

## Nonlinear elastic problems in dislocation theory: a gauge approach

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1991 J. Phys. A: Math. Gen. 24 3237

(<http://iopscience.iop.org/0305-4470/24/14/012>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 01/06/2010 at 11:02

Please note that [terms and conditions apply](#).

## Nonlinear elastic problems in dislocation theory: a gauge approach

V A Osipov

Joint Institute for Nuclear Research, Laboratory of Theoretical Physics, Head Post Office  
PO Box 79, Moscow, USSR

Received 25 February 1991

**Abstract.** In the framework of the nonlinear theory of elasticity the new perturbation method based on the gauge approach is developed to study static dislocations continuously distributed in materials. The self-consistent system of field equations for defect dynamics is presented up to the second-order approximation. The solution for the straight screw dislocations is obtained. The problem of an electron localization in crystals with screw dislocations is considered. The localized electron states are found to appear only in the second-order approximation for  $M = 0$  where  $M$  is the angular quantum number.

### 1. Introduction

The gauge theory of defects is one of the modern trends in elasticity theory [1-3]. The Edelen and Kadić (EK) gauge model constructed first in 1983 [1] allows us to study both the elastic properties of materials with continuously distributed dislocations and disclinations and the defect dynamics. The field equations of defect dynamics presented in [1] are essentially nonlinear in their origin, so we are, in fact, dealing with nonlinear theory. Nonlinear elastic problems in dislocation theory have been investigated for a long time (see, e.g., [4] and references therein). Several different methods which employ the nonlinear theory of elasticity for treating dislocation theory are known at present time. Two of them were developed especially to determine the stress and strain fields generated by dislocations continuously distributed in materials [5-7]. For convenience, in the following we shall refer to a recent review [4] where the full details of both methods can be found.

It is clear that the exact solutions of a system of coupled nonlinear differential equations of defect dynamics are of most interest. Unfortunately, such solutions have not yet been obtained. The only known exact monopole-like solution found recently (see [8]) is for static disclinations in the framework of the EK gauge model. This solution gives us information about the core of the disclinations (the core radius is found to depend on the model parameters). Otherwise, perturbation methods should be used.

The approximation procedure, based on a homogeneous scaling of the gauge group generators, was developed in [1]. It was shown that in the first-order approximation elasticity theory is recovered, in the second-order dislocation dynamics is modelled, whereas in the third-order both the dislocation and disclination dynamics are modelled. Note that even the linearized system of equations for defect dynamics is difficult to solve in most cases. For further simplification one can put all the elastic displacement

variables equal to zero. In this case, the characteristic phenomena are described by solutions with singularities and, in the first-order approximation, the static solutions for edge and screw dislocations are found to be in agreement with classical ones [1].

The purpose of the present paper is to show that the EK gauge model allows us to study the dislocation problems in the higher order approximations fairly easily even if we put all the elastic displacement variables equal to zero. The plan of the paper is as follows. In section 2 we construct the general scheme and consider the governing equations as well as the constitutive relationships up to the second-order approximation. The method for determining the stress and strain fields is illustrated in section 3 using as an example the straight-screw dislocations in an isotropic elastic medium. In section 4 we study the problem of an electron localization in materials with screw dislocations where the importance of the second-order solutions is demonstrated. Section 5 is devoted to concluding comments.

### 2. The general scheme

Let us start from the Lagrangian that is invariant under the inhomogeneous action of the gauge translational group T(3) and takes the following form [1]:

$$L = L_\chi + L_\phi \tag{1}$$

where

$$L_\chi = (\rho_0/2) B_A^i \delta_{ij} B_B^j - [\lambda (E_{AB} \delta^{AB})^2 + 2\mu E_{AB} \delta^{AC} \delta^{BD} E_{CD}] / 8 \tag{2}$$

describes the elastic properties of the material, and

$$L_\phi = -(s_1/2) \delta_{ij} D_{ab}^i k^{ac} k^{bd} D_{cd}^j \tag{3}$$

describes the dislocations.

The strain tensor in (2) is determined to be

$$E_{AB} = B_A^i \delta_{ij} B_B^j - \delta_{AB} \tag{4}$$

where

$$B_a^i = \partial_a \chi^i + \phi_a^i \tag{5}$$

is the distortion tensor. In (5)  $\partial_a \chi^i$  describes the integrable part of the distortion, and the second term arises from the breaking of the homogeneity of the action of the translation group T(3). The state vector  $\chi^i(X^a) = \chi^i(X^A, T)$  in (5) characterizes the configuration at time  $T$  in terms of the coordinate cover  $(X^A)$  of a reference configuration, and  $\phi_a^i$  are associated with dislocation fields. Tensor  $D_{ab}^i$  in (3) is determined as follows:

$$D_{ab}^i = \partial_a \phi_b^i - \partial_b \phi_a^i. \tag{6}$$

In (2) and (3)  $\lambda$  and  $\mu$  are the Lamé constants,  $\rho_0$  is the mass density in the reference configuration,  $s_1$  is the coupling constant,  $k^{AB} = -\delta^{AB}$ ,  $k^{44} = 1/y$  and  $k^{ab} = 0$  for  $a \neq b$  and  $y$  is the positive 'propagation parameter'. The equations of balance of the linear momentum have the form well known in a classical elasticity theory

$$\partial_a p_i - \partial_A \sigma_i^A = 0 \tag{7}$$

where the explicit expression for the stress tensor

$$\sigma_i^A = (\frac{1}{2}) \delta_B^A \delta_{ij} (\partial_C \chi^j + \phi_C^j) (\lambda \delta^{BC} \delta^{FD} E_{FD} + 2\mu \delta^{RB} \delta^{SC} E_{RS}) \tag{8}$$

and the momentum

$$p_i = \rho_0 \delta_{ij} (\partial_4 \chi^j + \phi_4^j). \tag{9}$$

The Euler-Lagrange equations with respect to  $\phi_a^i$  are

$$\delta_{ij} \delta^{BD} [\partial^A (\partial_A \phi_D^i - \partial_D \phi_A^i) - (1/y) \partial_4 (\partial_4 \phi_D^i - \partial_D \phi_4^i)] = (1/2s_1) \sigma_j^B \tag{10}$$

and

$$(1/y) \delta_{ij} \partial^A (\partial_A \phi_4^i - \partial_4 \phi_A^i) = (1/2s_1) p_j. \tag{11}$$

Restricting our attention to the static case, we reduce (7) to (11) to the form

$$\partial_A \Sigma_i^A = 0 \quad \text{and} \quad \delta_{ij} \delta^{BD} \partial^A (\partial_A \phi_D^i - \partial_D \phi_A^i) = \kappa^2 \Sigma_j^B \tag{12}$$

where  $\Sigma_E^m = (1/\mu) \sigma_E^m$  and  $\kappa^2 = \mu/2s_1$ . In general, we must solve the system (12) together with the constitutive relations (4) and (8). Surely, it is a difficult problem. Instead, we shall use the linearization procedure based on the scaling of the gauge group generators. Following [1], let us introduce the displacements  $u^i(X^B)$  by the substitution  $\chi^i(X^B) = \delta_A^i X^A + u^i(X^B)$  and then put all the elastic displacements equal to zero. With the scaling parameter  $\varepsilon$ , the components of the distortion tensor can be written as  $B_A^i = \partial_A \chi^i + \varepsilon \phi_A^i$ , or, in our case,  $B_A^i = \delta_A^i + \varepsilon \phi_A^i$ , where  $\phi_A^i$  is expanded in the series in ascending powers of  $\varepsilon$ :  $\phi_A^i = {}_0\phi_A^i + \varepsilon_1 \phi_A^i + \varepsilon^2 {}_2\phi_A^i + \dots$

Substituting this expansion in (4) and (8), we obtain that both  $E_{AB}$  and  $\Sigma_i^A$  can be expressed as a power series in a parameter  $\varepsilon$

$$E_{AB} = \sum_{n=1}^{\infty} \varepsilon^n E_{AB} \quad \Sigma_i^A = \sum_{n=1}^{\infty} \varepsilon^n \Sigma_i^A \tag{13}$$

in which

$${}_1E_{AB} = 2{}_0\phi_A^i \delta_{iB} \tag{13a}$$

$${}_2E_{AB} = 2{}_1\phi_A^i \delta_{iB} + {}_0\phi_A^i \delta_{ij} {}_0\phi_B^j \tag{13b}$$

$${}_1\Sigma_i^A = (1/\mu) {}_1\sigma_i^A = {}_1E_{SB} \delta_i^B \delta^{SA} + (L/2) \delta_i^A \delta^{FD} {}_1E_{FD} \tag{13c}$$

$${}_2\Sigma_i^A = {}_2E_{SB} \delta_i^B \delta^{SA} + {}_0\phi_B^j \delta_{ji} \delta^{BD} \delta^{SA} {}_1E_{DS} + (L/2) (\delta_i^A \delta^{FD} {}_2E_{FD} + {}_0\phi_B^j \delta_{ji} \delta^{AB} \delta^{FD} {}_1E_{FD}). \tag{13d}$$

Here  $L = \lambda/\mu$ , and we have used the explicit gauge conditions  $\phi_2^1 = \phi_1^2$ ,  $\phi_3^1 = \phi_1^3$  and  $\phi_3^2 = \phi_2^3$  that are convenient in our analysis (see [1]).

Let us note that the equilibrium equations  $\partial_A \Sigma_i^A = 0$  must be satisfied in any order approximation. The remaining field equations in (12) take the following form:

$$\delta_{ij} \delta^{BD} \partial^A (\partial_{A0} \phi_D^i - \partial_{D0} \phi_A^i) = \kappa^2 {}_1\Sigma_j^B \quad \text{(first order)} \tag{14a}$$

$$\delta_{ij} \delta^{BD} \partial^A (\partial_{A1} \phi_D^i - \partial_{D1} \phi_A^i) = \kappa^2 {}_2\Sigma_j^B \quad \text{(second order)}. \tag{14b}$$

A general plan for a solution, which can be applied to any order approximation, has been presented in [1]. Namely, first we must find classes of solutions of the equilibrium equations. Next, solve (13c) and (13d) for the  $\phi$ s in terms of the  $\Sigma$ s. Finally, obtain the  $\phi$ s as explicit functions of position by solving the governing equations (14a) and (14b).

For the sake of simplicity, we confine our attention here to problems with axial orientation. This is the case for edge and screw dislocations which are of interest here.

We assume that the problem depends upon  $X$  and  $Y$  only, i.e.  $\partial(\dots)/\partial z = 0$ . Then, the suitable form for  ${}_n\Sigma_A^i$  that satisfies the equilibrium equations can be chosen as

$${}_n\Sigma_A^i = \begin{pmatrix} \partial_{yn}^2 g & -\partial_y \partial_{xn} g & -\partial_{yn} f \\ -\partial_y \partial_{xn} g & \partial_{xn}^2 g & \partial_{xn} g \\ -\partial_{yn} f & \partial_{xn} f & {}_n p \end{pmatrix}. \tag{15}$$

At this stage, functions  ${}_n g = {}_n g(x, y)$ ,  ${}_n f = {}_n f(x, y)$  and  ${}_n p = {}_n p(x, y)$  are supposed to be arbitrary, and  $\partial_x = \partial/\partial x$ ,  $\partial_x^2 = \partial^2/\partial x^2$ .

Let us consider the first-order approximation. Using (13a) we can rewrite (13c) as

$$2_0\phi_A^i = {}_1\Sigma_A^i - L\delta_A^i \text{Tr } {}_0\phi \tag{16}$$

where we have taken the symmetrical form of (15) into account, and  $\text{Tr } {}_0\phi = \delta_{i0}^B \phi_B^i$ . From (16) one obtains that

$$2_0\phi_A^i = {}_1\Sigma_A^i - a\delta_A^i \text{Tr } {}_1\Sigma \tag{17}$$

where  $a = L/(3L+2) = \nu/(\nu+1)$ , and  $\nu$  is the Poisson constant. As follows from (15),  $\text{Tr } {}_1\Sigma = \Delta_1 g + {}_1 p$  with  $\Delta = \partial_x^2 + \partial_y^2$ . Thus, the strain-stress relationships take the form

$${}_1 E_{AB} = {}_1\Sigma_A^i \delta_B^i - a\delta_{AB}(\Delta_1 g + {}_1 p). \tag{18}$$

It should be noted that both the governing equations (14a) and relationships (18) are just the same as those obtained using the method described in Kr oner *et al* (see [4]). To compare their expressions with ours, one must take into account the fact that, first,  $E_{AB}$  in [4] is twice the usual determination of the strain tensor and second, the dislocation density  $\alpha^{Ai}$  may be introduced as in [1]:  $\alpha^{Ai} = \epsilon^{ABC}(\partial_B \phi_C^i - \partial_C \phi_B^i)$ .

Let us consider the second-order approximation. The solutions of the first-order approximation are supposed to be known, and we must determine  ${}_1\phi_A^i$  as functions of  ${}_2\Sigma_A^i$ , i.e. solve (13d). Performing straightforward calculations, we finally obtain

$$2_1\phi_A^i = {}_2\Sigma_A^i - a\delta_A^i(\text{Tr } {}_2\Sigma) - F_A^i + G_A^i \tag{19}$$

where

$$F_A^i = 3_0\phi_B^i \delta_{k0}^B \phi_A^k + L_0\phi_A^i \text{Tr } {}_0\phi \tag{20}$$

$$G_A^i = a\delta_A^i [2_0\phi_E^k \delta_{kl} \delta^{ED} {}_0\phi_D^l + L(\text{Tr } {}_0\phi)^2] \tag{21}$$

and  $\text{Tr } {}_2\Sigma = \Delta_2 g + {}_2 p$ . Substituting (19) in (14b), we obtain the governing equations in the second-order approximation

$$\partial_y^2 [(1-a)\Delta_2 g - a_2 p - (F_1^i - G_1^i)] + \partial_x \partial_y F_2^1 = 2\kappa^2 \partial_y^2 g \tag{22a}$$

$$\partial_x^2 [(1-a)\Delta_2 g - a_2 p - (F_2^i - G_2^i)] + \partial_x \partial_y F_2^1 = 2\kappa^2 \partial_x^2 g \tag{22b}$$

$$(1-a)\Delta_2 p - a\Delta\Delta_2 g - \Delta(F_3^i - G_3^i) = 2\kappa^2 {}_2 p \tag{23}$$

and

$$\Delta_2 f = 2\kappa^2 {}_2 f. \tag{24}$$

Note that the equation for determining  ${}_2 f$  is removed from the system. Summing (23a) and (23b), we obtain

$$\Delta[(1-a)\Delta_2 g - a_2 p - 2\kappa^2 {}_2 g] = \Psi(x, y) \tag{25}$$

$$(1-a)\Delta_2 p - a\Delta\Delta_2 g - 2\kappa^2 {}_2 p = \Phi(x, y) \tag{26}$$

where

$$\Psi(x, y) = \partial_y^2(F_1^1 - G_1^1) + \partial_x^2(F_2^2 - G_2^2) - 2\partial_x\partial_y F_2^1$$

and  $\Phi(x, y) = \Delta(F_3^3 - G_3^3)$ . In addition to (25) and (26), one of equations (22a) and (22b) must be satisfied. Clearly, the general solution of (25) and (26) is still complex. It should be noted, however, that thus far we have considered  $\kappa$  to be an arbitrary parameter. This parameter characterizes the ratio of the elastic energy to the dislocation one. As has been mentioned in [1], the different choices for the order of  $\epsilon$  of the ratio  $\mu/s_1$  lead to models describing different phenomena. The classical results of the elasticity theory may be obtained in the physically meaningful limit  $\kappa \rightarrow 0$  (or, more precisely,  $\kappa^2 \sim \epsilon$ ). As can be seen, for  $\kappa^2 \sim \epsilon$  the second-order approximation equations (25) and (26) must be rewritten in the following form:

$$\Delta\Delta_2g = \frac{1-a}{1-2a} \left[ \Psi(x, y) + \frac{a}{1-a} \Phi(x, y) + 2\kappa^2 \left( \Delta_1g + \frac{a}{1-a} {}_1p \right) \right] \tag{27}$$

$$\Delta_2p = \frac{1}{1-a} [a\Delta\Delta_2g + \Phi(x, y) + 2\kappa^2 {}_1p] \tag{28}$$

where (27) serves to determine  ${}_2g$  whereas (28) allows us to determine  ${}_2p$  in terms of  ${}_2g$ . Thus, we can obtain the full solution of the problem for  $\kappa^2 \sim \epsilon$ . Let us realize this programme for a concrete example.

### 3. An example: straight screw dislocations

In the framework of the gauge model the first-order approximation for the straight screw dislocations continuously distributed in materials along the  $Z$ -axis has been considered in [1]. It was shown that  ${}_1\Sigma$  is the trace-free matrix with  ${}_1g = {}_1p = 0$ . In this case, the field equations (14a) are reduced to  $\Delta_1f = 2\kappa^2 {}_1f$  with the most general solution  ${}_1f = CK_0(\sqrt{2}\kappa r)$ , where  $K_0$  is the modified Bessel function of the second kind of order zero and  $r^2 = X^2 + Y^2$ . From (15) and (17) one obtains

$${}_1\Sigma_i^A = 2_0\phi_i^A = \sqrt{2}C(\kappa/r)K_1(\sqrt{2}\kappa r) \begin{pmatrix} 0 & 0 & -Y \\ 0 & 0 & X \\ -Y & X & 0 \end{pmatrix}. \tag{29}$$

Note that in a general case (29) gives the exponential decay for large distances  $r$  from the dislocation line, whereas the stress field is known in classical theory to decay as  $1/r$ . As we have previously noted, the classical results may be obtained by putting  $\kappa^2 \sim \epsilon$ . In this case, (14a) is reduced to  $\Delta_1f = 0$  and hence we obtain the well known first-order solution which in cylindrical coordinates, takes the form  ${}_1\sigma_{\phi z} = \mu C/r$ . The constant  $C$  is determined to be  $C = {}_1b/2\pi$  where  $b = \epsilon_1 b$  is the third component of the Burger's vector. It is clear that an analogous result follows directly from (29) in the limit  $\kappa \rightarrow 0$ .

Since  $\text{Tr } {}_0\phi = 0$ , tensors  $F_A^i$  and  $G_A^i$  take a simpler form. Namely,

$$F_A^i = 3_0\phi_B^i \delta_{k0}^B \phi_A^k \quad \text{and} \quad G_A^i = 2a\delta_{A0}^i \phi_E^k \delta_{k0}^E \phi_D^i.$$

Taking (29) into account we can obtain the exact form of  $\Psi(x, y)$  and  $\Phi(x, y)$ . First of all, let us rewrite  $\Psi(x, y)$  as

$$\Psi(x, y) = \left(\frac{3}{2}\right) [\partial_y^2(\partial_y {}_1f)^2 + \partial_x^2(\partial_x {}_1f)^2 + 2\partial_x\partial_y(\partial_y {}_1f)(\partial_x {}_1f)] - \Delta G \tag{30}$$

where  $G = G_1^1 = G_2^2 = G_3^3$ . Making use of the fact that in our case  $f$  is a radial function, we get

$$\Psi(x, y) = \Psi(r) = \left(\frac{3}{2}\right)[(\partial_{r_1}^2 f)^2 + (2/r)(\partial_{r_1} f)(\partial_{r_1}^2 f) + (\partial_{r_1} f)(\partial_{r_1}^3 f)] - a\Delta(\partial_{r_1} f)^2 \quad (31)$$

and

$$\Phi(x, y) = \Phi(r) = (3/4 - a)\Delta(\partial_{r_1} f)^2. \quad (32)$$

Taking into account the exact form of  $f$ , we rewrite (31) and (32) as

$$\Psi(r) = 3\kappa^2 C^2[(K_1')^2 + (2/r)K_1 K_1' + K_1 K_1''] - 2a\kappa^2 C^2 \Delta K_1^2 \quad (33)$$

$$\Phi(r) = 2\kappa^2 C^2(3/4 - a)\Delta K_1^2 \quad (34)$$

where  $K_1 = K_1(t)$ ,  $t = \sqrt{2}\kappa r$ , and  $K_1' = \partial_t K_1$ . In the limit  $\kappa \rightarrow 0$ ,  $\Psi(r)$  is reduced to  $\Psi(r) = (3 - 8a)C^2/2r^4$ , and  $\Phi(r) = (3 - 4a)C^2/r^4$ . Thus, (27) can be finally written as

$$\Delta\Delta_2 g = 4N/r^4 = (N/2)\Delta\Delta(\ln r)^2 \quad (35)$$

where  $N = (b/2\pi)^2(3 - 5a)/8(1 - 2a)$ . This result is in good agreement with that in [4]. The only constant  $N$  in [4] is determined in a more complex form. We note, however, that for  $\nu = \frac{1}{2}$  ( $a = \frac{1}{3}$ ) the expression for  $N$  in [4] becomes simpler and agrees with ours. Thus, we reproduce all results of [4]. Namely, in cylindrical coordinates the stress tensor has the following form:

$${}_2\sigma_{\phi z} = {}_2\sigma_{r\phi} = 0 \quad (36)$$

$${}_2\sigma_{rr} = (N/r^2) \ln r + 2d_1 + d_2/r^2 \quad (37)$$

$${}_2\sigma_{\phi\phi} = (-N/r^2) \ln r + 2d_1 + (N - d_2)/r^2 \quad (38)$$

where  $d_1$  and  $d_2$  are constants which can be determined by the boundary conditions. Thus, a further analysis of the problem depends on the choice of boundary conditions. It is usually assumed that the stress tensor  $\sigma_{rr}$  vanishes at the core boundary, i.e.  ${}_2\sigma_{rr} = 0$  at  $r = r_0$  where  $r_0$  is the core radius. It is beyond the scope of our paper to present the explicit expressions for  ${}_2\sigma$  for this case. It is clear that they should be the same as those obtained by the method in Kröner *et al* (see [4]).

#### 4. Electron states of screw dislocations

In this section we consider the concrete physical problem where remarkable effects appear only in the second-order approximation. Namely, let us study the long-wave electron states localized at screw dislocations. It is well known that the deformation potential arising from the long-range strain field in the presence of dislocations may result in localized electronic states with energies close to the conduction band (see, e.g., [9-14]). It should be noted, however, that the localized states of an electron on an edge dislocation appear in the first-order approximation whereas for screw dislocations this effect is essentially weaker. So, in [14] and [15] the anharmonic approximation was used to describe long-wave quasi-particle states localized at screw dislocations. Let us consider this problem in the framework of the gauge approach.

Making use of the effective mass and deformation potential theories, we get the stationary Schrödinger equation

$$[\Delta + m^*G(\text{Tr } E_{AB})/\hbar^2]\Psi = -(2m^*E/\hbar^2)\Psi. \quad (39)$$

Here  $m^*$  is an effective electron mass and  $G$  is a constant which characterizes the interaction of electrons with acoustic waves and can be defined in the isotropic case as  $G = (\frac{2}{3})E_F$ , where  $E_F$  is the Fermi energy. Note that the only strain component that can affect the electron energy in this case is the dilatation. The previously mentioned analysis shows that, in the first-order approximation, the strain matrix for screw dislocations is traceless (see (29)). Hence, we must take into account solutions obtained in the second-order approximation.

As follows from (13b), in the second-order approximation we get  $\text{Tr}_2 E_{AB} = 2 \text{Tr}_1 \phi + \Sigma_0 \phi^2$ , where we have denoted  $\Sigma_0 \phi^2 = {}_0\phi_A^i \delta_{ij} \delta^{AB} {}_0\phi_B^j$ . Making use of (15), (19) and (29) we find

$$\text{Tr}_2 E_{AB} = (1 - 3a)[\Delta_2 g + {}_2p - 2\Sigma_0 \phi^2]. \tag{40}$$

Restricting our consideration to the case  $\kappa^2 \sim \epsilon$  and using the results of the previous section we get finally

$$\text{Tr} E_{AB} = \epsilon^2 \text{Tr}_2 E_{AB} = C^2(1 - 3a)/8(1 - 2a)r^2 \tag{41}$$

where an additional inessential constant is dropped and  $C$  is defined now as  $C = b/2\pi$ .

Let us return to (39). Since  $\text{Tr} E_{AB}$  depends only on  $r$ , the wavefunction in (39) may be chosen as a product of the radial and angular parts  $\Psi(r, \theta) = R \exp(iM\theta)$ , where  $M$  ( $M = 0, \pm 1, \pm 2, \dots$ ) is the angular quantum number. In this case one obtains for the radial part  $R$

$$\partial_r^2 R + (1/r)\partial_r R + (2m^*/\hbar^2)[E - U]R = 0 \tag{42}$$

where

$$U = -(G/2) \text{Tr} E_{AB} + \hbar^2 M^2 / 2m^* r^2. \tag{43}$$

Taking (41) into account we find finally

$$U = -G(b/2\pi)^2(1 - 2\nu)/16(1 - \nu)r^2 + \hbar^2 M^2 / 2m^* r^2 \tag{44}$$

where we have used the condition  $a = \nu/(\nu + 1)$ . Let us consider the qualitative analysis of (42). If  $U > 0$ , the localized states are not present in the electron spectrum. Conversely, for  $U < 0$  there is an infinite number of discrete levels with  $E < 0$  condensed to the point  $E = 0$ .

Let us note that the first term in (44) is negative due to the fact that  $\nu \leq \frac{1}{2}$ . Hence, if  $M = 0$ , we always (apart from the limiting case  $\mu = 0$ ) have the localized electron states in materials with screw dislocations. On the other hand, if  $M \neq 0$ , the sign of (44) depends on the value of the parameter  $\alpha$  where  $\alpha = 32\pi^2 \hbar^2 M^2(1 - \nu) / Gm^* b^2(1 - 2\nu)$ . Setting here  $G = (\frac{2}{3})E_F$  and using the known relation  $E_F = (\hbar^2/2m^*)(6\pi^2 \rho/g)^{2/3}$ , where  $\rho$  is the density of conducting electrons and  $g$  denotes the degeneracy of electron levels, we draw the conclusion that  $\alpha > 1$  for all real materials (from dielectrics to metals). It means that for  $M \neq 0$  we have always  $U > 0$ , i.e. the localized electron states do not appear in this case.

It is of interest to note that analogous results have been found in [14] where, however, the only case  $M = 0$  has been considered and the phenomenological constant  $g_2$  has been introduced. Our approach enables us to determine via the main model parameters this constant in a way:  $g_2 = -G(1 - 2\nu)/16(1 - \nu)$ . Since  $\nu \leq \frac{1}{2}$  we always have  $g_2 \leq 0$  thus leading to an electron localization.



## 5. Conclusion

The perturbation method developed here in the framework of the  $EK$  gauge model is simple and can be useful in determining the stress and strain fields in dislocated bodies. The presented procedure is quite general and can be applied to other types of dislocations. However, the calculations within the second-order approximation seem to be more tedious. Nevertheless, as has been shown in [1], the results of the classic theory may be obtained in the limit when  $s_1$  becomes very large, that is when  $\kappa$  tends to zero. In this case the analysis is essentially simplified.

Our analysis shows that the gauge theory reproduces the stress fields associated with screw dislocations up to the second-order approximation without any consideration of accompanying displacement fields. It has been noted first in [1] that the field equations of the gauge theory replace the compatibility conditions of linear elasticity theory. We have shown that this assertion is valid in the framework of the nonlinear theory.

We have considered the problem of an electron localization at screw dislocations. The effect of binding of electrons to screw dislocations due to the long-range strain field is found to take place in the second-order approximation.

## References

- [1] Kadić A and Edelen D G B 1983 A Gauge Theory of Dislocations and Disclinations *Lecture Notes in Physics* vol 174 ed H Araki, J Ehlers, K Hepp, R Rippenhahn, H A Weidenmüller and J Zittarz (Berlin: Springer)
- [2] Króner E (ed) 1982 *Gauge Field Theories of Defects in Solids* (Stuttgart: Max-Planck Institut)
- [3] Kleinert H 1988 *Gauge Theory of Stresses and Defects* (Singapore: World Scientific)
- [4] Gairola B K D 1980 *Dislocations in Solids* vol 1 ed F R N Nabarro (Amsterdam: North-Holland) p 223
- [5] Króner E and Seeger A 1959 *Arch. Rational Mech. Analysis* **3** 97
- [6] Pfeiderer H, Seeger A and Króner E 1960 *Z. Naturf. A* **15** 758
- [7] Willis J R 1967 *Int. J. Engng. Sci.* **5** 171
- [8] Osipov V A 1990 *Phys. Lett. A* **146** 67
- [9] Landauer R 1954 *Phys. Rev.* **94** 1386
- [10] Emtage P R 1967 *Phys. Rev.* **163** 865
- [11] Voronov V P and Kosevich A M 1980 *Sov. J. Low Temp. Phys.* **6** 371
- [12] Lifshitz I M and Pushkarov Kh 1970 *Sov. Phys.-JETP Lett.* **11** 456
- [13] Winter S 1977 *Phys. Status Solidi b* **79** 637
- [14] Kosevich A M 1978 *Sov. J. Low Temp. Phys.* **4** 902
- [15] Maradudin A A 1970 Fundamental Aspects of Dislocation Theory *NBS Special Publication* 317 part 1 (Washington, DC: US Govt Printing Office) p 205