1 - \kappa r K_1(\kappa r)\Big\}, \tag{10}$$

and in cylindrical coordinates

$$F_r = F_x \cos\varphi + F_y \sin\varphi = \frac{\mu b_z b'_z}{2\pi r} \Big\{1 - \kappa r K_1(\kappa r)\Big\},$$
$$F_\varphi = F_y \cos\varphi - F_x \sin\varphi = 0. \tag{11}$$

Thus, the force between two screw dislocations is also a radial force in the nonlocal case. The force expression (11) has some interesting features. A maximum of F_r can be found from Eq. (11) as

$$|F_r|_{\max} \simeq 0.399\kappa \frac{\mu b_z b'_z}{2\pi}, \quad \text{at} \quad r \simeq 1.114\kappa^{-1}. \tag{12}$$

When the nonlocal atomistic effect is neglected, $\kappa^{-1} \to 0$, Eq. (11) gives the classical result

$$F_r^{cl} = \frac{\mu b_z b'_z}{2\pi r}. \tag{13}$$

To compare the classical force with the nonlocal one, the graphs from Eqs. (11) and (13) are plotted in Fig. 15.1. It can be seen that near the dislocation line the nonlocal result is quite different from the classical one. Unlike the classical expression, which diverges as $r \to 0$ and gives an infinite force, it is zero at $r = 0$. For $r > 6\kappa^{-1}$ the classical and the nonlocal expressions coincide.

4.2. PARALLEL EDGE DISLOCATIONS

We analyze now the force between two parallel edge dislocations with (anti)parallel Burgers vector. For an edge dislocation with $\xi_z = 1$ with Burgers vector b'_x we have in Cartesian coordinates

$$F_x = \sigma_{yx} b'_x = \frac{\mu b_x b'_x}{2\pi(1-\nu)} \frac{x}{r^4} \Big\{ (x^2 - y^2) - \frac{4}{\kappa^2 r^2}(x^2 - 3y^2) - 2y^2 \kappa r K_1(\kappa r) + 2(x^2 - 3y^2) K_2(\kappa r) \Big\}, \tag{14}$$

$$F_y = -\sigma_{xx} b'_x = \frac{\mu b_x b'_x}{2\pi(1-\nu)} \frac{y}{r^4} \Big\{ (y^2 + 3x^2) + \frac{4}{\kappa^2 r^2}(y^2 - 3x^2) - 2y^2 \kappa r K_1(\kappa r) - 2(y^2 - 3x^2) K_2(\kappa r) \Big\}.$$

F_x is the driving force for conservative motion (gliding) and F_y is the climb force. The glide force has a maximum/minimum in the slip plane (zx-plane) of

$$|F_x(x,0)| \simeq 0.260\kappa \frac{\mu b_x b'_x}{2\pi(1-\nu)}, \quad \text{at} \quad |x| \simeq 1.494\kappa^{-1}. \tag{15}$$

The maximum/minimum of the climb force is found as

$$|F_y(0,y)| \simeq 0.546\kappa \frac{\mu b_x b'_x}{2\pi(1-\nu)}, \quad \text{at} \quad |y| \simeq 0.996\kappa^{-1}. \tag{16}$$

It can be seen that the maximum of the climb force is greater than the maximum of the glide force (see Fig. 15.2). The glide force F_x is zero at $x = 0$ ($\varphi = \frac{1}{2}\pi$). This corresponds to one equilibrium configuration of the two edge dislocations. In classical elasticity the glide force is also zero at the position $x = y$ ($\varphi = \frac{1}{4}\pi$). But in nonlocal elasticity we obtain from Eq. (14) the following expression for the glide force

$$F_x(\varphi = \pi/4) = \frac{\mu b_x b'_x \sqrt{2}}{4\pi(1-\nu)} \frac{1}{r} \Big\{ \frac{4}{\kappa^2 r^2} - \kappa r K_1(\kappa r) - 2K_2(\kappa r) \Big\}. \tag{17}$$

Its maximum is

$$|F_x(\varphi = \pi/4)|_{\max} \simeq 0.151\kappa \frac{\mu b_x b'_x \sqrt{2}}{4\pi(1-\nu)}, \quad \text{at} \quad r \simeq 0.788\kappa^{-1}. \tag{18}$$

The $F_x(\varphi = \pi/4)$ gives only a valuable contribution in the region $r \lessapprox 12\kappa^{-1}$. Therefore, only for $r > 12\kappa^{-1}$ the position $\varphi = \frac{1}{4}\pi$ is an equilibrium configuration. The climb force F_y is zero at $y = 0$.

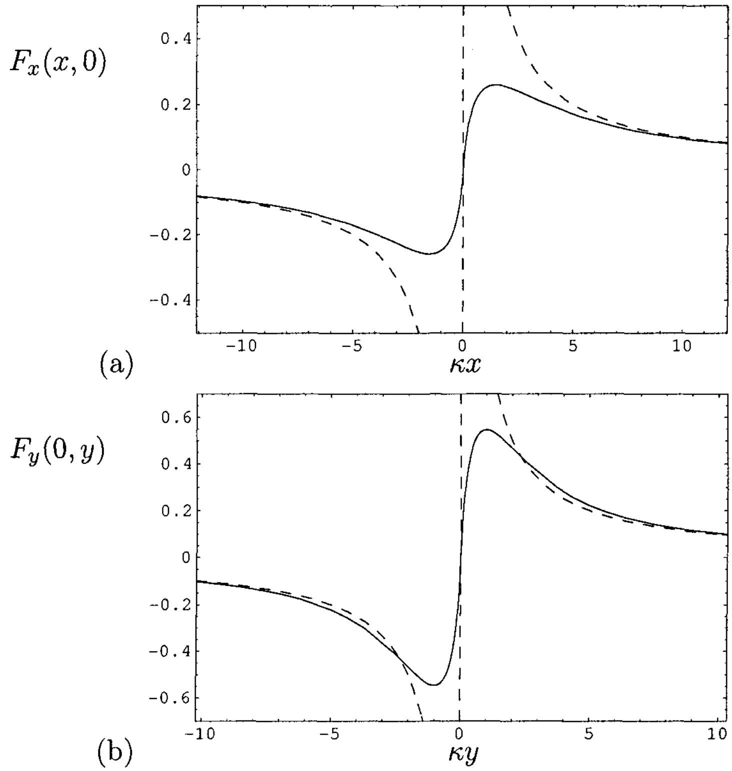

Figure 15.2. The glide and climb force components near the dislocation line: (a) $F_x(x, 0)$ and (b) $F_y(0, y)$ are given in units of $\mu b_x b'_x \kappa/[2\pi(1-\nu)]$. The dashed curves represent the classical force components.

From Eq. (14) the force can be given in cylindrical coordinates as

$$F_r = \frac{\mu b_x b'_x}{2\pi(1-\nu)} \frac{1}{r}\left\{\Big(1 - \kappa r K_1(\kappa r)\Big) - \cos 2\varphi\left(\frac{4}{\kappa^2 r^2} - \kappa r K_1(\kappa r) - 2K_2(\kappa r)\right)\right\},$$

$$F_\varphi = \frac{\mu b_x b'_x}{2\pi(1-\nu)} \frac{\sin 2\varphi}{r}\left\{1 - \frac{4}{\kappa^2 r^2} + 2K_2(\kappa r)\right\}. \qquad (19)$$

The force between edge dislocations is not a central force because a tangential component F_φ exists. Both the components F_r and F_φ depend on r and φ. The dependence of φ in F_r is a new feature of the nonlocal result (19) not present in the classical elasticity. Unlike the "classical" case, the force F_r is only zero at $r = 0$ and F_φ is zero at $r = 0$ and $\varphi = 0$, $\frac{1}{2}\pi$, π, $\frac{3}{2}\pi$, 2π. The force F_r in (19) has an interesting dependence of the angle φ. In detail, we obtain

$$\text{(i) } \varphi = 0,\, \pi: \quad F_r = \frac{\mu b_x b'_x}{2\pi(1-\nu)} \frac{1}{r}\left\{1 - \frac{4}{\kappa^2 r^2} + 2K_2(\kappa r)\right\}, \tag{20}$$

$$|F_r|_{\max} \simeq 0.260\, \frac{\mu b_x b'_x \kappa}{2\pi(1-\nu)}, \quad \text{at} \quad r \simeq 1.494\kappa^{-1},$$

$$\text{(ii) } \varphi = \frac{\pi}{4}, \frac{3\pi}{4}, \frac{5\pi}{4}, \frac{7\pi}{4}: F_r = \frac{\mu b_x b'_x}{2\pi(1-\nu)} \frac{1}{r}\{1 - \kappa r K_1(\kappa r)\}, \tag{21}$$

$$|F_r|_{\max} \simeq 0.399\, \frac{\mu b_x b'_x \kappa}{2\pi(1-\nu)}, \quad \text{at} \quad r \simeq 1.114\kappa^{-1},$$

$$\text{(iii) } \varphi = \frac{\pi}{2}, \frac{3\pi}{2}: F_r = \frac{\mu b_x b'_x}{2\pi(1-\nu)} \frac{1}{r}\left\{1 + \frac{4}{\kappa^2 r^2} - 2\kappa r K_1(\kappa r) - 2K_2(\kappa r)\right\},$$

$$|F_r|_{\max} \simeq 0.547\, \frac{\mu b_x b'_x \kappa}{2\pi(1-\nu)}, \quad \text{at} \quad r \simeq 0.996\kappa^{-1}. \tag{22}$$

On the other hand, F_φ has a maximum at $\varphi = \frac{1}{4}\pi, \frac{5}{4}\pi$ and a minimum at $\varphi = \frac{3}{4}\pi, \frac{7}{4}\pi$. They are

$$|F_\varphi| \simeq 0.260\kappa \frac{\mu b_x b'_x}{2\pi(1-\nu)}, \quad \text{at} \quad r \simeq 1.494\kappa^{-1}. \tag{23}$$

The classical result for the force reads in cylindrical coordinates

$$F_r^{cl} = \frac{\mu b_x b'_x}{2\pi(1-\nu)} \frac{1}{r}, \quad F_\varphi^{cl} = \frac{\mu b_x b'_x}{2\pi(1-\nu)} \frac{\sin 2\varphi}{r}. \tag{24}$$

To compare the nonlocal result with the classical one, diagrams of Eqs. (19) and (24) are drawn in Fig. 15.3. The force calculated in nonlocal elasticity is different from the classical one near the dislocation line at $r = 0$. It is finite and has no singularity in contrast to the classical result. For $r > 12\kappa^{-1}$ the classical and the nonlocal expressions coincide.

5. CONCLUSION

The nonlocal theory of elasticity has been used to calculate the Peach-Koehler force due to screw and edge dislocations in an infinitely extended body. The Peach-Koehler force calculated in classical elasticity is infinite near the dislocation core. The reason is that the classical elasticity is invalid in dealing with problems of micro-mechanics. The nonlocal elasticity gives expressions for the Peach-Koehler force which are physically more reasonable. The forces due to dislocations have no singularity.

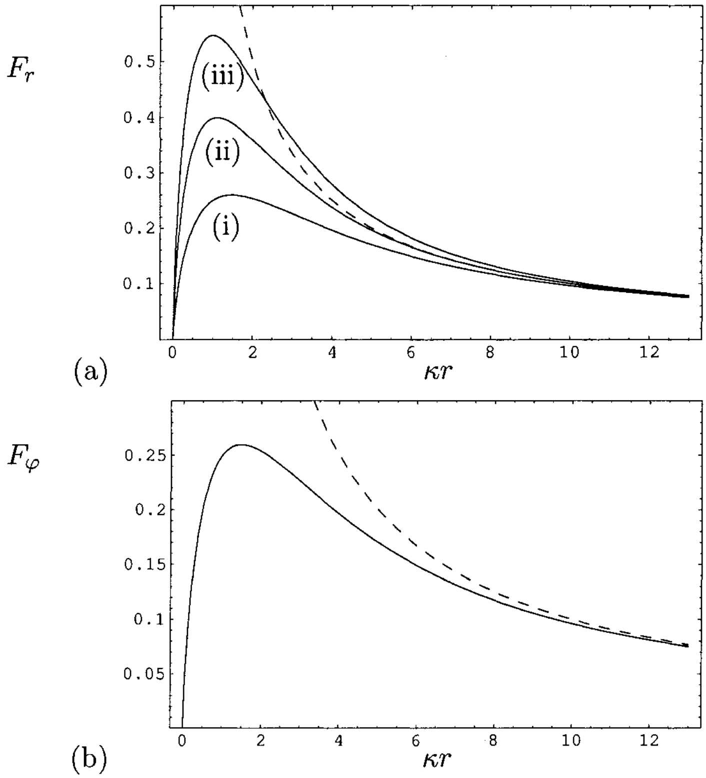

Figure 15.3. The force near the dislocation line: (a) F_r and (b) F_φ with $\varphi = \frac{1}{4}\pi$, $\frac{5}{4}\pi$ are given in units of $\mu b_x b'_x \kappa / [2\pi(1-\nu)]$. The dashed curves represent the classical force components.

They are zero at $r = 0$ and have maxima or minima in the dislocation core. The finite values of the force due to dislocations may be used to analyze the interaction of dislocations from the micro-mechanical point of view.

Acknowledgments

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