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The problem of energy of kinks of dislocation lines

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THE PAPER deals with the problem of energy of inflections (kinks) of dislocation lines in the pseudo-continuum model of D. Rogula. The calculations are performed for the simple model of an isotropic pseudo-continuum thus enabling us to take into account the dispersion phenomena occurring in the crystal and certain details of the structure of dislocations. The energy is evaluated for the case of stationary dislocations; the resulting formula is suitable for further discussion and separates the influences of the structure of the medium from those of the dislocation structure.

Praca poświęcona jest badaniu energii przegięcia na linii dyslokacji w modelu pseudo-kontinuum Roguli. Obliczenia przeprowadzone są dla prostego modelu pseudo-kontinuum izotropowego; pozwala on uwzględnić dyspersję w krysztale oraz szczegóły struktury dyslokacji. Energia obliczona jest dla przypadku dyslokacji stacjonarnej. Otrzymano dogodny do dyskusji wzór, pozwalający na badanie wpływu dyspersji, kształtu przegięcia i struktury dyslokacji na energię przegięć.

В работе исследуется энергия перегиба на дислокационной линии в рамках модели псевдоконтинуума Рогули. Расчеты выполнены для случая простой модели изотропного псевдоконтинуума; эта модель позволяет учесть дисперсию в кристалле и детали структуры дислокации. Энергия вычислена для случая стационарной дислокации. Получена удобная для анализа формула, в которой влияние структуры материала и структуры дислокации разделены.

THE CAUSE of failures of all former attempts at determination of the energy of kinks of dislocation lines may be attributed mainly to an unsuitable choice of the model of continuum containing the dislocation. The definition of kink as a transition domain in the slip plane, connecting two rectilinear dislocation segments lying along the atom lines in a crystal indicates that the notion of an kink is principally related to the crystal. In a continuous medium, we should speak rather of a dislocation consisting of a number of rectilinear segments inclined one to an other at certain angles. Investigations of kinks on the basis of continuous media cannot be fruitful, and it proves necessary to take into account the crystalline structure of the medium and also the structure of the kink itself. The model which satisfies the above requirements and is, at the same time, energetically consistent and mathematically correct is the pseudo-continuum model (ROGULA 1965, KUNIN 1966). This paper is based on the pseudocontinuum model introduced by ROGULA.

The dislocation equations have the same form as in a continuous medium, namely:

$$\varrho\dot{v}_i - S_{ik,k} = 0, \quad \varepsilon_{klm}\beta_{im,l} = \alpha_{im}, \quad \dot{\beta}_{lm} - v_{l,m} = +J_{lm}. \tag{1}$$

Here β_{ij} is the distortion tensor, v_i — dislocation velocity, α_{ij} — dislocation density tensor, J_{ij} — dislocation flux tensor, and S_{ik} corresponds to the Kirchhoff stress tensor. The tensors and J are subject to additional conditions

(2) $$\alpha_{ik,k} = 0, \quad \dot{\alpha}_{ik} - \varepsilon_{klm} J_{im,l} = 0;$$

S is a functional of β, and in the linear approximation

(3) $$S_{ij}(\mathbf{x}) = \sigma_{ij}(\mathbf{x}) = \int c_{ijlm}(\mathbf{x}-\mathbf{x}')\beta_{lm}(\mathbf{x}')d_3x'.$$

The Eqs. (1) and (2), in spite of their continual form, describe the discrete system; all functions appearing in these equations are obtained by means of interpolation of discrete functions defined on the discrete system represented by the crystal. The proper selection of the class of interpolation functions is of essential significance for the pseudo-continuum model. From the considerations of small vibrations of crystals it follows that they should be rational functions of three variables representing Fourier transforms of distributions with a compact support in the closure of the first Brillouin zone. The class of functions is denoted by PC. Each function $f(\mathbf{x})$ of the PC class corresponds to a discrete function f^n increasing at infinity not more rapidly than a polynomial. When the crystal class is changed, the PC class must also be changed.

When the relation (3) is satisfied, and the tensors α and J are known, we are able to find a general solution of the Eqs. (1) with the conditions (2), expressing β and v in terms of α, J and G — that is, to determine the Green function for small acoustic vibrations. It is the solution of the following equation:

$$\varrho \frac{\partial^2}{\partial t^2} G_{in}(\mathbf{x}, \mathbf{x}', t, t') - \int d_3x'' c_{iklm}(\mathbf{x}-\mathbf{x}'') \frac{\partial^2}{\partial x''_m \partial x''_k} G_{ln}(\mathbf{x}'', \mathbf{x}', t, t') = \delta^P(\mathbf{x}-\mathbf{x}')\delta(t-t')\delta_{in},$$

where

$$\delta^P(\mathbf{x}-\mathbf{x}') = \frac{1}{(2\pi)^3} \int_B d_3k e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}.$$

Consequently, the expressions for β and v have the form

(4) $$\beta_{ij}(\mathbf{x}, t) = \int d_3x' dt' G_{in}(\mathbf{x}-\mathbf{x}', t-t') \cdot \Big[\varrho \frac{\partial J_{nj}(\mathbf{x}', t')}{\partial t'} - \int d_3x'' c_{nklm}(\mathbf{x}'-\mathbf{x}'') \varepsilon_{mjs} \frac{\partial}{\partial x''_k} \alpha_{ls}(\mathbf{x}'', t') \Big],$$

(5) $$v_i(\mathbf{x}, t) = \int d_3x' dt' G_{in}(\mathbf{x}-\mathbf{x}', t-t') \int d_3x'' c_{nklm}(\mathbf{x}'-\mathbf{x}'') \frac{\partial}{\partial x''_k} J_{lm}(\mathbf{x}'', t').$$

A discussion of these equations in the general, anisotropic case is somewhat complicated and intricate; on the other hand, it is not generally possible to determine the exact anisotropic structure of the tensor α. In our case, let us confine ourselves to the isotropic pseudo-continuum defined by the following conditions:

1. Tensor $c_{iklm}(\mathbf{k})$ depends solely on the absolute value of the vector $\mathbf{k}$;

2. The tensorial structure of c_{iklm} is the same as for the classical elastic continuum,

$$c_{ijlm}(k) = \varrho[c_1^2(k)-c_2^2(k)]\,\delta_{ij}\delta_{lm}+\varrho c_2^2(k)\,[\delta_{il}\delta_{jm}+\delta_{im}\delta_{jl}]. \tag{6}$$

3. The Brillouin zone is replaced by a sphere of radius $k_m \approx \pi/b$. The isotropic continuum enables determination of the kink energy, both the dispersion within the crystal and the structural details of dislocation being taken into account. It seems that we can dispense with a simultaneous investigation of anisotropy, which is of secondary importance for energy considerations.

The elastic energy of a dislocation line in the pseudo-continuum is determined as follows:

$$W = \frac{1}{2}\int\int c_{nklm}(\mathbf{x}-\mathbf{x}')\beta_{nk}(\mathbf{x})\beta_{lm}(\mathbf{x}')\,d_3x\,d_3x' = \frac{1}{2}\frac{1}{(2\pi)^3}\int c_{nklm}(\mathbf{k})\beta_{nk}(\mathbf{k})\beta_{lm}(-\mathbf{k})\,d_3k. \tag{7}$$

Tensorial structure of this expression is analogous to that of an elastic continuum; however, we shall take into account the spatial dispersion which yields the dependence of c_{nklm} on $\mathbf{k}$. The energy is determined in the space $\mathbf{x}$, but it will be instantaneously transformed to the $\mathbf{k}$-space, since it is known that in problems dealing with crystals it may serve as the most adequate mathematical tool. If our considerations were confined to stationary dislocations, $\beta_{ij}(\mathbf{x})$ would be given by the formula

$$\beta_{ij}(\mathbf{x}) = -\int\int d_3x'\,d_3x''\,c_{nklm}(\mathbf{x}'-\mathbf{x}'')G_{in}(\mathbf{x}-\mathbf{x}')\,\varepsilon_{mjs}\frac{\partial}{\partial x_k''}\alpha_{ls}(\mathbf{x}''), \tag{8}$$

$\beta_{ij}(\mathbf{x})$ is a function of class PC and thus may be represented by the integral

$$\beta_{ij}(\mathbf{x}) = \frac{1}{(2\pi)^3}\int e^{i\mathbf{k}\cdot\mathbf{x}}\beta_{ij}(\mathbf{k})\,d_3k, \tag{9}$$

where

$$\beta_{ij}(\mathbf{k}) = c_{nklm}(\mathbf{k})G_{in}(\mathbf{k})\varepsilon_{mjs}ik_k\alpha_{ls}(\mathbf{k}). \tag{10}$$

The expression (10) being inserted into the Eq. (7), the general expression for energy is obtained. Tensor c appears in that expression three times, G — twice; consequently, W contains several scores of terms which makes any calculations extremely tedious. Let us then try to find a different, simpler form of the expression. Differentiation of both sides of the Eq. (7) with respect to time yields

$$\dot{W} = \int\int \frac{\partial\beta_{uk}(\mathbf{x},t)}{\partial t}c_{nklm}(\mathbf{x}-\mathbf{x}')\beta_{lm}(\mathbf{x}',t)\,d_3x\,d_3x'.$$

Using the Eqs. (1), (2), this expression is transformed to

$$\dot{W} = \int\int v_{i,k}(\mathbf{x},t)c_{nklm}(\mathbf{x}-\mathbf{x}')\beta_{lm}(\mathbf{x}',t)\,d_3x\,d_3x' + \int J_{nk}(\mathbf{x},t)c_{nklm}(\mathbf{x}-\mathbf{x}')\beta_{lm}(\mathbf{x}',t)\,d_3x\,d_3x',$$

J_{nk} is now represented in the form:

$$J_{nk} = \frac{\partial \tilde{\beta}_{nk}}{\partial t} + \varphi_{n,k}$$

whence

$$\dot{W} = \int\int \frac{\partial \tilde{\beta}_{nk}(\mathbf{x}, t)}{\partial t} c_{nklm}(\mathbf{x}-\mathbf{x}')\beta_{lm}(\mathbf{x}', t) d^3x d^3x'$$
$$+ \int\int [\varphi_{n,k}(\mathbf{x}, t) + v_{n,k}(\mathbf{x}, t)] c_{nklm}(\mathbf{x}-\mathbf{x}')\beta_{lm}(\mathbf{x}', t) d_3x d_3x'.$$

Integrating this expression by parts, and using the equations of motion we finally obtain, for stationary dislocations, the formula

(11) $$W = \frac{1}{2}\int\int \tilde{\beta}_{nk}(\mathbf{x}) c_{nklm}(\mathbf{x}-\mathbf{x}')\beta_{lm}(\mathbf{x}') d_3x d_3x'.$$

Here $\tilde{\beta}$ and β satisfy the following relations

(12) $$\begin{gathered} \varepsilon_{klm}\beta_{im,l} = \alpha_{ik}, \qquad \varepsilon_{klm}\tilde{\beta}_{im,l} = \alpha_{ik}, \\ \frac{\partial \beta_{nk}}{\partial t} = J_{nk} + v_{n,k}, \qquad \frac{\partial \tilde{\beta}_{nk}}{\partial t} = J_{nk} - \varphi_{n,k}; \end{gathered}$$

φ is an arbitrary function. β should fulfil, in addition, the equations of motion:

$$\int c_{nklm}(\mathbf{x}-\mathbf{x}')\beta_{lm,k}(\mathbf{x}') d_3x' = 0.$$

An additional condition is also imposed upon $\tilde{\beta}$

(13) $$\tilde{\beta}_{nk,k} = 0.$$

The value of $\tilde{\beta}$, which satisfies all the conditions prescribed above, has the form:

(14) $$\tilde{\beta}_{ij}(\mathbf{k}) = -\frac{ik_k \varepsilon_{kjs}\alpha_{is}(\mathbf{k})}{k^2}.$$

Finally, the energy of an arbitrary dislocation may be written in the following form:

(15) $$W = \frac{1}{16\pi^3}\int d_3k\, c_{nklm}(k) c_{rwip}(k) G_{nr}(\mathbf{k})\varepsilon_{pka}\varepsilon_{smb}k_w k_s \alpha_{ia}(\mathbf{k})\alpha_{lb}(-\mathbf{k})\frac{1}{k^2};$$

α is the dislocation density tensor. It is defined by means of the Burgers vector (which might be interpreted as a quantity determining the dislocation intensity) and a certain function depending on the form and structure of the dislocation,

(16) $$\alpha_{ik}(\mathbf{x}) = b_i \int\limits_L \chi(\mathbf{x}-\mathbf{x}') dx'_k.$$

The integration is performed along the dislocation line.

The function $\chi(\mathbf{x}-\mathbf{x}')$ itself depends on the model of dislocation assumed — e.g., the dislocation line corresponds to a delta-like function.

The Fourier transform of $\alpha_{ik}(\mathbf{x})$ has the form

(17) $$\alpha_{ik}(\mathbf{k}) = b_i\chi(\mathbf{k}) \int\limits_L e^{i\mathbf{k}\cdot\mathbf{x}} dx_k.$$

Substituting this expression in the Eq. (16), we obtain:

$$W = \frac{1}{16\pi^3} \int d_3 k A_{abil}(\mathbf{k}) b_i b_l \chi(\mathbf{k}) \chi(-\mathbf{k}) \psi_{ab}(\mathbf{k}), \tag{18}$$

where

$$A_{abil} = c_{nklm}(\mathbf{k}) c_{rwip}(\mathbf{k}) G_{nr}(\mathbf{k}) \varepsilon_{pka} \varepsilon_{smb} \frac{k_w k_s}{k^2}, \tag{19}$$

$$\psi_{ab}(\mathbf{k}) = \int_L e^{-i\mathbf{k}\cdot\mathbf{x}} dx_a \int_L e^{i\mathbf{k}\cdot\mathbf{x}'} dx_l'. \tag{20}$$

Let us now pass to the expression determining the energy of two kinks on a dislocation line. Assume a definite reference frame in which the dislocation line coincides

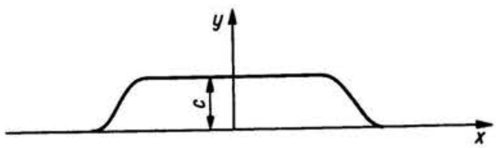

FIG. 1.

with the OX-axis, the slip plane is OXY, and the Burgers vector has the components $\mathbf{b} = [b_1, b_2, 0]$. The dislocation line itself is then given by the function $y = y(x)$.

Let us consider the integrals appearing in the expressions (20) for the dislocation line with two kinks shown in Fig. 1.

$$a = 1 \quad \int_L e^{\pm i\mathbf{k}\cdot\mathbf{x}} dx = \int_{-\infty}^{\infty} e^{\pm ik_1 x} e^{\pm ik_2 y(x)} dx = 2\pi\delta(k_1) + 2\int_0^{\infty} \cos k_1 x (e^{\pm ik_2 y(x)} - 1) dx = 2\pi\delta(k_1) + f_1^{\pm},$$

$$a = 2 \quad \int_L e^{\pm i\mathbf{k}\cdot\mathbf{x}} dy = 2i \int_0^{\infty} \sin k_1 x e^{\pm ik_2 y(x)} y'(x) dx = f_2^{\pm},$$

$$a = 3 \quad \int_L e^{\pm i\mathbf{k}\cdot\mathbf{x}} dz = 0.$$

Analogous expressions for a straight-line dislocation lying along the OX-axis have the form

$$a = 1 \quad \int_L e^{\pm i\mathbf{k}\cdot\mathbf{x}} dx = 2\pi\delta(k_1),$$

$$a = 2 \quad \int_L e^{\pm i\mathbf{k}\cdot\mathbf{x}} dy = 0,$$

$$a = 3 \quad \int_L e^{\pm i\mathbf{k}\cdot\mathbf{x}} dz = 0.$$

The energy of two kinks is determined as the limiting value (the distance between the kinks tending to infinity of the difference between the energy of a dislocation with two kinks and a straight line dislocation, since only then — at a very large distance between the kinks — various additional terms (connected with self-energies of straight line dislocation segments and with the interactions between these segments and kinks)

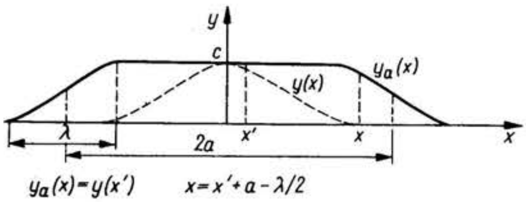

FIG. 2.

cancel each other; W_L denotes here the energy of dislocation with two kinks W_0 — the energy of straight line dislocation, $2a$ is the distance between the kinks.

If the kinks move away from each other, in the expression for W_L only functions $f_i^\pm$ determining the functions ψ_{ab} are changed, namely

$$f_1^\pm = \int_0^\infty \cos k_1 x(e^{\pm ik_2 y_a(x)}-1)\,dx = \int_0^\infty \cos k_1 x[e^{\pm ik_2 y(x-a+\lambda/2)}-1]\,dx \tag{21}$$

$$= \int_{-a+\lambda/2}^\infty \cos k_1(x'+a-\lambda/2)[e^{\pm ik_2 y(x')}-1]\,dx'$$

$$= \int_{-a+\lambda/2}^0 \cos k_1(x'+a-\lambda/2)[e^{\pm ik_2 c}-1]\,dx' + \int_0^\infty \cos k_1(x'+a-\lambda/2)[e^{\pm ik_2 y(x')}-1]\,dx'$$

$$= (e^{\pm ik_2 c}-1)\frac{\sin k_1(a-\lambda/2)}{k_1} + \int_0^\infty \cos k_1(x+a-\lambda/2)[e^{\pm ik_2 y(x)}-1]\,dx.$$

In a similar manner, $f_2^\pm$ is calculated, though in this case it will be an integral expression, since the λ parameter has been so selected that $y'(x) \neq 0$ only for $x \in \langle a-\lambda/2,\ a+\lambda/2\rangle$.

Introduce the following notations:

$$\varphi_\pm(x) = e^{\pm ik_2 y(x)}-1, \quad \vartheta_\pm(x) = e^{\pm ik_2 y(x)} y'(x).$$
$$A_\pm = e^{\pm ik_2 c}-1.$$

Functions $f_1^\pm$ may then be written as

$$f_1^\pm = 2A_\pm \frac{\sin k_1(a-\lambda/2)}{k_1} + 2\int_0^\infty \cos k_1(x+a-\lambda/2)\varphi_\pm(x)\,dx,$$

(22)

$$f_2^\pm = \pm 2i \int_0^\infty \sin k_1(x+a-\lambda/2)\vartheta_\pm(x)\,dx,$$

and the expressions for ψ_{ab} — in the form

$$\psi_{11} = 2\pi\delta(k_1)\left[2(A_+ + A_-)\frac{\sin k_1(a-\lambda/2)}{k_1} + 2\int \cos k_1(x+a-\lambda/2)(\varphi_+ + \varphi_-)dx\right]$$

$$+4A_+A_-\frac{\sin^2 k_1(a-\lambda/2)}{k_1^2} + 4\frac{\sin k_1(a-\lambda/2)}{k_1}\int \cos k_1(x+a-\lambda/2)[A_+\varphi_-(x)$$

$$+A_-\varphi_+(x)]dx + 4\int\int \cos k_1(x+a-\lambda/2)\cos k_1(x'+a-\lambda/2)\varphi_+(x)\varphi_-(x')dx dx',$$

$$(23)\qquad \psi_{12} = 4iA_-\frac{\sin k_1(a-\lambda/2)}{k_1}\int \sin k_1(x+a-\lambda/2)\vartheta_+(x)dx$$

$$+4i\int\int \cos k_1(x+a-\lambda/2)\sin k_1(x'+a-\lambda/2)\varphi_-(x)\vartheta_+(x')dx dx',$$

$$\psi_{21} = 4iA_+\frac{\sin k_1(a-\lambda/2)}{k_1}\int \sin k_1(x+a-\lambda/2)\vartheta_-(x)dx$$

$$-4i\int\int \cos k_1(x+a-\lambda/2)\sin k_1(x'+a-\lambda/2)\varphi_+(x)\vartheta_-(x')dx dx',$$

$$\psi_{22} = 4\int\int \sin k_1(x+a-\lambda/2)\sin k_1(x'+a-\lambda/2)\vartheta_+(x)\vartheta_-(x')dx dx'.$$

In the expressions for ψ_{12} and ψ_{21} the following terms have been disregarded:

$$2\pi\delta(k_1)\cdot 2i\int \vartheta_\pm(x)\sin k_1(x+a-\lambda/2)dx$$

since after integration they yield zero contributions. The ψ_{ab} are still represented in a somewhat complicated form which makes further calculations difficult and causes certain ambiguities in interpretation. In order to avoid these difficulties let us reduce the expressions for ψ_{ab} to a simpler form, and consider them in detail. Integration by parts yields:

$$\int \cos k_1(x+a-\lambda/2)\varphi_\pm(x)dx = -A_\pm\frac{\sin k_1(a-\lambda/2)}{k_1}$$

$$\mp\frac{ik_2}{k_1}\int \sin k_1(x+a-\lambda/2)\vartheta_\pm(x)dx$$

and hence

$$\frac{4\sin k_1(a-\lambda/2)}{k_1}\int \cos k_1(x+a-\lambda/2)[A_-\varphi_+(x)+A_+\varphi_-(x)]dx$$

$$= -8A_+A_-\frac{\sin^2 k_1(a-\lambda/2)}{k_1^2} + \frac{4ik_2}{k_1}\sin k_1(a-\lambda/2)\int \sin k_1(x+a-\lambda/2)\times$$

$$\times[A_+\varphi_-(x)+A_-\varphi_+(x)]dx + \int\int \cos k_1(x+a-\lambda/2)\cos k_1(x'+a-\lambda/2)\times$$

$$\times\varphi_+(x)\varphi_-(x')dx dx' = 4A_+A_-\frac{\sin^2 k_1(a-\lambda/2)}{k_1^2}$$

$$-\frac{4ik_2}{k_1}\sin k_1(a-\lambda/2)\int \sin k_1(x+a-\lambda/2)[A_+\vartheta_-(x)-A_+\vartheta_-(x)]dx$$

$$+4\frac{k_2^2}{k_1^2}\int\int \sin k_1(x+a-\lambda/2)\sin k_1(x'+a-\lambda/2)\vartheta_+(x)\vartheta_-(x')dx dx'.$$

Finally,

$$\psi_{11} = 2\pi\delta(k_1)\frac{2ik_2}{k_1}\int \sin k_1(x+a-\lambda/2)\,[\vartheta_-(x)-\vartheta_+(x)]\,dx$$
$$+4\frac{k_2^2}{k_1^2}\int\int \sin k_1(x+a-\lambda/2)\sin k_1(x'+a-\lambda/2)\vartheta_+(x)\vartheta_-(x')\,dx\,dx',$$

(24) $$\psi_{12} = -4\frac{k_2}{k_1}\int\int \sin k_1(x+a-\lambda/2)\sin k_1(x'+a-\lambda/2)\vartheta_+(x)\vartheta_-(x')\,dx\,dx',$$

$$\psi_{21} = \psi_{12}.$$

The fact that a term proportional to a still appears in the expression for ψ_{11} seems to be an aggravation since the first term, after integration with $\delta(k_1)$ over k_1 yields:

$$4\pi ik_2\int [a+x-\lambda/2]\,[\vartheta_-(x)-\vartheta_+(x)]\,dx.$$

Apparent, however is the difficulty that this term appears for finite values of a only, and if we are dealing with the entire expression for ψ_{11} at very large values of a — i.e., when $a/c \gg 1$ and $a/\lambda \gg 1$, the terms proportional to a, cancel each other. More precisely: when $a \to \infty$

$$\sin k_1(x+a-\lambda/2)\sin k_1(a+x'-\lambda/2) \approx \sin^2 k_1 a + \frac{1}{2}k_1(x+x'-\lambda)\sin 2k_1 a$$

and

$$\lim_{a\to\infty}\int \frac{\sin^2 k_1 a}{ak_1^2}\,dk_1 = \pi,$$

$$\int [\vartheta_-(x)-\vartheta_+(x)]\,dx = -\int\int \vartheta_+(x)\vartheta_-(x')\,dx\,dx' = -2(1-\cos k_2 c).$$

The problem consists in the observation that the expression for ψ_{11} is multiplied by the function $A_{11jl}(\mathbf{k})$. If it is integrated with $\delta(k_1)$, we obtain $A^0_{11jl}(\mathbf{k})$ — i.e. $A_{11jl}(\mathbf{k})$, in which $k_1 = 0$; on the other hand, the second term in ψ_{11} is multiplied by the entire expression $A_{11j}(\mathbf{k})$; thus the term $A^0_{11jl}(\mathbf{k})$ is simultaneously added and subtracted from that expression; the latter term is independent of k_1. The integral over k_1 is evaluated directly and the terms proportional to a are cancelled. (More strictly, it should be added here that we are not dealing now with the dependence of χ on k_1. Anticipating the results to follow, it may be stated that χ is entirely independent of k_1). The "price" paid consists in the fact that the expression ψ_{11} is now multiplied by $[A_{11jl}(\mathbf{k})-A^0_{11jl}(\mathbf{k})]$, and not by $A_{11jl}(k)$.

The energy is now written in the form:

(25) $$W = \frac{1}{4\pi^3}\int d_3k\int\int \sin k_1(a+x-\lambda/2)\sin k_1(a+x'-\lambda/2)\vartheta_+(x)\vartheta_-(x')\chi(\mathbf{k})\chi(-\mathbf{k})\times$$
$$\times\left[A_{22il}(\mathbf{k})-\frac{k_2}{k_1}\big(A_{12il}(\mathbf{k})+A_{21il}(\mathbf{k})\big)+\frac{k_2^2}{k_1^2}\big(A_{11il}(\mathbf{k})-A^0_{11il}(\mathbf{k})\big)\right]b_i b_l$$

It is time to pass to the functions $A_{abjl}(\mathbf{k})$. Let us observe that the integration over k_1, k_2, k_3 is performed in intervals with symmetric boundaries, and the integrand must be an even function of k_1, k_2, k_3. It turns out that only the functions A_{ab11} and A_{ab22}

give non-zero contributions and there are no terms proportional to $b_1 b_2$. We can conclude that the energy of two kinks on a dislocation characterized by the Burgers vector $\mathbf{b} = [b_1, b_2, 0]$ is a sum of the corresponding expressions for a screw dislocation with the Burgers vector b_1, and for an edge dislocation with the Burgers vector b_2. This fact is common for the self-energy and the energy of interaction — no "interference" terms are present.

Introducing the notations

$$\beta(k) = \frac{c_1^2(k) - c_2^2(k)}{c_1^2(k)}, \quad \alpha(k) = c_2^2(k)\beta(k) \tag{26}$$

all the necessary functions A_{abil} may be determined according to the Table 1.

Table 1

A_{abil}	$i = l = 1$	$i = l = 2$
A_{11il}	$c_2^2(k)\frac{k_2^2+k_3^2}{k^4} - 2\alpha(k)\frac{k_1^2(k_2^2+k_3^2)}{k^6}$	$2\alpha(k)\left[\frac{2k_3^2}{k^4} + \frac{k_1^2 k_2^2}{k^6}\right]$
A_{22il}	$2\alpha(k)\left[\frac{2k_3^2}{k^4} + \frac{k_1^2 k_2^2}{k^6}\right]$	$c_2^2(k)\frac{k_1^2+k_3^2}{k^4} - 2\alpha(k)\frac{k_2^2(k_1^2+k_3^2)}{k^6}$
A_{12il}	$-c_2^2(k)\frac{k_1 k_2}{k^4}\left[1 - 2\beta(k)\frac{k_1^2}{k^2}\right]$	$-2\alpha(k)\frac{k_1 k_2}{k^4}\left[1 - \frac{k_2^2}{k^2}\right]$
A_{21il}	$-2\alpha(k)\frac{k_1 k_2}{k^4}\left[1 - \frac{k_1^2}{k^2}\right]$	$-c_2^2(k)\frac{k_1 k_2}{k^4}\left[1 - 2\beta(k)\frac{k_2^2}{k^2}\right]$

The energy may also be written in a more compact form,

$$W = \frac{1}{4\pi^3}\int d_3 k\, \psi(k_1, k_2)\,[b_1^2 A_1(\mathbf{k}) + b_2^2 A_2(\mathbf{k})]\,\chi(\mathbf{k})\chi(-\mathbf{k}). \tag{27}$$

Here

$$A_i(\mathbf{k}) \overset{\text{df}}{=} [A_{11ii}(\mathbf{k}) - A_{11ii}^0(\mathbf{k})]\frac{k_2^2}{k_1^2} + A_{22ii}(\mathbf{k}) - \frac{k_2}{k_1}[A_{12ii}(\mathbf{k}) + A_{21ii}(\mathbf{k})],$$

$$\psi(k_1, k_2) = \iint \sin k_1(x + a - \lambda/2)\sin k_1(x' + a - \lambda/2)\vartheta_+(x)\vartheta_-(x')\,dx\,dx'.$$

Using the table, the values of A_i are determined in the explicit form:

$$\begin{aligned} A_1(\mathbf{k}) &= 4\alpha(\mathbf{k})\frac{k_3^2}{k^4} - c_2^2(k)\frac{k_2^2}{k^2(k_2^2+k_3^2)}, \\ A_2(\mathbf{k}) &= c_2^2(k)\frac{1}{k^2} - 4\alpha(k)\frac{k_2^2 k_3^2}{k^2(k_2^2+k_3^2)^2} - 4\alpha(k)\frac{k_2^2 k_3^2}{k^4(k_2^2+k_3^2)}. \end{aligned} \tag{28}$$

The total energy of two kinks is given by the final formula

$$(29)\qquad W=\frac{1}{8\pi^3}\int d_3k\,\chi(\mathbf{k})\chi(-\mathbf{k})\Bigg[b_1^2\Bigg(4\alpha(k)\frac{k_3^2}{k^4}-c_2^2(k)\frac{k_2^2}{k^2(k_2^2+k_3^2)}\Bigg)$$

$$+b_2^2\Bigg(c_2^2\frac{1}{k^2}-4\alpha(k)\frac{k_2^2k_3^2}{k^2(k_2^2+k_3^2)^2}-4\alpha(k)\frac{k_2^2k_3^2}{k^4(k_2^2+k_3^2)}\Bigg)\Bigg]\int\int e^{ik_2[y(x)-y(x')]}y'(x)y'(x')\times$$

$$\times[\cos k_1(x-x')+\sin 2k_1 a\sin k_1(x+x'-\lambda)-\cos 2k_1 a\cos k_1(x+x'-\lambda)]\,dx\,dx'.$$

This is the sum of self-energies and of the energy of interaction of the kinks. Applying an asymptotic procedure, we may simply state that the terms independent of a describe the self-energy, while the remaining terms — the energy of interaction. A more detailed analysis of that problem will be presented in another paper. Meanwhile, it should be observed that the form of expression (29) is convenient for further considerations. First of all, the integrand is a product of three functions, each of which is connected with a separate property of the medium and of the dislocation.

Dispersion of the medium is described by $A(\mathbf{k})$, or more precisely: by the dependence of c_1^2 and c_2^2 on the wave vector $\mathbf{k}$. Selecting these functions appropriately, we obtain non-dispersive, weakly or strongly dispersive media.

The shape of a kink and the dependance of the energy on it is described by the function $\psi(\mathbf{k})$, and more precisely — the function $y(x)$ appearing in it, as also the parameter λ connected with the kinks width.

The function $\chi(\mathbf{k})$ is modeling the structure of the dislocation line itself: its form depends on the model of the dislocation assumed: a line or a strip. The latter case corresponds to an extended dislocation — i.e., consisting of partial dislocations whose total Burgers vector is equal to **b**. Dislocations of that type are usually encountered in real crystals.

The effects of all individual factors will be considered in more detail by separate investigation of the self-energy and the energy of interaction of the inflections.

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