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дубна

E17-90-71

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EXTENSION OF THE KADIĆ-EDELEN GAUGE MODEL: ELECTRONIC PROPERTIES OF DEFECT SYSTEMS

Submitted to "Physica A"

1990

1. Introduction

The gauge constructions in the theory of materials with defects have been successfully developed in the last ten years (see, e.g., [1-3]). The complete gauge field theory for materials with dislocations and disclinations has first been presented in [1]. The approach developed by Kadić and Edelen includes the combinations of the Yang-Mills (YM) minimal coupling theory, the conventional equations for defect dynamics and the Cartan structure equations. It has been shown that the space group $G_{sp} = SO(3) \triangleright T(3)$ may be viewed as a 6-parameter gauge group that leaves the Lagrangian of elasticity theory invariant. Breaking of the homogeneity of the action of SO(3) was shown to give rise to disclinations and rotational dislocations, while homogeneity breaking of T(3) gives rise to translational dislocations. As a final result, the field theory Lagrangian that describes the deformable elastic continuum together with the dislocation and disclination fields has been derived in [1].

Note that the Kadić-Edelen (KE) gauge model allows us to study the defect dynamics. It is known, however, that the mobility of dislocations in semiconductors depends on the electronic states of materials (see, e.g., [4]). Moreover, the core of disclination acts as an acceptor (donor) thus leading to the formation of the dislocation subband in the midgap of the electronic spectrum [5-7]. The subject of our investigation in the present article is the electronic properties of defect systems. We show that the electronic properties of materials with dislocations and disclinations may be viewed in the framework of the gauge approach. For this purpose, we extend the Lagrangian of the KE model by adding the electronic terms in the gauge invariant form.

The plan of the paper is as follows. In section 2 the KE gauge model is considered. The Lagrangian as well as the field equations are presented. As an illustration of the possibilities of the method, the exact monopole-like solution for static disclinations obtained first in [8] is presented. The effective Lagrangian for the electronic subsystem is constructed in section 4. The electron fields are considered to transform by the spinor representation of the gauge group SO(3). Spinor components are suggested to be the electron states with spin up and spin down, respectively. It is of interest that the primary free electrons are found to interact with disclination fields. We have solved the Schrödinger equation in the external potential given by the static vortex-like disclinations. The term describing the interaction of electron fields with acoustic waves is derived in section 4b. In this case electrons are shown to interact with both the dislocation and disclination fields. Restricting here attention to phenomena where only disclination fields play a significant role, we have analyzed the Schrödinger equation in the presence of the interaction term. As a result of the interaction, the localization of electrons in the region of the core of the monopole-like disclination is established. Section 5 is devoted to concluding comments.

We have used here (unless otherwise stated) the same notation as in [1]. Namely, lower case Greek indices, $\alpha,\beta,\ldots$, take their values from the set $I=\{1,2,3\}$. The same is true for indices denoted by capital letters, $A,B,\ldots$, and by lower case Latin letters, $i,j,k,\ldots$, starting with the letter i. Lower case Latin letters at the beginning of the alphabet, a,b,..., take their values from the index sets J={1,2,3,4}. As usual, the summation for repeated indices is assumed. The labels i,j,k,α,β, and γ are the G_{sp} labels, whereas the labels a,b,c,... and A,B,C,... are the space labels.

2. The Kadić-Edelen gauge model

The Lagrangian that is invariant under the inhomogeneous action of the gauge group G_{sp} takes the following form [1]:

$$L = L_\chi + L_\phi + L_W , \tag{2.1}$$

where

$$L_\chi = (\rho_0/2) B^i_4 \delta_{ij} B^j_4 - [\lambda (E_{AB}\delta^{AB})^2 + 2\mu E_{AB}\delta^{AC}\delta^{BD}E_{CD}]/8 \tag{2.2}$$

describes the elastic properties of the material,

$$L_\phi = -(s_1/2)\delta_{ij} D^i_{ab} k^{ac} k^{bd} D^j_{cd} \tag{2.3}$$

describes the dislocations, and

$$L_W = -(s_2/2) C_{\alpha\beta} F^\alpha_{ab} g^{ac} g^{bd} F^\beta_{cd} \tag{2.4}$$

describes the disclinations. The strain tensor in (2.2) is determined as

$$E_{AB} = B^i_A \delta_{ij} B^j_B - \delta_{AB} , \tag{2.5}$$

where

$$B^i_a = \partial_a \chi^i + \gamma^i_{\alpha j} \chi^j W^\alpha_a + \phi^i_a \tag{2.6}$$

is the distortion tensor. In (2.6) $\partial_a \chi^i$ describes the integrable part of the distortion, the second term arises from the inhomogeneous action of the rotation group SO(3), and third 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 (2.6) characterizes the configuration at time T in terms of the coordinate cover (X^A) of a reference configuration, W^{α}_{a} are the compensating gauge fields associated with disclination fields, whereas ϕ^{i}_{a} are associated with dislocation fields. Tensors D^{i}_{ab} and F^{α}_{ab} are determined as follows:

$$D^{i}_{ab}=\partial_a\phi^{i}_{b}-\partial_b\phi^{i}_{a}+\gamma^{i}_{\alpha j}(W^{\alpha}_{a}\phi^{j}_{b}-W^{\alpha}_{b}\phi^{j}_{a}+F^{\alpha}_{ab}\chi^{j}), \qquad (2.7)$$

and

$$F^{\alpha}_{ab}=\partial_a W^{\alpha}_{b}-\partial_b W^{\alpha}_{a}+C^{\alpha}_{\beta\gamma}W^{\beta}_{a}W^{\gamma}_{b}. \qquad (2.8)$$

In (2.2-2.4) λ and μ are the Lamé constants, ρ_0 is the mass density in the reference configuration, s_1 and s_2 are the coupling constants, $C_{\alpha\beta}$ are the components of the Cartan-Killing metric of the subgroup SO(3), $C^{\alpha}_{\beta\gamma}$ are the structure constants of the Lie algebra SO(3), and $\gamma^{i}_{\alpha j}$ are the generating matrices of the group SO(3). In (2.4) the quantities g^{ab} are given by $g^{AB}=-\delta^{AB}$, $g^{44}=1/\zeta$, and $g^{ab}=0$ for $a\neq b$, whereas in (2.3) $k^{AB}=-\delta^{AB}$, $k^{44}=1/y$, and $k^{ab}=0$ for $a\neq b$. The parameters ζ and y are the two positive "propagation parameters". The field equations that determine the functions χ^{i}, W^{α}_{a} and ϕ^{i}_{a} are given in Appendix.

The physical substantiation of the KE model as well as some other details may be found directly in [1]. It is necessary to take account of the fact, however, that only defects continuously distributed in materials can be considered in the framework of this model. Moreover, as was mentioned in [9], the gauge translational and rotational degrees of freedom were treated in [1] separately, which is of interest only in the regime of dilute defect distribution. Some of these problems have been studied in [9,10] where the gauge theory of defects for discrete systems was developed by using simplicial and differential geometric methods.

The field equations given in Appendix are a system of coupled nonlinear differential equations which is very difficult to solve in the general case. To study most of the problems of practical interest, the linearization procedure developed in [1] may be used. This procedure involves the scaling of the gauge group with a group scaling parameter ε. As was shown in [1], in the first order approximation the elasticity theory is recovered. In the second order approximation the dislocation fields appear whereas the disclinations enter the equations only in the third and higher order approximation. However, as was mentioned in [1], there are other possibilities, one of which is examined in the next section.

3. The exact monopole-like solution for static disclinations

Let us consider the disclination Lagrangian $L=L_{\chi}+L_{W}$ where the dislocation fields ϕ^{i}_{a} are ignored from the beginning. In this case (A10) and (A1) can be rewritten as follows:

$$\partial_a G^{ab}_{\alpha} - C^{\beta}_{\gamma\alpha} W^{\gamma}_{a} G^{ab}_{\beta} = T^{b}_{\alpha}/2, \tag{3.1}$$

and

$$\partial_a Z^{a}_{i} - Z^{a}_{j} W^{\alpha}_{a} \gamma^{j}_{\alpha i} = 0 \quad , \tag{3.2}$$

where the condition (A12) takes now the form $T^{a}_{\alpha}=\gamma^{i}_{\alpha j} Z^{a}_{i} \chi^{j}$. At this stage we choose the regular representation for the rotation group SO(3): $\gamma^{i}_{\alpha j}= \varepsilon_{i\alpha j}$, where $\varepsilon_{i\alpha j}$ is the full antisymmetric tensor, $\varepsilon_{123}=1$; $C_{\alpha\beta}=\delta_{\alpha\beta}$, and $C^{\gamma}_{\alpha\beta}=-C^{\gamma}_{\beta\alpha}$, where $C^{1}_{23}=1$.

Note that the system (3.1-3.2) is similar to that in the YM field theory with the Higgs triplet. Since the underlying group for the YM theory, SU(2), and SO(3) have isomorphic Lie algebras, the known solutions in particle physics may be suitable in defect dynamics. Indeed, as was first shown in [1], if the disclination energy density coefficient s_2 is very large, the right-hand side of (3.1) tends to zero thus reducing (3.1) to the free YM equation. The static solution of such an equation (well known as the solution of Yang and Wu (see,e.g.,[11])) was used in [1] to describe the far field of a static disclination.

On the other hand, in [8] the static monopole-like ansatz for (3.1,3.2) has been chosen in the form

$$\chi^{1}(X^{A}) = \delta^{1}_{A}F(r)X^{A}/r \qquad (3.3)$$

and

$$W^{\alpha}_{A}(X^{B}) = \delta^{\alpha\beta}\epsilon_{\beta AB}X^{B}/r^{2}, \qquad W^{\alpha}_{4} = 0, \qquad (3.4)$$

where $r^2= X^{A}X_{A}$. In accordance with the boundary conditions (A5) and (A11), the function $F(r)$ in (3.3) must tend to the constant value, F, as $r\to\infty$, while the disclination fields W^{α}_{A} tend to zero as $1/r$. Let us note also that the solution (3.4) is already antiexact in accordance with (A14) since $X^{A}W^{\alpha}_{A}+TW^{\alpha}_{4}\equiv 0$.

Clearly, (3.4) is the solution of Yang and Wu that is singular as $r\to 0$, while (3.3) is the exact monopole form analogous to that for the Higgs triplet in field theory. Note that the singular behaviour is peculiar to dislocations and disclinations and may be explained due to the fact that the elasticity theory formulae are not valid for small r.

Let us show that the right-hand part of (3.1) turns out into zero at our choice of (3.3,3.4). The stress tensor σ^{1}_{A} determined in (A2) may now be written as

$$\sigma^{A}_{1}= X_{1}X^{A}g(r)\{\lambda[g^{2}(r)-3]/2+\mu[g^{2}(r)-1]\}/r^{2}, \qquad (3.5)$$

where $g(r)=\partial F(r)/\partial r$. Clearly, σ_i^A is symmetric. Thus, the right-hand side of (3.1) takes the form $\varepsilon_{i\alpha j}x^i x^A x^j=0$, and we obtain the free YM equation. The deformation tensor $E_{AB}=(x_A x_B/r^2)g^2(r)-\delta_{AB}$, and the distortion tensor $B_A^i=(x^i x_A/r^2)g(r)$. As can be easily seen, (3.2) reduces to

$$\partial_r g(r)[3Ag^2(r)-B] = -2[Ag^3(r)-Bg(r)]/r, \tag{3.6}$$

where $A=\lambda/2+\mu$, and $B=3\lambda/2+\mu$. Carrying out the integration in (3.6) we obtain the following condition:

$$|Ag^3(r)-Bg(r)| = g_0/r^2, \tag{3.7}$$

where g_0 is an integration constant. The stress tensor takes now the form

$$\sigma_i^A = g_0 X_i X^A/r^4, \tag{3.8}$$

which agrees with the result of [1], but is valid for all r (with the exception of the small region near r=0 where the elasticity theory does not work). We would like to remind that in [1] only the region of large r has been considered. Note that the solution (3.3,3.4) has a vortex-like behaviour. Due to the nonlinear character of (3.7) the new principal feature, as compared to the monopole solution, arises. Namely, the analysis of (3.7) shows two distinctly defined regions characterized by the dimensional parameter $r_0=(27g_0^2A/4B^3)^{1/4}$.

The solutions of (3.7) are found to be [8]

$$g(r) = \begin{cases} g_1(r)=N_0\cosh[\frac{1}{3}\cosh^{-1}r_0^2/r^2], & r\le r_0 \\ g_2(r)=-N_0\cos[\frac{1}{3}\cos^{-1}r_0^2/r^2+\frac{\pi}{3}], & r\ge r_0\ , \end{cases} \tag{3.9}$$

where $N_0=2(B/3A)^{1/2}$. Obviously, the symmetric solution $g^*(r)=-g(r)$ is also present. It is convenient to introduce the universal dimensionless parameter $t=r/r_0$. For $t\to 0$ $g(t)$ diverges as $t^{-2/3}$. For $t\to\infty$ $g(t)$ tends to zero as t^{-2}. At $t=1$ $g(t)$ has a jump from the value N_0 to $-N_0/2$. Fig.1 shows the function $g_n(t)=g(t)/N_0$. One can see that $g(t)$ essentially changes its behaviour when t passes the point $t=1$. To restore now the function $F(r)$ we perform numerical calculations (the integration constant is set to be zero here). The result is presented in Fig.1. The region $t\leq 1$ determines the core of the disclinations, i.e., the region where deformations take maximal values. Beyond the core the state vector χ^i changes slowly and tends to a constant value as $t\to\infty$.

The topological charge (or, equivalently, the Frank index) can be defined as follows (see, e.g.,[12]):

$$N = (1/8\pi F^3)\int \varepsilon^{ijk}\varepsilon_{ABC}\partial_i\chi^A\partial_j\chi^B\partial_k\chi^C d^3x. \qquad (3.10)$$

After straightforward calculations we obtain that $N=1$ for (3.3). It should be noted that disclinations with the Frank index $N\approx 1$ are now not so well studied in solids to be compared with the case $N\ll 1$. The reason is that the investigation of disclinations with $N\approx 1$ as well as cores of disclinations meets considerable mathematical problems because the nonlinear relation between stresses and strains must be taken into account. As we have shown here, the gauge model of defects allows us to describe the disclinations with $N=1$ quite well.

4. Electronic properties of defect systems

Let us introduce the electronic fields $\Psi_n(x^a)$ transforming under the action of the rotation gauge group SO(3) according to

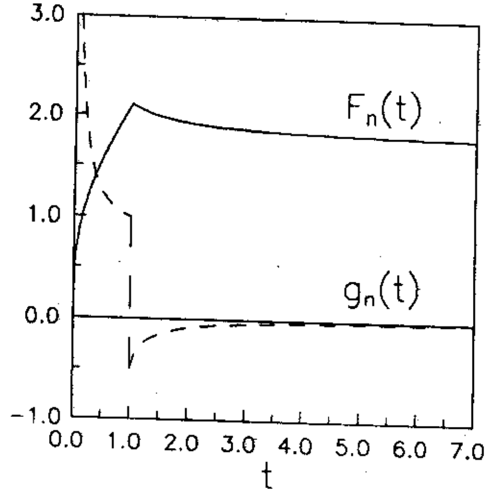

Fig.1. The functions $F_n(t)=F(t)/N_0r_0$ (solid line) and $g_n(t)=g(t)/N_0$ (dashed line) are presented. The point t=1 ($r=r_0$) corresponds to the disclination core radius.

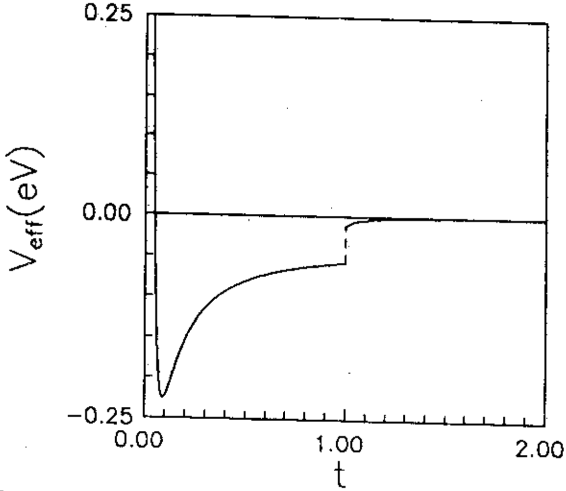

Fig.2. The effective potential (4.19) is shown. The parameter set is used: 4B/3A=2, J=1/2, $m^*=0.5MeV$, $r_0=5a_0$, $a_0=5Å$, $E_F=0.03eV$, so that $K_1=0.06eV$ and $K_2=0.0032eV$.

$$\delta^{\alpha}\Psi_j = iT^{\alpha}_{jk}\Psi_k, \qquad [T^{\alpha},T^{\beta}]=i\varepsilon^{\alpha\beta\gamma}T^{\gamma}. \tag{4.1}$$

We have taken the spinor representation for fields Ψ_j (j=1,2). In this case $T^{\alpha}=\tau^{\alpha}/2$ where τ^{α} are the Pauli matrices. Two states Ψ_1 and Ψ_2 may be associated with the spin up and spin down electron states, respectively.

a) *Effective Lagrangian (free case)*

Let us consider the long-wave electronic states. We derive the effective Lagrangian for the electronic subsystem that is invariant under the inhomogeneous action of the gauge group G_{sp} in the form

$$L_{\Psi}= \{i\hbar[\Psi^{+}D_4\Psi-(D_4\Psi^{+})\Psi] - (\hbar^2/m^*)(D_A\Psi^{+})D^A\Psi\}/2, \tag{4.2}$$

where Ψ is the two-component spinor, m^* is an effective electron mass, and the covariant divergence for electron fields is determined as

$$(D_a\Psi)_j = \partial_a\Psi_j - igT^{\alpha}_{jk}W^{\alpha}_a\Psi_k, \tag{4.3}$$

where g is the group constant (in what follows we shall consider the case g=1). Thus, we obtain in (4.2) that the primary free electron fields interact additionally with the disclination fields while the interaction with dislocation fields, ϕ^{i}_{a}, do not appear in the free case. Clearly, the variation of (4.2) with respect to W^{α}_{a} adds new terms to the Euler-Lagrange equation (A10). Moreover, the variation of (4.2) with respect to Ψ gives an additional equation. We do not know at present how to carry out the complete analysis of the self-consistent system of equations for defect dynamics in the presence of the electron fields. We see, however, two types of problems which can be studied. First, we can investigate the electronic properties of defect systems considering the Schródinger equation in the external potential given by the dislocations and (or) disclinations. Second, we can study the influence of the electron fields on defect dynamics.

We shall consider here the first problem. Namely, let us study the electronic properties of continuum media in the presence of the vortex-like disclination (3.4). The variation of (4.2) with respect to Ψ gives the Schródinger equation which takes the following form in the stationary case:

$$-(\hbar^2/2m^*)(\partial_A - i\tau^\alpha W^\alpha_A/2)^2\Psi = E\Psi . \qquad (4.4)$$

We restrict attention here to static disclinations ($W^\alpha_4=0$). Using the gauge condition $\partial^A W^\alpha_A=0$, one obtains from (4.4)

$$[\partial^2 - i\tau^\alpha W^\alpha_A \partial^A - W^\alpha_A W^{\alpha A}/4]\Psi = -(2m^* E/\hbar^2)\Psi, \qquad (4.5)$$

where $\partial^2=\partial_A\partial^A$. Substituting the solution (3.4) in (4.5), one gets

$$[\partial^2 - i\varepsilon_{\alpha AJ}\tau^\alpha(x^J/r^2)\partial^A - 1/2r^2]\Psi = -(2m^* E/\hbar^2)\Psi. \qquad (4.6)$$

This equation may be solved in the usual way. Let us introduce the operator of the total angular momentum

$$M^\alpha = M^\alpha_{orb} + I^\alpha, \qquad (4.7)$$

where $M^\alpha_{orb}=-i\hbar\varepsilon^{\alpha AB}x_A\partial_B$ denotes the ordinary angular momentum, and $I^\alpha=\hbar\tau^\alpha/2$ denotes an isospin. Breaking up ∂^2 into the radial and angular parts, $\partial^2=\partial^2_R+(1/r^2)\partial^2_{\phi,\theta}$, we rewrite (4.6) in the form

$$[\partial^2_R + (1/r^2)\partial^2_{\phi,\theta} - (M^\alpha_{orb}\tau^\alpha)/\hbar r^2 - 1/2r^2]\Psi = -(2m^* E/\hbar^2)\Psi. \qquad (4.8)$$

Since $M^2_{orb}=-\hbar^2\partial^2_{\phi,\theta}$, we finally obtain

$$[\partial^2_R - M^2/\hbar^2 r^2 + 1/4r^2]\Psi = -(2m^* E/\hbar^2)\Psi. \qquad (4.9)$$

The solution of (4.9) is well known. The wave function Ψ may be presented in the form $\Psi(r,\phi,\theta)=R_J(r)Y^J_{lm}(\phi,\theta)$, where Y^J_{lm} are the spherical spinors which satisfy $M^2Y^J_{lm}=\hbar^2J(J+1)Y^J_{lm}$, $M_zY^J_{lm}=\hbar mY^J_{lm}$ and

$$R_J(r) = C_J(kr)^{-1/2}J_s(kr). \qquad (4.10)$$

Here J_s is the Bessel function, $s=\sqrt{J(J+1)}$, and C_J can be determined from the normalization condition. The quantum numbers take the following values: $J=l\pm(1/2)$ at $l\neq0$; $J=1/2$ at $l=0$, and $m=-J,\dots,J$, where l $(l=0,1,\dots\infty)$ is the orbital quantum number. The energy spectrum E is similar to that for the free motion, $E=\hbar^2k^2/2m^*$. Thus, we obtain that the presence of the vortex-like disclination only slightly modifies the electronic properties of continuum media.

b) *Effective Lagrangian (general case)*

Here, we consider the electronic properties of defect systems when the deformation potential which characterizes the interaction of electrons with acoustic waves is taken into account. We construct the interaction Lagrangian in the following gauge invariant form:

$$L_{int}= -\Psi^+(x^A)W_d(x^A)\Psi(x^A), \qquad (4.11)$$

where the deformation potential in the isotropic case may be defined as

$$W_d(x^C)=-(G/2)SpE_{AB}(x^C), \qquad (4.12)$$

and G is the interaction constant. Let us remind that E_{AB} is determined in (2.5). In the defect free case we easily obtain from (4.12) the known expression for the deformation potential (see, e.g.,[13]) where the constant G is determined as $G=(2/3)E_F$, and E_F is the Fermi energy. Thus, the complete theory includes now elastic fields, dislocations, disclinations, and electron fields. The effective Lagrangian takes the form

$$L = L_{\chi} + L_{\phi} + L_{W} + L_{\Psi} + L_{int}, \tag{4.13}$$

where $L_{\chi}, L_{\phi}, L_{W}, L_{\Psi}$ and L_{int} are determined in (2.2-2.4), (4.1), and (4.11), respectively. Note that electron fields in (4.11) interact with both the dislocation fields ϕ^{i}_{A} and the disclination fields W^{α}_{A}. In the present paper, we restrict our attention only to disclination fields. Namely, we consider the static monopole-like disclination (3.3,3.4) as the external field to the Schródinger equation. An analogous problem has been studied in relativistic field theory [14]. It has been shown that the Dirac equation for massless fermions possesses the zero-energy fermion bound state in the presence of the static t'Hooft-Polyakov monopole. As a consequence, fermion number is broken thus leading to the strong baryon-number breaking in monopole-fermion interactions [15]. In our (non-relativistic) case we expect the appearance of discrete levels in the electron spectrum in the presence of the monopole-like disclinations.

Taking into account the interaction term (4.11), we rewrite the Schródinger equation (4.4) in the form

$$[\partial^2 - i\tau^{\alpha} W^{\alpha}_{A} \partial^{A} - W^{\alpha}_{A} W^{\alpha A}/4 + m^{*} G E_{AB} \delta^{AB}/\hbar^2]\Psi = -(2m^{*}E/\hbar^2)\Psi. \tag{4.14}$$

We consider the case when the dislocation fields are absent whereas the disclination fields are taken to have the monopole-like form (3.3,3.4). Thus, (4.14) can be rewritten as

$$[\partial^2_R - M^2/\hbar^2 r^2 + 1/4r^2 + m^{*} G (g^2(r) - 3)/\hbar^2]\Psi = -(2m^{*}E/\hbar^2)\Psi. \tag{4.15}$$

The wave function in (4.15) may again be chosen as a product of the radial and angular parts. In this case one obtains for the radial part R

$$\partial_R^2 R + (2m^*/\hbar^2)[E - (J(J+1)-1/4)\hbar^2/2m^*r^2 + Gg^2(r)/2 - 3G/2]R = 0. \quad (4.16)$$

It is of interest that the constant term in (4.16) is determined as $3G/2=E_F$. Thus, the electron energy is really measured relative to the Fermi energy. We reduce (4.16) to the usual form

$$\partial_R^2 R + (2m^*/\hbar^2)[\tilde{E} - V_{eff}]R = 0, \quad (4.17)$$

where $\tilde{E}=E-E_F$ and

$$V_{eff} = -(E_F/3)g^2(r) + [J(J+1)-1/4]\hbar^2/2m^*r^2. \quad (4.18)$$

Using (3.9), we rewrite (4.18) in the following form:

$$V_{eff} = \begin{cases} -K_1\cosh^2[\frac{1}{3}\cosh^{-1}(1/t^2)]+K_2/t^2, & t\le 1 \\ -K_1\cos^2[\frac{1}{3}\cos^{-1}(1/t^2)+\frac{\pi}{3}]+K_2/t^2, & t\ge 1\ , \end{cases} \quad (4.19)$$

where $K_1=4BE_F/3A$ and $K_2=[J(J+1)-1/4]\hbar^2/2m^*r_0^2$ are the positive dimensional parameters. The analysis of (4.19) allows us to obtain the full information about the electron spectrum. Let us study first the qualitative behaviour of V_{eff}. For $t\to 0$ the second term in (4.19) tends to infinity as t^{-2} whereas the first term diverges as $-t^{-4/3}$. For $t\to 1^-$ one obtains $V_{eff}\to K_2-K_1$. For $t\to 1^+$ $V_{eff}\to K_2-K_1/4$. For $t\to\infty$ the first term in (4.19) tends to zero as $-t^{-4}$ whereas the second term as t^{-2}. It is clear that the potential well always arises in the region $t\le 1$. The characteristic parameters of the potential well essentially depend on the values of K_1 and K_2. When K_2 decreases (or, equivalently, K_1 increases), the minimum of V_{eff} moves to the left and the depth of the potential well rapidly increases. Such a behaviour takes place in a wide range of the parameters. We have investigated (4.19) numerically taking a parameter set related to semimetals (E_F=0.03eV). The typical curve for V_{eff} is shown in Fig.2.

Thus, we find that in accordance with our proposal the discrete levels must appear in the electron spectrum due to the presence of the static monopole-like disclination. Moreover, it follows immediately from Fig.2 that the electron states with $E<E_F$ are localized in the region of the core of disclination. This result agrees quite well with that for the electron localization in the region of the core of dislocation (see, e.g., [4-6,16,17]).

5. Summary

Let us note the main results obtained in the paper.

1. We extend the KE gauge model by including electron fields. The effective Lagrangian that describes elastic fields, dislocations, disclinations, as well as electron fields is constructed in the gauge invariant form. In the framework of this model one can study both the influence of electron fields on the defect dynamics (using, for example, the quasiclassical approximation for electron fields) and the electronic properties of materials with defects.
2. We obtained the exact monopole-like solution for static disclinations with the Frank index N=1. The stress tensor is found to depend only on the model parameters (λ and μ) and on the disclination core radius (r_0).
3. We investigated the long-wave electronic states of materials with disclinations. When the interaction between electron fields and acoustic waves is taken into account, the electrons with the energy $E<E_F$ are obtained to be localized in the region of the core of the monopole-like disclination.

In the present paper, we restricted attention to disclinations. Note that disclinations are not so well studied in solids to be compared with dislocations. The reason is that disclinations are seldom observed in ordinary 3-dimensional crystals. Nevertheless, they are important in liquid crystals, polymers, and amorphous bodies. Our interest in disclinations comes from the known results obtained first in the relativistic field theory for the t'Hooft-Polyakov monopole. There is no doubt that the investigation of electronic properties of materials with dislocations in the framework of the gauge model are of considerable interest. The work in this direction should be continued.

Appendix

The field equations of defect dynamics

Here we present the field equations of defect dynamics obtained first in [1]. The Euler-Lagrange equations with respect to χ^i take the form

$$\partial_4 p_i - \partial_A \sigma^A_i = \gamma^j_{\alpha i}(W^\alpha_4 p_j - W^\alpha_A \sigma^A_j + F^\alpha_{ab} R^{ab}_j), \qquad \text{(A1)}$$

where the explicit expression for the stress tensor

$$\sigma^A_i = (1/2)\delta^A_B \delta_{ij}(\partial_C \chi^j + \gamma^j_{\alpha k} W^\alpha_C \chi^k + \phi^j_C)(\lambda\delta^{BC}\delta^{FD}E_{FD} + 2\mu\delta^{RB}\delta^{SC}E_{RS}), \qquad \text{(A2)}$$

and the momentum

$$p_i = \rho_0 \delta_{ij}(\partial_4 \chi^j + \gamma^j_{\alpha k} W^\alpha_4 \chi^k + \phi^j_4). \qquad \text{(A3)}$$

R^{ab}_i is determined as follows:

$$R^{ab}_i = \partial L/\partial D^i_{ab} = -s_1 \delta_{ij} k^{ac} k^{bd}[\partial_c \phi^j_d - \partial_d \phi^j_c + \gamma^j_{\alpha k}(W^\alpha_c \phi^k_d - W^\alpha_d \phi^k_c) + \gamma^j_{\alpha k} F^\alpha_{cd} \chi^k]. \qquad \text{(A4)}$$

Note that (A1) are the equations of balance of the linear momentum. When W^α_a are equal to zero (pure dislocated material) (A1) reduces to the well-known in classical elasticity theory form $\partial_A \sigma^A_i = \partial_4 p_i$. As was shown in [1], the two types of the boundary conditions may be written for (A1):

a) the Dirichlet data (traction-free spatial boundaries)

$$\delta\chi^i|_{\partial E_4} = 0 \qquad (\chi^i|_{\partial E_4} \text{ specified}), \tag{A5}$$

b) the homogeneous Neumann data (zero initial and final momentum)

$$Z^a_i \pi_a|_{\partial E_4} = 0 . \tag{A6}$$

Here and below, $\partial E_4(\partial E_3)$ are the spatial boundaries of the 4(3)-dimensional Euclidean space, respectively, π_a is a top-down generated basis for the $\binom{4}{3}$- dimensional space $\Lambda^3(E_4)$, μ_B is a top-down generated basis for the space $\Lambda^2(E_3)$, and $Z^a_i = \partial L/\partial B^i_a$, where

$$Z^A_i = -\sigma^A_i, \qquad Z^4_i = p_i . \tag{A7}$$

The Euler-Lagrange equations with respect to ϕ^i_a are

$$\partial_a R^{ab}_j - \gamma^i_{\alpha j} W^\alpha_a R^{ab}_i = Z^b_j/2, \tag{A8}$$

where R^{ab}_i is determined in (A4). The boundary conditions are the homogeneous Neumann data

$$R_i|_{\partial E_4} = 0. \tag{A9}$$

The variation with respect to W^α_a gives

$$\partial_a G^{ab}_\alpha - C^\beta_{\gamma\alpha} W^\gamma_a G^{ab}_\beta = T^b_\alpha/2, \tag{A10}$$

where $G^{ab}_\alpha = \partial L/\partial F^\alpha_{ab}$ and $T^a_\alpha = (\partial L/\partial W^\alpha_a)|_{F^\alpha_{ab}}$. The boundary conditions for (A10) are obtained to be the natural Neumann data

$$G^{aB}_\alpha \mu_B|_{\partial E_3} = 0. \tag{A11}$$

Additionally to the Euler-Lagrange equations, we write here the important relationship between dislocations, disclinations, and stresses

$$T^a_\alpha = \gamma^i_{\alpha j}(Z^a_i \chi^j + 2R^{ab}_i \phi^j_b), \tag{A12}$$

and the integrability conditions

$$\gamma^{i}_{\alpha j}\sigma^{A}_{i}B^{j}_{A} = 0 \ , \qquad (A13)$$

which determine the balance of moment of momentum.

Finally, we note that the theory [1] has been constructed in such a way that the nonexact gauge condition must be satisfied. Namely,

$$x^{a}\phi^{i}_{a}=0, \qquad x^{a}W^{\alpha}_{a}=0. \qquad (A14)$$

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Received by Publishing Department
on February 6, 1990.