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## LETTER TO THE EDITOR

# Localized electron states in elastic materials with disclinations

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**Abstract.** In the framework of a gauge approach the problem of an electron localization in elastic materials with disclinations is investigated. The straight wedge disclinations, both topologically stable and unstable, as well as the disclination monopole, are considered. It is shown that for the topologically stable wedge, a disclination strongly localized in the core region electron states appears. For the topologically unstable negative wedge disclination and disclination monopole, the localization process is found to depend essentially on the depth of the deformation potential. The levels of localized electrons as well as the exact form of the normalized wavefunctions of the ground state are obtained numerically.

As is well known (see, e.g., [1]), the presence of defects even in minor concentrations can essentially modify electronic properties of materials, first of all semiconductors. This problem was studied in detail for point impurities [2] and linear translational defects—dislocations [3–6]. In both cases, the interaction of an electron with the longitudinal acoustic vibrations can result in localization of the electron at defects. The electron states in disclinated materials are less well understood. Qualitative analysis performed recently [7, 8] showed the possibility for the binding of electrons to negative disclinations.

In this letter, we study numerically the problem of an electron localization in disclinated materials in the context of the gauge model proposed in [9]. This model is the natural extension of the Edelen–Kadić gauge model [10] for an elastic continuum with dislocations and disclinations. The interaction of electrons with elastic media is considered in the framework of the deformation-potential theory. The validity of the effective mass approximation is assumed. When the defect fields are considered as the external ones, the stationary Schrödinger equation takes the following general form (cf [7])

$$\left[ - \sum_{A,B} \frac{\hbar^2}{2m_{AB}^*} D_A D_B + V(\mathbf{r}) \right] \Psi_E(\mathbf{r}) = E \Psi_E(\mathbf{r}). \quad (1)$$

Here  $m_{AB}^*$  is the effective electronic mass tensor, and  $V(\mathbf{r})$  is the deformation potential. The electron energy  $E$  is measured relative to the bottom of the conduction band in the undeformed crystal. As is seen, the most important deviation from the standard model is the replacement of the conventional derivative  $\partial_A = \partial/\partial x_A$  by the covariant one  $D_A$ . In the presence of dislocations, the translational symmetry of elastic media is broken, so that the gauge group is  $T(3)$ . In this case [11], the covariant derivative coincides with the conventional one, so that we arrive at the standard model known in dislocation theory [3–6].

For disclinations the gauge group is the rotational one. There are two kinds of symmetry which are appropriate for disclination problems. The first one is the spherical symmetry

which occurs for point disclinations such as the known 'hedgehog' in liquid crystals [12]. In this case the gauge group is  $G = \text{SO}(3)$  and the covariant derivative is determined to be  $(D_A \Psi)_j = \partial_A \Psi_j - i \varepsilon_{jk}^\alpha W_A^\alpha \Psi_k$  where  $W_A^\alpha$  are the gauge fields due to disclinations and  $\varepsilon_{jk}^\alpha$  is a completely antisymmetric tensor. The second kind of symmetry is the cylindrical one that holds for linear disclinations. In this case only rotations in the plane normal to the defect line are of importance, so that the gauge group reduces to  $G = \text{SO}(2)$ . The covariant derivative then takes the form  $D_A \Psi = (\partial_A - i W_A) \Psi$ . Thus, for rotational defects a perturbation appears not only in the potential energy due to the deformation potential, but in the kinetic energy as well.

Let us restrict consideration to acoustic deformations. As is known [1], in general, there are six independent components of the deformation-potential tensor. For cubic crystals they can be reduced to two components, so that the deformation potential takes the form

$$V(\mathbf{r}) = -G_d S p E_{AB}(\mathbf{r}) - G_u \sum_{A,B} \eta_{AB}(\mathbf{r}) (m_{AB}^*)^{-1} D_A D_B \quad (2)$$

where  $E_{AB}$  is the strain tensor,  $\eta_{AB} = E_{AB} - \frac{1}{3} \delta_{AB} S p E_{AB}$ , and  $G_d$  and  $G_u$  are the deformation potential constants. In the following, we will restrict consideration to isotropic materials where carriers belong to a singlet band centred at  $k = 0$ , where  $k$  is the wavevector. This is often the case for the conduction band in materials of zincblende or wurtzite structures. The only strain component that can affect the energy of such a band is the dilatation, i.e. only the first term in (2) has to be taken into account. Accordingly, the effective mass tensor reduces to a scalar  $m^*$ .

Let us consider the linear disclination oriented along the  $z$ -axis. In this case, the exact solution of the problem was found to have a vortex-like form. Particularly, the gauge fields  $W_A$  were found to be [13]:

$$W_r = 0 \quad W_\theta = W(r) = \nu/r \quad W_z = 0 \quad (3)$$

where  $\nu$  is the Frank index. The exact solution of the problem has been obtained for two cases: (a) small  $\nu$ ; this corresponds to the partial topologically unstable disclinations, and (b)  $\nu = 1$ ; a complete topologically stable disclination.

It is important to note that in either case the dilatation was found to depend only on the radial vector  $r$  in the  $xy$  plane. The electron wavefunction can be chosen as  $\Psi_E(x, y, z) = \Psi_E(r, \phi) \Psi_E(z)$ . Then, the stationary Schrödinger equation (1) is rewritten in the following form:

$$\left( -\frac{1}{r} \frac{d}{dr} r \frac{d}{dr} + \frac{(j-\nu)^2}{r^2} - \frac{2m^* G_d}{\hbar^2} S p E_{AB} \right) u_E^j(r) = k^2 u_E^j(r). \quad (4)$$

Here we have used the *ansatz*  $\Psi_E(\mathbf{r}) = \sum_j u_E^j(r) e^{ij\theta} / \sqrt{2\pi}$ ,  $j = 0, \pm 1, \pm 2, \dots$  and  $k^2 = 2m^* E / \hbar^2$ . The effective potential in (4) consists of two parts, the deformation-potential energy and the so-called centrifugal energy.

Let us note once more that the most important distinction from the case of dislocations and point impurities is that the interaction of an electron with the gauge field due to disclinations modifies the kinetic term as well. It is clear that this modification will result in a principally new situation for the localization process. A theoretical analysis of dislocated materials showed [5, 6] that the localized electron states always exist (at least with  $j = 0$ ) provided that the deformation potential is the attractive one. This is not the case for topologically unstable disclinations with the fractional Frank index where even for  $j = 0$  there exists a compensating positive term in (4) caused by the centrifugal energy. Hence the problem of the electron localization in this case requires an additional analysis. To proceed further we need the explicit form of the deformation potential.

Let us consider first a disclination with a small Frank index in a cylinder with an inner radius  $R_c$  and an external radius  $R$ . Taking into account the explicit form of the strain tensor (see, e.g. [14, 15]), the effective potential in (4) is written as

$$U_j(r) = \frac{\nu(1-2\sigma)}{2(1-\sigma)} G_d \left[ 2 \ln \frac{r}{R} + 1 + \frac{2R_c^2}{R^2 - R_c^2} \ln \frac{R_c}{R} \right] + \frac{(j-\nu)^2 \hbar^2}{2m^* r^2} \quad (5)$$

where  $\sigma$  is the Poisson constant. A simple qualitative analysis shows that the potential (5) is repulsive for  $\nu < 0$  (it corresponds to the positive disclination [14]) and, obviously, the localized electronic states do not appear in this case. On the other hand, for  $\nu > 0$  (negative disclination) the effective potential (5) may be the attractive one. This case is of interest to us here.

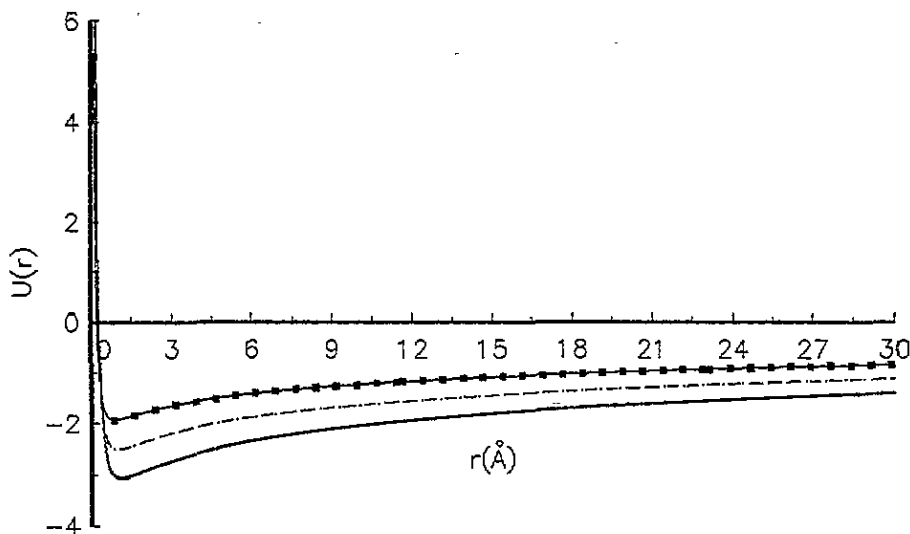
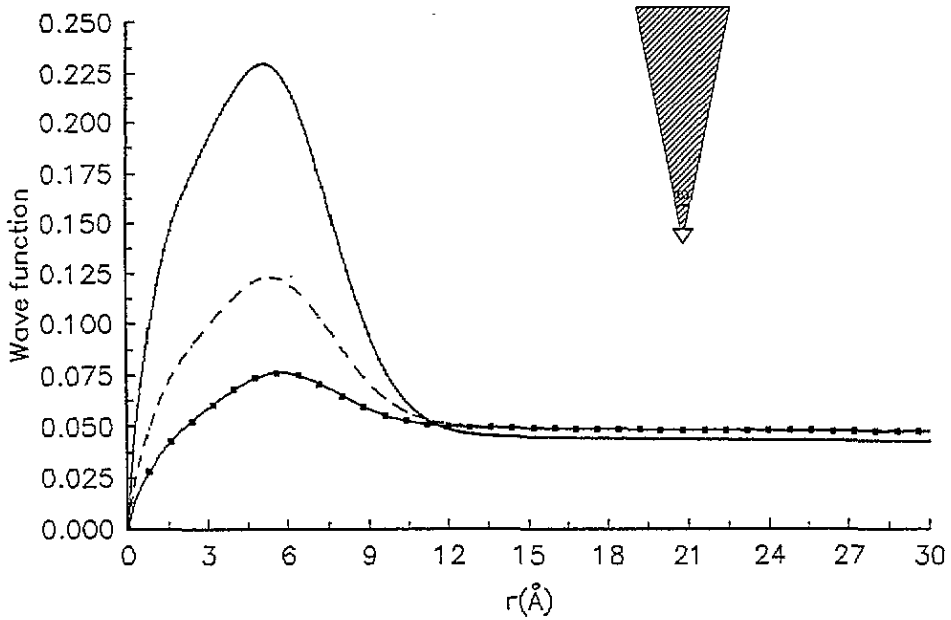
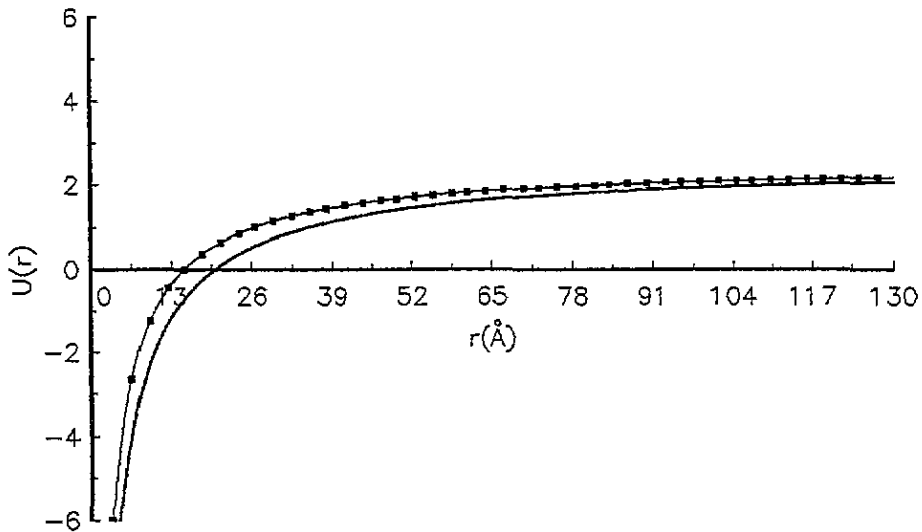


Figure 1. The effective potential (5) (in eV) for the small-angle straight wedge disclination:  $\nu = 0.1$ —solid line,  $\nu = 0.08$ —dashed line,  $\nu = 0.06$ —squares. The parameter set used is:  $R = 5 \times 10^{-6}$  cm,  $m^* = 5 \times 10^4$  eV,  $G_d = 10$  eV,  $\sigma = 0.41$ ,  $j = 0$ .

We performed numerical calculations with the wide set of parameters. The physically interesting region in  $R$  is  $R \sim 10^{-6}$ – $10^{-5}$  cm which corresponds to the mesoscopic structural level of the plastic deformation. As is known (see, e.g. [15]), in crystallites of this size the creation of the small-angle (partial) disclinations becomes energetically preferable in comparison with dislocations of the same geometry. Notice that in this case  $R/R_c \sim 10^2$ , so that the last term in the square brackets of (5) is negligible. Figure 1 shows the effective potential (5) for different  $\nu$ . Depth of the potential well is found to vary over a wide range with the model parameters used. At  $\nu = 0.1$ , the lowest electron levels are found to be  $E_0^{j=0} = -0.41$  eV,  $E_0^{j=1} = -0.38$  eV,  $E_1^{j=1} = -0.09$  eV, and  $E_1^{j=0} = 0.07$  eV. At  $\nu = 0.08$ ,  $E_0^{j=0} = -0.27$  eV, whereas at  $\nu = 0.06$ ,  $E_0^{j=0} = -0.17$  eV. The discrete electron levels become deeper when the depth of the well increases. The electron wavefunctions are presented in figure 2. As is seen, a logarithmic potential results in a gradual decrease of the electron wavefunctions with  $r$ . Therefore, in fact, this state is not a localized state but it corresponds to a resonance state. Notice that the amplitude of the wave functions decreases rapidly with decreasing of  $\nu$ . An exact solution for topologically stable linear disclination which corresponds to the complete straight wedge disclination has been found

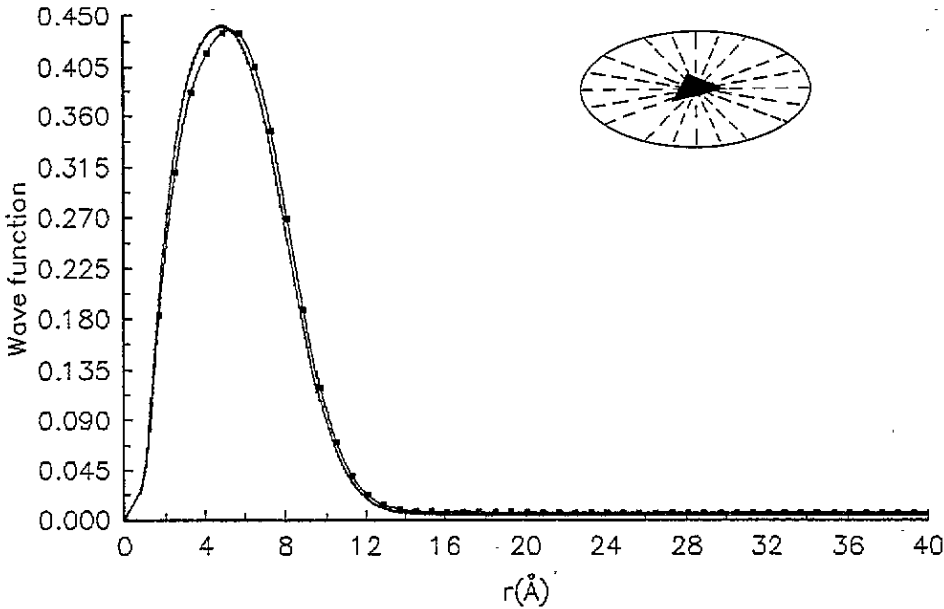


**Figure 2.** The wavefunctions of the ground state for the small-angle straight wedge disclination (schematically shown as an insert in the upper right-hand corner,  $\omega = 2\pi\nu$ ) with  $\nu = 0.1$ —solid line,  $\nu = 0.08$ —dashed line,  $\nu = 0.06$ —squares. The parameter set is the same as in figure 1.



**Figure 3.** The effective potential  $\phi$  (in eV) for the complete straight wedge disclination with  $\nu = 1$ :  $r_0 = 20$  Å—solid line,  $r_0 = 15$  Å—squares. The parameter set used is:  $m^* = 5 \times 10^4$  eV,  $G_d = 10$  eV,  $D = 1$ ,  $j = 1$ .

in [13]. It is important to note that this solution contains the information about the core region of the disclination. Namely, we found the explicit form of the deformation potential



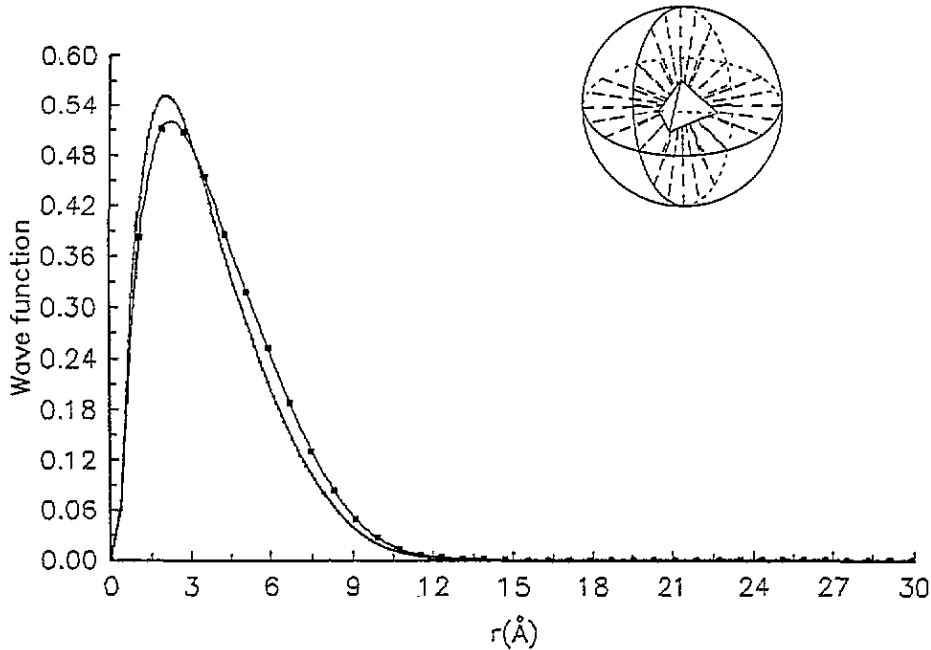
**Figure 4.** Normalized wavefunctions of the ground state for the complete straight wedge disclination (schematically shown as an insert in the upper right-hand corner) with  $\nu = 1$ . Designations and the parameter set are the same as those in figure 3.

in a wide space region including the core of a defect. The effective potential was written as follows [7]

$$U_j(r) = \begin{cases} G_d - DG_d \cosh^2 \left[ \frac{1}{3} \cosh^{-1}(r_0/r) \right] + K(j)/r^2 & r \leq r_0 \\ G_d - DG_d \cos^2 \left[ \frac{1}{3} \cos^{-1}(r_0/r) + \frac{2}{3} \pi l \right] + K(j)/r^2 & r \geq r_0 \end{cases} \quad (6)$$

where  $D = 4(\lambda + \mu)/3(\lambda + 2\mu)$ ,  $\lambda$  and  $\mu$  are the Lamé constants,  $K(j) = (j - \nu)^2 \hbar^2 / 2m^*$ . The point  $r = r_0$  in (6) turns out to be the boundary between two regions: the core region where deformations are large, and the region beyond the core where deformations decrease slowly and tend to a constant value at  $r \rightarrow \infty$ . In this letter, we will analyse the case  $l = 0$ . One can see that for  $j = 1$ , the potential (6) becomes the attractive one, and, therefore, the discrete levels exist at any set of the model parameters. This conclusion is confirmed by numerical calculations. Figure 3 shows the effective potential for different  $r_0$ . The corresponding wavefunctions are presented in figure 4. At  $r_0 = 20 \text{ \AA}$  the lowest electron level is  $E_0^{j=1} = -2.5 \text{ eV}$ . For the state with  $j = 0$  the localization takes place as well but with the lower amplitude, and  $E_0^{j=0} = -0.62 \text{ eV}$ . As  $r_0$  increases, the depth of the potential well rapidly increases and the first electron level becomes remarkably deeper. Conversely, for small  $r_0$ , the well is shallow and the lowest level lies close to the edge of the continuum electron spectrum. For  $r_0 = 15 \text{ \AA}$ ,  $E_0^{j=1} = -0.83 \text{ eV}$ .

Strictly speaking, description of the strongly localized electron states is beyond the applicability of the effective mass approximation. That is why the results concerning deep electron levels must be considered only as the qualitative ones. Let us remark, however, that sometimes the use of the effective mass approximation for description of strongly localized electron states (e.g., electrons localized in the core region of a dislocation [16] or electrons



**Figure 5.** Normalized wavefunctions of the ground state for the disclination monopole (schematically shown as an insert in the upper right-hand corner)  $r_0 = 10 \text{ \AA}$ —solid line,  $r_0 = 9 \text{ \AA}$ —squares. The parameter set used is:  $m^* = 5 \times 10^4 \text{ eV}$ ,  $G_d = 6 \text{ eV}$ ,  $B = 1$ ,  $J = 0.5$ .

localized in the plane, see discussion in [17]) gives even a quantitative agreement with experimental results.

Let us consider the point-like disclination with the exact solution [18] called the disclination monopole. The gauge fields  $W_A$  were found to be [18]

$$W_A^\alpha(x^B) = \varepsilon_{AB}^\alpha \frac{x^B}{r^2}. \quad (7)$$

Because of the spherical symmetry, the solution of (1) can be chosen in the form  $\Psi(x^A) = \Psi(r)\Psi(\theta, \phi)$ . Then, for the radial wavefunction equation (1) is written as

$$\left[ \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{2m^*}{\hbar^2} (E - U_j(r)) \right] \Psi_E(r) = 0 \quad (8)$$

where the effective potential takes the form [18]

$$U_j(r) = \begin{cases} (3/2)G_d - BG_d \cosh^2 \left[ \frac{1}{3} \cosh^{-1}(r_0/r)^2 \right] + K(J)/r^2 & r \leq r_0 \\ (3/2)G_d - BG_d \cos^2 \left[ \frac{1}{3} \cos^{-1}(r_0/r)^2 + \frac{2}{3}\pi l \right] + K(J)/r^2 & r \geq r_0. \end{cases} \quad (9)$$

Here  $B = 2(3\lambda + 2\mu)/3(\lambda + 2\mu)$ ,  $K(J) = [J(J + 1) - 1/4]\hbar^2/2m^*$ ,  $J = 1/2$  at  $j = 0$ ,  $J = j \pm 1/2$  at  $j = 1, 2, \dots$ . Qualitative analysis showed [19] that a potential well can occur in the core region. For a sufficiently deep well, the discrete electron levels and the localized states can appear.

Let us study this problem in detail by solving (8) with the potential (9) numerically. Figure 5 shows the exact form of the wavefunctions for different  $r_0$ . One can see that the localized states really appear but their amplitudes decrease with decreasing of  $r_0$ . It should be noted that there is an important difference between the results obtained for the

disclination monopole and those for a complete wedge disclination. Namely, as was found above, the localized electron state always exists for the complete wedge disclination, at least for  $j = 1$ . In the case of the disclination monopole, the last term in (9) turns out to be non-zero for any  $j$ . Thus the potential well may appear to be too shallow to localize the electron. In fact, the depth of the well is found to be very sensitive to the value of  $r_0$ . At  $r_0 = 10 \text{ \AA}$  the lowest electron level is  $E_0^{j=1/2} = -3.3 \text{ eV}$  whereas at  $r_0 = 9 \text{ \AA}$   $E_0^{j=1/2} = -1.1 \text{ eV}$ .

Let us summarize the main results. We showed that the binding of electrons to a small-angle straight wedge disclination can take place only for the negative disclination. The amplitude and the position of the resonance electron state depend on the depth of the potential well. The first excited state is that with  $j = 1$ . For the complete straight wedge disclination ( $\nu = 1$ ) the localization was found to always be present for a state with  $j = 1$ . In contrast to the small-angle defect, the first excited state in this case is the state with  $j = 0$ . In both these cases, an electron is free to move along the  $z$ -axes. For a disclination monopole, the localization takes place only for a sufficiently deep potential well. When this takes place, an electron becomes completely captured by the disclination.

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