FIELD THEORY OF CRYSTAL DEFECT STRUCTURE

A.I. OLEMSKOI AND A.V. KHOMENKO

Sumy State University
2, Rimskii-Korsakov St., 40007 Sumy, Ukraine

Abstract. A description of single defects is carried out within the gauge theory where the compensating field represents the elastic shear and the material field, being a complex order parameter, describes long–range correlations in variation of potential relief of structural units (atoms). Dislocation as a localized material field of the shear and disclination as a localized rotation field are represented on the basis of simple variant of U(1) theory. A description of a point defect leads to non Abelian SU(2) theory with components of gauge field being relevant to different polarizations of elastic wave.

1. Introduction

At present time the geometrical models of crystal defects based on obvious or topological considerations are worked out and generally accepted [1, 2]. They allow the continual description of elastic fields created by these defects [2]. Nevertheless, these models do not describe the real structure of defects kernels. For example, there is no explanation for anomalous high values of a diffusion coefficient along dislocation tubes.

Thus, the problem appears, within the framework of which the material field accounting the atomic structure of defects should be described and a force field created by these defects has to be reproduced. It turns out that the basis for representation of the former is the conception of rearrangeable potential relief [3]. It allows self–consistent picture representing defect structure within field approach.

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2. Field Theory of Crystal Defects

Let us consider the spatial distribution of a field that characterizes the structure level of defects at steady state. For this purpose, it is necessary to introduce a field $U(\mathbf{x})$ conjugated to a material field $\rho(\mathbf{x})$ that characterizes distribution of structural units on the initial (atom) level. The later field realizes a basis of irreducible representations of initial group of the system symmetry. The distribution of the material field specifies thermodynamic potential $\Phi\{\rho(\mathbf{x})\}$ whose variation gives conjugate field [3]

$$U(\mathbf{x}) = \frac{\delta\Phi(\mathbf{x})}{\delta\rho(\mathbf{x})} \tag{1}$$

being determined analogously to energy of elementary excitations of many-particle system [4]. Physically, this field represents the potential relief of structural units on the initial level (for example, the field $U(\mathbf{x})$ gives the Paierls relief for dislocation distribution [5]).

A system deviation from equilibrium results in excitation of ensemble of structural units, which is displayed in a smearing of the potential relief. Related probability of steady state distribution $U(\mathbf{x})$ is determined by Boltzmann–like form

$$P\{U(\mathbf{x})\} \propto \exp\left(-\frac{V\{U(\mathbf{x})\}}{\Theta}\right) \tag{2}$$

which is given by the corresponding functional of the synergetic potential $V\{U(\mathbf{x})\}$ and excitation intensity Θ [3]. By definition, the functional order parameter that characterizes new defect level is given by long-range correlations of variation $\delta U(\mathbf{x}') = U(\mathbf{x}') - \langle U(\mathbf{x}')\rangle$ with respect to a deviation $\delta U(\mathbf{x}) = U(\mathbf{x}) - \langle U(\mathbf{x})\rangle$ fixed at $\mathbf{x} = \mathbf{const}$:

$$\lim_{|\mathbf{x}'-\mathbf{x}|\to\infty} \frac{\langle\delta U(\mathbf{x})\ \delta U(\mathbf{x}')\rangle}{\langle|\delta U(\mathbf{x})|^2\rangle} \equiv \varepsilon^2(\mathbf{x}) \tag{3}$$

where the averaging is performed over distribution (2). Here, the change in characteristic length on new level is displayed as follows: if the potential relief $U(\mathbf{x})$ oscillates over small distances $x \sim a$ being microscopic, then macroscopic order parameter $\varepsilon(\mathbf{x})$ varies at much more distances $x \geq \xi$ which scale $\xi \gg a$ corresponds to new level. To take into account such scaling, it is convenient to introduce complex field of order parameter

$$\epsilon(\mathbf{x}) = \varepsilon(\mathbf{x})e^{i\varphi(\mathbf{x})} \tag{4}$$

where variation of the phase $\varphi(\mathbf{x})$ is observed at microscopic distances $x \sim a$. Then, transition from initial scale a to new one ξ implies spontaneous breaking conformal invariance being realized below within the framework of a gauge field scheme.

The simplest case of a scalar parameter (4) is characterized by the symmetry group U(1) that makes *external* four–dimensional coordinate x_μ, $\mu = 0, 1, 2, 3$ ambiguous for new level (here $x_0 = ct$, c is velocity of transversal sound) [3]. This ambiguity reflects the appearance of defects and can be compensated by prolongation of the derivative:

$$\partial^\mu \equiv \frac{\partial}{\partial x_\mu} \Rightarrow \nabla^\mu \equiv \partial^\mu + \Gamma^\mu, \quad \mu = 0, 1, 2, 3 \tag{5}$$

where Γ^μ is the 4–potential of the corresponding gauge field. From geometrical point of view Γ^μ is the connectivity in the stratification, which is a nontrivial generalization of the direct product of a manifold of initial structural units and gauge group U(1) [6]. To study new structure level, it is convenient to use associated stratification, considering at each point x^μ not the transformations of the gauge group, but the corresponding potential Γ^μ whose value is associated with 4–vector of displacements $A^\mu \equiv (\varphi, \mathbf{u})$, $\mu = 0, 1, 2, 3$ by the equality $\Gamma^\mu = -\mathrm{i} g A^\mu$ where g is elastic charge [3].

Within four–dimensional representation, we consider the simplest Ginzburg-Landau scheme whose material Lagrangian

$$\mathcal{L}_m \equiv L_m - L_c \tag{6}$$

is determined by usual term

$$L_m = \frac{\beta}{2} |\nabla^\mu \epsilon|^2 - V(\epsilon) \tag{7}$$

with gradient constant $\beta > 0$ and synergetic potential $V(\epsilon)$. The diminution L_c takes into account a specific integral condition for field distribution being relevant to a defect:

$$\oint \Gamma_\mu \mathrm{d}x^\mu = w \oint \mathrm{d}\varphi = 2\pi w n, \quad n = 0, \pm 1, \dots \tag{8}$$

According to this condition, defects play the role of elementary carriers of gauge fields to make a manifold of defect crystal multiply connected. It is easily to see that the constraint (8) is a result of spontaneous breaking of conformal invariance related to the Lagrangian

$$L_c = \nu_\mu \left(\nabla^\mu \varepsilon - w \varepsilon \partial^\mu \varphi\right) \tag{9}$$

with respect to variation of Lagrange multiplier ν_μ. Actually, relevant differential constraint reads:

$$(\partial^\mu + \Gamma^\mu)\varepsilon = w \varepsilon \partial^\mu \varphi. \tag{10}$$

Since the external coordinate x^μ corresponds to a change in the phase $\varphi(x^\mu)$ at distances $x^\mu \sim a$ while the internal coordinate should describe a variation of the amplitude $\epsilon(x^\mu)$ at $x^\mu \geq \xi$, one obtains the condition $\xi = a/w$ which fixes the scale ξ by the assignment of the parameter $w \ll 1$ (a is given *a priori*). On the other hand, the gauge choice

$$\Gamma^\mu = \partial^\mu(-\ln\varepsilon + w\varphi), \tag{11}$$

reducing Eq. (10) to identity, gets many–valued field Γ^μ obeying to the constraint (8) needed.

The equation for material field following from Eq. (6) takes the form

$$\partial^\mu\partial_\mu\epsilon = \Gamma^\mu\Gamma^*_\mu\epsilon + \beta^{-1}\frac{\partial V}{\partial\epsilon^*} \tag{12}$$

where the gauge condition $\partial^\mu\Gamma_\mu = 0$ has been taken into account. Here, the order parameter ϵ varies at correlation length ξ, whereas the 4–displacement $A^\mu \equiv (\varphi, \mathbf{u})$ related to the gauge field $\Gamma^\mu = -igA^\mu$ does at microscopic distance a. Then, elastic charge g and correlation length ξ are determined by equalities

$$g = \frac{1}{\xi a}; \qquad \xi^2 = \frac{\beta}{|A|}, \quad A \equiv \left.\frac{\partial^2 V}{\partial\varepsilon^2}\right|_{\varepsilon = 0} \tag{13}$$

and the scale ratio $w \equiv a/\xi \ll 1$ takes the magnitude

$$w = ga^2. \tag{14}$$

3. Description of Disclination and Dislocation

Within the framework of the field approach developed, let linear defects be represented as autolocalized regions possessing rearranged potential relief. A defect kernel is described by distribution $\epsilon(\mathbf{r})$ of a relief rearrangement parameter over spatial components of radius–vector $\mathbf{r}$. A conjugated field is specified by an elastic component of a 4-vector of static displacement $A^\mu_e = (\varphi_e, \mathbf{u}_e)$ reduced to 4-potential of a gauge field. Corresponding strengths

$$\chi_e = -\frac{\partial\mathbf{u}_e}{c\partial t} - \mathrm{grad}\varphi_e, \quad \omega_e = \mathrm{curl}\ \mathbf{u}_e \tag{15}$$

represent elastic components of shift and rotation vectors. The material component $A^\mu_m = (\varphi_m, \mathbf{u}_m)$ is related to coherent displacement of minima and smearing of a potential relief. The gauge symmetry is connected with invariance of medium characteristics relative to translation and rotation of a specimen as a whole. A charge (13) is determined by inherent atomic distance a and correlation length ξ to be characteristics of the material field. Moreover, there is the third scale

$$\lambda = \frac{\nu}{c}; \qquad \nu \equiv \frac{\eta}{\rho}, \quad c^2 \equiv \frac{\mu}{\rho} \tag{16}$$

to determine a length of elastic field smearing (here ρ, η and μ are density, shear viscosity and related elastic modulus of medium, respectively). The system behavior is determined by value of Landau–Ginzburg parameter

$$\kappa = \frac{\lambda}{\xi} \equiv \frac{\eta}{\xi\sqrt{\rho\mu}}. \tag{17}$$

In weakly excited state the crystal possesses so large shear viscosity η that one has the values $\kappa \gg 1$. Under such a condition distributions of material and elastic fields have soliton–like form type of Gross–Pitayevskii soliton [3]. Here, rotation field $\omega(\mathbf{r})$ corresponds to disclination whereas shear field $\chi(\mathbf{r})$ does to dislocation. Let study conditions for realization of the first type solutions.

In real crystal there are stress concentrators always. Let one of them creates a homogeneous rotation field ω_{ext} over distances $x \le \lambda$. If, in addition, the local rearrangement of atomic system takes place over distances $x \le \xi$, at critical value $\omega_{\text{ext}} = \omega_c$ the situation is realized when variation of thermodynamic potential

$$\Phi = \mathcal{L}_m + L_f \tag{18}$$

becomes decreasing. Here, material component $\mathcal{L}_m$ is given by Eqs. (6), (7), (9) with synergetic potential

$$V = \frac{A}{2}|\epsilon|^2 + \frac{B}{4}|\epsilon|^4 \tag{19}$$

where A and B are material constants. The field addition is specified as

$$L_f = \frac{1}{4}\left(\partial^\mu A^\nu - \partial^\nu A^\mu\right)^2 - \frac{1}{c}A^\mu j_\mu \tag{20}$$

where $A^\mu(\mathbf{r}, t)$ is a 4-potential of the gauge field, c is sound velocity, $j^\mu = (\rho c, \mathbf{j})$ is a 4–current.

Using expressions (6), (7), (9), (18) — (20), it is easy to show that a condition $\Delta\Phi = 0$ for variation of thermodynamic potential is realized if external field is reduced to critical one ω_c defined by relation

$$\omega_c^2 = \frac{1}{2}|a|\varepsilon_0^2 \tag{21}$$

where ε_0 is the order parameter at steady state. The variation of thermodynamic potential connected with creation of new phase

$$\Delta\Phi \equiv \int [\Phi(\epsilon) - \Phi(\epsilon = 0)]\, d\mathbf{r} \tag{22}$$

takes the explicit form [4]

$$\Delta\Phi = \rho c^2\omega_c^2 \int \left[-\left(1 - \mathbf{u}_e^2\right)\varepsilon^2 + \frac{1}{2}\varepsilon^4 + \kappa^{-2}\left(\frac{d\varepsilon}{d\mathbf{r}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \mathrm{curl}\ \mathbf{u}_e\right)^2 \right] d\mathbf{r}. \tag{23}$$

Here $\mathbf{u}_e$ is elastic displacement, the coordinate $\mathbf{r}$ is measured in units of the length λ. Then, static Euler equations

$$\kappa^{-2}\nabla^2\varepsilon = -(1 - \mathbf{u}_e^2)\varepsilon + |\epsilon|^2\varepsilon, \tag{24}$$

$$-\mathrm{curl\ curl}\ \mathbf{u}_e = |\epsilon|^2\mathbf{u}_e \tag{25}$$

and variation of thermodynamic potential (23) are equivalent to corresponding equations of Ginzburg – Landau – Abrikosov theory for a vortical (mixed) state of a superconductor [4] where an elastic component $\mathbf{u}_e$ of displacement vector is meant as vector potential and a rotation vector $\omega_e = \mathrm{curl}\ \mathbf{u}_e$ is understood as magnetic field. Having in mind this analogy, let the main results of theory [4] apply to the case under consideration.

The mixed state is realized provided $\kappa > 1/\sqrt{2}$ within the interval of rotation field $\omega_{c1} < \omega_{\rm ext} < \omega_{c2}$ where

$$\omega_{c1} = \frac{\ln\kappa}{\sqrt{2}}\omega_c, \quad \omega_{c2} = \sqrt{2}\kappa\omega_c. \tag{26}$$

Near ω_{c2} the closed packed lattice of vortical threads is formed: at $\omega_{\rm ext} = \omega_{c2}$ threads density N per unit of area is maximum and amounts to value $N_{\max} = 1/\pi\xi^2$; at $\omega_{\rm ext}$ decreasing in a region $\omega_{c2} - \omega_{\rm ext} \ll \omega_{c2}$ it varies according to the equality

$$\frac{N}{N_{\max}} = \frac{\omega_{\rm ext}}{\kappa} - \frac{\overline{\varepsilon^2}}{2\kappa^2} \tag{27}$$

where average over volume $\overline{\varepsilon^2}$ is connected with a rotation vector magnitude $\omega_{\rm ext}$ by equality

$$\overline{\varepsilon^2} = \frac{2\kappa}{\beta(2\kappa^2 - 1)}(\kappa - \omega_{\rm ext}), \quad \beta \equiv \overline{\varepsilon^4}/(\overline{\varepsilon^2})^2 = 1.1596. \tag{28}$$

The average value

$$\overline{\omega_e} = \omega_{\rm ext} - \overline{\varepsilon^2}/2\kappa = \omega_{\rm ext} - (\kappa - \omega_{\rm ext})/\beta(2\kappa^2 - 1) \tag{29}$$

is smaller than applied field in a quantity being equal to the average of a medium polarization

$$\overline{\omega_m} = -\overline{\varepsilon^2}/2\kappa = -(\kappa - \omega_{\text{ext}})/\beta(2\kappa^2 - 1). \qquad (30)$$

The maximum value of a rotation vector field is reached in threads cores, and the minimum one $\omega_{\min} = \omega_{\text{ext}} - \sqrt{2}(\kappa - \omega_{\text{ext}})/(2\kappa^2 - 1)$ — in the centers of triangles formed by threads. The average variation of thermodynamic potential (18) caused by medium rotation

$$\overline{\Delta\Phi} = \rho c^2 \omega_c^2 \left(\frac{1}{2} + \overline{\omega_e^2} - \frac{\overline{\varepsilon^4}}{2} \right) = \rho c^2 \omega_c^2 \left[\frac{1}{2} + \overline{\omega}_e^2 - \frac{(\kappa - \overline{\omega}_e)^2}{1 + \beta(2\kappa^2 - 1)} \right] \qquad (31)$$

is the function of the average turning $\overline{\omega}_e$ differentiation with respect to which results in Eq. (29).

Near the lower critical value ω_{c1} threads density $N = (\kappa/2\pi)\overline{\omega}_e$ is not large and they can be treated independently. Taking into account that $u_e(r)$ varies at distances $r \sim 1$ and $\varepsilon(r)$ does at $r \sim \kappa^{-1}$, the displacements are determined by Eq. (25) with $|\epsilon|^2 \approx 1$ and $\kappa \gg 1$:

$$u_e = -\kappa^{-1} K_1(r) \qquad (32)$$

where $K_1(\mathbf{r})$ is the Hankel function of imaginary argument. Respectively, the order parameter is determined by Eq. (24) with $u_e = 1/\kappa r$:

$$\begin{aligned} \varepsilon &\simeq c_1 r \quad \text{at} \quad r \ll \kappa^{-1}, \\ \varepsilon^2 &\simeq 1 - (\kappa r)^{-2} \quad \text{at} \quad r \gg \kappa^{-1} \end{aligned} \qquad (33)$$

where c_1 is positive constant. According to Eq. (32) one has $u_e \approx -1/\kappa r$ at $r \ll 1$ and $u_e \approx -\sqrt{\pi/2\kappa^2}\, r^{-1/2} e^{-r}$ at $r \gg 1$. The dependence $\overline{\omega}_e(\omega_{\text{ext}})$ is of steadily increasing nature: at $\omega_{\text{ext}} = \omega_{c1}$ it has the vertical tangent and with ω_{ext} growth it asymptotically approaches to the straight line $\overline{\omega}_e = \omega_{\text{ext}}$. Thermodynamic potential per thread length unit is $(2\pi/\kappa^2)\ln\kappa$. The ω_e value in a thread center is twice as large as ω_{c1}.

The described system of vortical threads related to rotation field ω_{ext} corresponds to periodical distribution of rectilinear disclinations. In the same way, it can be shown that the mixed state formed by threads in a shear field χ_{ext} is possible as well to be corresponded to a system of rectilinear dislocations. To prove the above, it is necessary to determine the law of strength field decrease near the threads. Within the framework of the field scheme the function of this field components is performed by material components of strength vectors: ω_m — for disclination and χ_m — for dislocation. Thus, it is necessary to reestablish dependencies $\omega_m(r)$,

$\chi_m(r)$ by the obtained dependence $\mathbf{u}_e(r)$. In order to do this, let the elastic part of current be written down:

$$\mathbf{j}_e = -\beta g^2 c|\epsilon|^2 \mathbf{u}_e. \tag{34}$$

As it is evident from the motion equation written in the form

$$\Delta \mathbf{u} = \text{curl}\, \omega_m + \frac{\partial \chi_m}{c\partial t} + \frac{\mathbf{j}}{c}, \tag{35}$$

the material fields ω_m, χ_m relevant to defects causes the current

$$\mathbf{j}_m = c\, \text{curl}\, \omega_m + \frac{\partial \chi_m}{\partial t}. \tag{36}$$

At steady state one has $\mathbf{j}_e + \mathbf{j}_m = 0$ and for the case of simple rotation ($\chi_m = 0$) within actual region $\kappa^{-1} < r < 1$ where $u_e \propto r^{-1}$ it follows from Eqs. (34), (36) that creation of a localized rotation thread results in variation of the external field ω_{ext} by value $\omega_m \propto \ln r$. Respectively, in a shear field one has $\chi_m \propto r^{-1}$. Since it is in this way that the stress of the elastic field decreases near disclinations and dislocations [1], it can be concluded that the described mixed state represents an ensemble of crystal structure linear defects.

In real case the appearance of defects, being localized carriers of plastic deformation, is caused by stress concentrators providing the system transition into the region $\omega_{c1} < \omega_{\text{ext}} < \omega_{c2}$ (or $\chi_{c1} < \chi_{\text{ext}} < \chi_{c2}$) of mixed state even with lack of external load. The main condition of realization of this inequalities is utmost large values of the parameter κ ($1 \ll \ln \kappa \ll \kappa$) giving a very small lower critical field and the large upper one in accordance with Eqs. (26). Therefore, in a real crystal there is a stable system of lattice defects (with the exception of thread type crystals where in view of potential relief stiffness resulting in large values of a gradient parameter β the quantity κ is small).

The consideration carried out above shows that a linear defect represents an autolocalized formation corresponding to a small domain of rearranged potential relief $U(\mathbf{r})$ and to a considerable region of the elastic field distribution. The coordinate dependence of the corresponding fields is shown in Fig. 1a. Since relief $U(\mathbf{r})$ rearrangement in the region of a defect kernel is reduced to smearing into ensemble $\{U(\mathbf{r})\}$ and a field switching results in contribution of energy $-\chi_m(\mathbf{r})$ to the total potential, the potential relief picture near the defect has the form shown in Fig. 1b. It is smeared within a kernel region that causes increase of a tube diffusion coefficient due to considerably decrease of effective height of the barrier. The elastic field is expressed in variation of a reference level and quick oscillations of potential $U(\mathbf{r})$ at interatomic distances.

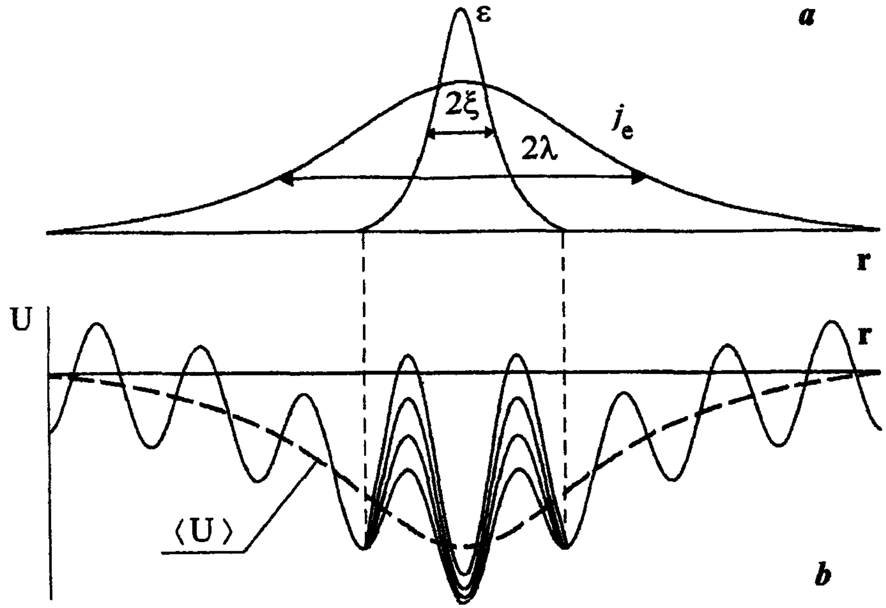

Figure 1. a: Coordinate dependence of material deformation field ε and elastic stress field j_e near a defect. b: Corresponding form of the potential relief

4. Non Abelian Field Theory of Point Defect

It seems at the first glance that the point defect, being the simplest one in geometrical form, have to be described by a simple variant of the field theory. Such insight is based on naive representation that the point defect is a result of shrinking three orthogonal dislocation loops [2]. But it needs to keep in mind that this model implies junction of dislocation kernels which arrives at a new type of the field singularity being fundamentally non-linear in nature. It turned out that, besides above solutions that belong to Abelian gauge groups, the SU(2)-symmetry leads to new solution related to topology change in distribution of plastic deformation being relevant to the point defect [3]. Let us consider main statements of corresponding field scheme.

In this case, the order parameter ϵ_a has three components numbered by polarizations $a = 1, 2, 3$ of related displacement waves. Moreover, two-component material field Ψ_a describes a structural unit distribution for each polarization a to realize a basis of the gauge group (the components correspond to excited and unexcited states — in accordance with dimensionality of generators $\hat{\tau}^\mu$ of the group SU(2) which are the Pauli matrices [6]). Material component of generic Lagrangian has the form [7]

$$L_m = \mathrm{i}\beta^{1/2}\overline{\Psi}_a\hat{\tau}^\mu\nabla_\mu^{ab}\Psi_b + \frac{\beta}{2}\left|\nabla_\mu^{ab}\epsilon_b\right|^2 - \omega j^a\epsilon_a - \frac{B}{4}\left|\epsilon_a\right|^4 \tag{37}$$

where β, ω and B are constants, $\nabla_\mu^{ab} = \partial_\mu\delta_{ab} + \varepsilon_{abc}\Gamma_\mu^c$, $j^a = \mathrm{i}\varepsilon_{abc}\overline{\Psi}^b\Psi^c$ is the current of structural units, ε_{abc} is structural constant which is reduced to the antisymmetric tensor. Similar to all non Abelian models, the Lagrangian (37) results in both asymptotic freedom and confinement. These facts reflect the long–range order in distribution of structural units over excited and unexcited states.

Variation of the action corresponding to Eq. (37) with respect to the fields $\Psi_a(x^\mu)$ results in equation of Weyl–type

$$(\hat{\tau}^\mu\partial_\mu\delta_{ab} - \mathrm{i}\varepsilon_{abc}\hat{\tau}^\mu\Gamma_\mu^c + \omega\beta^{-1/2}\varepsilon_{abc}\hat{I}\epsilon^c)\Psi^b = 0 \tag{38}$$

where $\hat{I}$ is 2×2 unit matrix. It is typical that the term that contains the order parameter (the plastic deformation field $\epsilon^c(x^\mu)$) performs the function of the mass of bare "fermions" that are reduced to the structural units distributed over excited and unexcited states. Using Eq. (38) allows to eliminate the field $\Psi_a(x^\mu)$ in the Lagrangian (37) to reduce the latter to the form (6) where potential $V(\epsilon^a)$ is given by Landau–type expansion with a minimum at the point $|\epsilon_0^a| = \mathrm{i}\omega|\Psi^a|$. This means that dispersion law (the mass) ω of bare "fermion" has to be of imaginary nature. As a result of exchange with Higgs bosons, corresponding to the field of plastic deformation, between the fermions, which are the structural units, the gauge symmetry is spontaneously broken. Longitudinal component ϵ^1 of the plastic deformation takes on a fixed value ϵ_0^1, and the two transversal components ϵ^2, ϵ^3 transform into Goldstone bosons of restoration of SU(2)–symmetry, i.e., they become the elastic components e^2 and e^3 of the strain field. Conversely, for the corresponding components Γ_μ^2 and Γ_μ^3 of the potential of the stress $\hat{\sigma}$, the dispersion law acquires a plastic character, while for the longitudinal component Γ_μ^1 it remains elastic.

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