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THE SELF-ENERGY OF STRAIGHT-LINE DISLOCATION SEGMENTS IN PSEUDO-CONTINUUM THEORY

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Abstract—Expressions for the self-energy of straight-line dislocation segments are derived on the basis of the pseudo-continuum theory. Final results are given in simple form and are shown to be valid even for very short segments of the order of 10 interatomic distances. The dependence of the energy expressions on the assumptions introduced is discussed. Dispersive terms are also derived and their influence on the values of the energy is studied. The results are compared with those obtained on the basis of the classical theory of elasticity. The use of the pseudo-continuum model obviates the necessity of introducing an ill-defined core parameter, because in this model the singularity on the dislocation line does not exist. It is the presence of this singularity in classical elasticity which necessitates the introduction of the core parameter. Numerical data illustrate the results obtained as summarized in two tables.

INTRODUCTION

The aim of the present paper is the determination of the energy of straight-line dislocation segments within the framework of the pseudo-continuum model (Rogula[1] 1965, Kunin[2] 1966). This model permits to describe discrete systems by means of the mathematical apparatus usually used for continua. The expressions determining the self-energy of dislocations per unit length obtained on the basis of classical linear elasticity contain an arbitrary parameter, namely the core radius. This is connected with the fact that at small distances from the dislocation line classical elasticity is no longer applicable, as exhibited by the feature of the energy expressions becoming divergent (infinite) when the core parameter approaches zero. The estimates of the value of this parameter used in the literature on dislocation theory[3–5] vary in the wide range of 1/4 to 5 times the magnitude of the Burgers vector.

By contrast, in pseudo-continuum theory there is no necessity at all to introduce such a parameter. This theory was employed successfully to determine the energy of defects of dislocation lines, such as kinks and jogs[6–8], a problem which the classical elasticity is not capable of treating because the size of these defects is of the order of atomic lattice distance.

The pseudo-continuum model could be interpreted as a certain nonlocal theory of a continuum, in the sense that, first, there is spatial dispersion and, second, the relation between the stress tensor and the dislocation tensor is of functional character. It is, however, important to be aware of the fact that a pseudo-continuum is describing discrete systems, while the object dealt with by nonlocal theories in the usual sense concerns continua with certain additional parameters, for example in the nature microstructure.

The pseudo-continuum theory exhibits, as is typical for nonlocal theories, nonuniqueness in defining many physical quantities, e.g. the strain energy density. This property allows to simplify to a considerable degree the energy expressions. As a consequence, the structure of the final results is such as to make the influence of various physical effects readily recognizable and, in addition, physical interpretation and comparison with classical theory becomes readily possible.

1. DESCRIPTION OF THE MODEL

It is the basic concept of the pseudo-continuum theory that the interpolation of any function defined over a discrete periodic structure is unique in terms of a function defined over a continuum. The uniqueness requirement indeed determines the class of interpolating functions. These are meromorphic functions and their Fourier transforms are distributions with a compact support in the closure of the first Brillouin zone[1, 2]. The elasticity tensor is replaced by a two-point tensorial function. The introduction of dislocations into the medium no longer permits the use of a displacement description u_i. Rather, two basic fields need to be introduced, namely, the distortion field β_{ij} and the velocity field v_i. Equations

$$\epsilon_{klm}\beta_{im,l} = 0, \qquad \dot{\beta}_{ik} - v_{i,k} = 0$$
$$(v_i = \dot{u}_i, \qquad \beta_{im} = u_{i,m})$$

for a medium without dislocations have to be replaced by equations

$$\epsilon_{klm}\beta_{il,m} = -\alpha_{ik}, \qquad \dot{\beta}_{ik} - v_{i,k} = J_{ik} \tag{1.1}$$

for a medium with dislocation, where α_{ik} denotes the dislocation density tensor, while J_{ik} denotes the dislocation flux density. We also have

$$\beta_{ik}(\bar{x}) = u_{i,k}(\bar{x}), \qquad \bar{x} \notin L$$

where L is the dislocation line and $\bar{x}$ denotes Cartesian coordinates. Equations (1.1) have to be supplemented by the conservation conditions

$$\alpha_{ik,k} = 0, \qquad \dot{\alpha}_{ik} + \epsilon_{klm}J_{im,l} = 0. \tag{1.2}$$

The equations of motion, in the absence of body forces, are

$$\rho\dot{v}_i - \sigma_{ik,k} = 0 \tag{1.3}$$

where ρ is the mass density and σ_{ik} is analogous to the stress tensor in continuum mechanics. It is defined in terms of the relation

$$\sigma_{ik}(\bar{x}) = \int c_{ikjl}(\bar{x} - \bar{x}')\beta_{jl}(\bar{x}')\,\mathrm{d}^3x'. \tag{1,4}$$

From eqns (1.1)–(1.4) we can obtain separate equations for the distorsion field and the velocity field. The solution to these equations is expressed in terms of the same Green's tensor. Renouncement of the displacement description seemingly increases the number of functions to be determined. The degree of difficulty, however, is not increased by this circumstance. The general solution of these equations may be found in [1]. The Green's functions depend on the elastic properties of the material, i.e. $c_{ikjl}(\bar{x} - \bar{x}')$. In the present study we restrict our attention to static problems for an isotropic pseudo-continuum. Then the components of c_{ikjl}, or rather their Fourier transforms, depend on the length of the wave vector $\bar{k}$ only, (but not on its direction) and the tensorial structure is the same as for the classical elasticity tensor. Thus

$$c_{ijkl}(\bar{k}) = \rho[c_1^2(k) - 2c_2^2(k)]\delta_{ij}\delta_{kl} + \rho c_2^2(k)[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}] \tag{1.5}$$

and the transform of the tensorial Green's function is

$$G_{ij}(\bar{k}) = \frac{1}{\rho k^2}\left[\frac{\delta_{ij}}{c_2^2(k)} + \frac{k_1 k_j}{k^2}\left(\frac{1}{c_1^2(k)} - \frac{1}{c_2^2(k)}\right)\right] \tag{1.6}$$

where c_1 and c_2 denote the longitudinal and transversal wave velocity, respectively. Even in the simple case of an isotropic pseudo-continuum these velocities depend on the wave vector. This is related to the fundamental feature of a pseudo-continuum, namely, in spite of a continuum form of the functions and equations, it describes periodic discrete systems with all its properties, the most significant being the dispersion. In the isotropic case the Brillouin zone is a sphere.

Finally, the isotropic properties lead to three independent restrictions as follows:

(1) Specific symmetries of the tensor c_{ijkl};
(2) Special form of functional dependence of c_{ijkl} on $\bar{k}$;
(3) Brillouin zone is a sphere.

2. DISLOCATION ENERGY IN PSEUDO-CONTINUUM

The dislocation energy in the pseudo-continuum is given as follows:

$$W = \frac{1}{2}\iint \beta_{ik}(\bar{x})c_{ikjl}(\bar{x}-\bar{x}')\beta_{jl}(\bar{x}')\,d^3x\,d^3x'$$
$$= \frac{1}{2}\frac{1}{(2\pi)^3}\int \beta_{ik}(\bar{k})c_{ikjl}(\bar{k})\beta_{kl}(-\bar{k})\,d^3k \tag{2.1}$$

where

$$\beta_{ij}(\bar{x}) = -\iint d^3x'\,d^3x''c_{nklm}(\bar{x}'-\bar{x}'')G_{in}(\bar{x}-\bar{x}')\epsilon_{mjs}\frac{\partial}{\partial x_k''}\alpha_{ls}(x'') \tag{2.2}$$

and

$$\beta_{ij}(\bar{k}) = \int e^{-i\bar{k}\bar{x}}\beta_{ij}(\bar{x})\,d^3x = -c_{nklm}(\bar{k})G_{in}(\bar{k})\epsilon_{mjs}ik_k\alpha_{ls}(\bar{k}). \tag{2.3}$$

The above expressions refer to the static case and, consequently, the flux J does not appear. The expressions for β_{ij} and W are given both in $\bar{x}$ and $\bar{k}$ space because in $\bar{x}$-space they are in the form of convolutions, and thus in $\bar{k}$-space they are in convenient form for further calculations. After inserting (2.3) into (2.1) we obtain rather complicated expressions defining the energy of a dislocation line of arbitrary shape. It is desirable to simplify these expressions and we return for this purpose to relations (2.1) for quasi-stationary dislocations. We assume that the time-rate of change of $J_{nk}(\bar{x}, t)$ and $v_i(\bar{x}, t)$ is so slow that $\dot{J}_{nk}$ and $\dot{v}_i$ may be set equal to zero. Relation (2.1) has to be replaced by

$$W(t) = \iint \beta_{ij}(\bar{x}, t)c_{ijkl}(\bar{x}-\bar{x}')\beta_{kl}(\bar{x}', t)\,d^3x\,d^3x'. \tag{2.4}$$

Differentiation of this expression with respect to time yields

$$\dot{W} = \iint \frac{\partial\beta_{ij}(\bar{x}, t)}{\partial t}c_{ijkl}(\bar{x}-\bar{x}')\beta_{kl}(\bar{x}', t)\,d^3x\,d^3x'. \tag{2.5}$$

Making use of the second eqn (1.1) we can transform (2.5) to

$$\dot{W} = \iint v_{i,j}(x, t)c_{ijkl}(\bar{x}-\bar{x}')\beta_{kl}(\bar{x}', t)\,d^3x\,d^3x' + \iint J_{ij}(x, t)c_{ijkl}(\bar{x}-\bar{x}')\beta_{kl}(x', t)\,d^3x\,d^3x'. \tag{2.6}$$

Let us represent J_{nk} in the form

$$J_{ij}(\bar{x}, t) = \frac{\partial\tilde{\beta}_{ij}}{\partial t} + \phi_{i,j}(\bar{x}, t) \tag{2.7}$$

where ϕ_i is an arbitrary vector function. Then

$$\dot{W} = \iint \frac{\partial\tilde{\beta}_{ij}(\bar{x}, t)}{\partial t}c_{ijkl}(\bar{x}-\bar{x}')\beta_{kl}(\bar{x}', t)\,d^3x\,d^3x'$$
$$+\iint [v_{i,j}(\bar{x}, t) + \phi_{i,j}(\bar{x}, t)]c_{ijkl}(\bar{x}-\bar{x}')\beta_{kl}(\bar{x}, t)\,d^3x\,d^3x'. \tag{2.8}$$

The second term of the above expression can be integrated by parts. If differentiation with respect to x_j is replaced by that with respect to x_j' (taking advantage of the functional dependence of c_{ijkl} on the difference $\bar{x}-\bar{x}'$) then a second integration by parts, together with use of the equation of motion (1.3) and the condition of quasi-stationary $\dot{v}_i = 0$, will show that this second term vanishes.

The resolution (2.7) does not define uniquely the functions ϕ_i and $\tilde{\beta}_{ij}$ which permits us to choose the latter function in the simplest possible way. (ϕ_i does not enter the expression for the energy.) Finally, the expression for the energy of stationary dislocations acquires the form

$$W = \frac{1}{2}\int\int \tilde{\beta}_{ij}(\bar{x})c_{ijkl}(\bar{x}-\bar{x}')\beta_{kl}(\bar{x}')\,\mathrm{d}^3x\,\mathrm{d}^3x'. \tag{2.9}$$

The relations which β and $\tilde{\beta}$ have to satisfy are

$$\epsilon_{klm}\beta_{im,l} = \alpha_{ik}, \qquad \epsilon_{klm}\tilde{\beta}_{im,l} = \alpha_{ik} \tag{2.10}$$

where α_{ik} are the same dislocation densities. Further, β satisfies the condition following from (1.3), namely

$$\int c_{nklm}(x-x')\beta_{lm,k}(\bar{x}')\,\mathrm{d}^3x' = 0.$$

By contrast, we impose on β the condition

$$\tilde{\beta}_{nk,k}(\bar{x}) = 0. \tag{2.11}$$

The Fourier transform of $\tilde{\beta}(\bar{x})$ which satisfies condition (2.10) and (2.11) is

$$\tilde{\beta}_{ij}(\bar{k}) = -\frac{ik_k\epsilon_{kjs}\alpha_{is}(\bar{k})}{k^2}. \tag{2.12}$$

Finally, the dislocation energy in a pseudo-continuum could be given by

$$W = \frac{1}{16\pi^3}\int c_{nklm}(\bar{k})c_{rwip}(\bar{k})G_{nr}(\bar{k})\epsilon_{pka}\epsilon_{smb}k_wk_s\alpha_{ia}(k)\alpha_{lb}(-k)\frac{\mathrm{d}^3k}{k^2}. \tag{2.13}$$

Let us notice that in a local theory the simplification as carried out above is not possible: in the process of integration by parts which gave us the opportunity to remove the dependence on the arbitrary function ϕ_i, we took advantage of the dependence of c_{ijkl} on $\bar{x}-\bar{x}'$, while in a classical continuum the elasticity tensor is simply a constant.

Now we wish to specialize the form of the dislocation density α_{ik}. We take it in the simplest form suitable for pseudo-continuum

$$\alpha_{ik}(\bar{x}) = b_i\int_L \delta_B(\bar{x}-\bar{x}')\,\mathrm{d}x'_k \tag{2.14}$$

where b_i is the Burgers vector and $\delta_B(\bar{x})$ is the pseudo-continuum analog of the delta Dirac function, defined by

$$\delta_B(\bar{x}) = \frac{1}{(2\pi)^3}\int_B \mathrm{e}^{i\bar{k}\cdot\bar{x}}\,\mathrm{d}^3k. \tag{2.15}$$

The integration is to be carried out over the first Brillouin zone B. It is to be noted that by contrast to the delta Dirac function, $\delta_B(\bar{x})$ is everywhere finite and satisfies the condition

$$\int \delta_B(\bar{x})\,\mathrm{d}^3x = 1 \tag{2.16}$$

and its Fourier transform equals unity. The Fourier transform of (2.14) is

$$\alpha_{ik}(\bar{k}) = b_i \int_L e^{-i\bar{k}\cdot\bar{x}}\, dx_k \tag{2.17}$$

where L, as before, denotes the dislocation line.

3. THE GENERAL EXPRESSION FOR THE SELF-ENERGY OF A STRAIGHT-LINE DISLOCATION SEGMENT

Let us consider a dislocation line L represented in Fig. 1. The energy of dislocation segments AB and DC is defined in the limit as $r \to \infty$ of the difference of two energies, namely, the energy W_2 of the dislocation line L and the energy W_0 of the dislocation line L_0 lying along the x-axis. Thereby both dislocation lines are characterized by the same Burgers vector. We thus have

$$W = \lim_{r\to\infty} (W_2 - W_0). \tag{3.1}$$

Now let us rewrite (2.13) in the form

$$W_2 = \frac{1}{16\pi^3} \int A_{abil}(\bar{k}) b_i b_l \psi_{ab}^{(2)}(\bar{k})\, d^3k \tag{3.2}$$

where

$$\psi_{ab}^{(2)} = \int_{L_2} e^{-i\bar{k}\cdot\bar{x}}\, dx_a \int_{L_2} e^{i\bar{k}\cdot\bar{x}}\, dx_b \tag{3.3}$$

and

$$A_{abil}(\bar{k}) = c_{nklm}(\bar{k}) c_{rwip}(\bar{k}) G_{nr}(\bar{k}) \epsilon_{pka} \epsilon_{smb} \frac{k_w k_s}{k^2}. \tag{3.4}$$

We consider the dislocation configuration with 2 segments as shown in Fig. 1 and we assume the Burgers vector to be $\bar{b} = [b_1, b_2, 0]$. Next we calculate the energy using expressions (3.1) and (3.2) and note that in the expression $\psi_{11} = \psi_{11}^{(2)} - \psi_{11}^{(0)}$ terms which are proportional to r are divergent. This singularity, however, can be removed. For this purpose, the expressions A_{11ab} have to be modified. Details of this procedure are given in [6] which is concerned with the energy of kinks. In that paper no restrictions upon the shape of the kink were introduced and thus those results are applicable in the present case. Finally, the total energy of two segments could be represented in the form

$$W_t = \frac{1}{8\pi^3} \int d^3k [b_1^2 A_1(k) + b_2^2 A_2(k)] \iint e^{ik_2(y(x)-y(x'))} y'(x) y'(x') [\cos k_1(x-x') + \sin k_1 r \sin k_1(x+x'-l) - \cos k_1 r \cos k_1(x+x'-l)]\, dx\, dx' \tag{3.5}$$

where

$$A_1(k) = 4\alpha(\bar{k}) \frac{k_3^2}{k^4} - c_2^2(\bar{k}) \frac{k_2^2}{k^2(k_2^2+k_3^2)} \tag{3.6}$$

$$A_2(k) = c_2^2(\bar{k}) \frac{1}{k^2} - 4\alpha(\bar{k}) \frac{k_2^2 k_3^2}{k^2(k_2^2+k_3^2)} \left(\frac{1}{k^2} + \frac{1}{k_2^2+k_3^2}\right) \tag{3.7}$$

$$\alpha(\bar{k}) = c_2^2(\bar{k}) \frac{c_1^2(\bar{k}) - c_2^2(\bar{k})}{c_1^2(\bar{k})}. \tag{3.8}$$

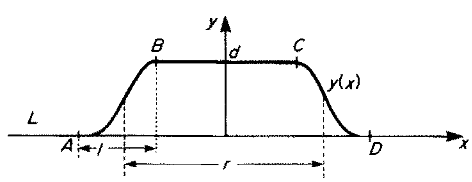

Fig. 1.

The self-energy of one of the segments, for example AB is

$$W=\frac{1}{16\pi^3}\int[(b_1{}^2A_1(k)+b_2{}^2A_2(k)]\psi(k_1,k_2)\,\mathrm{d}_3k \tag{3.9}$$

where

$$\psi(k_1,k_2)=\int_{L_2}\int_{L_2}y'(x)y'(x')\cos k_1(x-x')\exp\{ik_2[y(x)-y(x')]\}\,\mathrm{d}x\,\mathrm{d}x'. \tag{3.10}$$

Let us consider now the straight line segment AB, which could be described by the linear function (Fig. 2)

$$y(x)=d\left(1-\frac{x}{l}\right),\qquad x\in[0,l]. \tag{3.11}$$

After direct integration we obtain

$$\psi(k_1,k_2)=d^2\left[\frac{1-\cos(k_1l+k_2d)}{(k_1l+k_2d)^2}+\frac{1-\cos(k_1l-k_2d)}{(k_1l-k_2d)^2}\right]. \tag{3.12}$$

Let us notice that the self-energy does not depend on the position of the segment. Hence a convenient choice of the 0y-axis is possible. Even though the integration is carried out along the whole line in (3.10), a nonvanishing contribution will exist only in the range $x\notin[0,l]$ because for $x\notin[0,l]$, $y'(x)=0$. Furthermore, we restrict our study to segments perpendicular to semi-infinite dislocation lines. Then we set $l=0$ and obtain.

$$\psi(k_1,k_2)=\frac{2(1-\cos k_2d)}{(k_2d)^2}$$

and for the self-energy

$$W=\frac{\rho d^2}{16^3}\int[b_1{}^2A_1(\bar{k})+b_2{}^2A_2(\bar{k})]\frac{\sin^2\frac{k_2d}{2}}{\left(\frac{k_2d}{2}\right)^2}\,\mathrm{d}^3k. \tag{3.13}$$

4. DISPERSION, METHOD OF ANALYSIS AND ESTIMATION OF PARAMETERS

To restate, we are working in the framework of the theory of an isotropic pseudo-continuum. We set for the functions $c_i^2(k)$

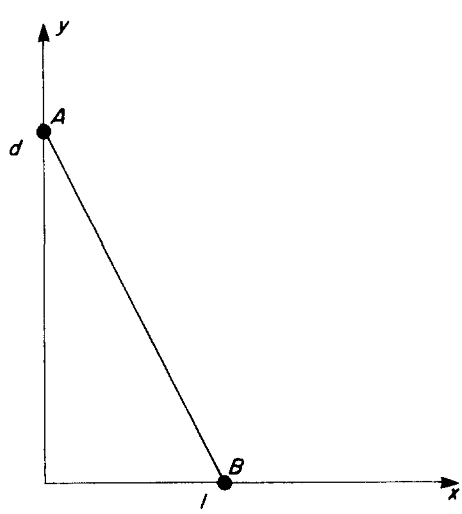

Fig. 2.

$$c_i^2(k) = c_i^2(0)\frac{\sin^2\left(\frac{\pi}{2}\frac{k}{K}\right)}{\left(\frac{\pi}{2}\frac{k}{K}\right)^2}, \qquad (i = 1, 2). \tag{4.1}$$

K is the radius of the isotropic Brillouin sphere. The form (4.1) corresponds in the discrete case to taking into account the interaction between nearest neighbors only (weak dispersion). Further, we assume the parabolic approximation of $c_i^2(k)/c_i^2(0)$:

$$h(k) = \frac{c_i^2(k)}{c_i^2(0)}(1 - Hk^2) = 1 - \frac{\pi^2}{24}\frac{k^2}{K^2}. \tag{4.2}$$

Formula (3.13) can now be rewritten in the form

$$W = \frac{\rho d^2}{16\pi^3}\int [b_1^2 A_1^0(\bar{k}) + b_2^2 A_2^0(k)]h(k)l(k)\,\mathrm{d}^3k. \tag{4.3}$$

A_1^0 and A_2^0 are obtained from A_1 and A_2 by replacing $c_2^2(k)$ and $\alpha(k)$ in (3.6) and (3.7) by the constants $c_2^2(0)$ and $\alpha(0)$, while $l(k)$ is defined by

$$l(k) = \frac{\sin^2\frac{k_2 d}{2}}{\left(\frac{k_2 d}{2}\right)^2}. \tag{4.4}$$

The shape of the function $l(k)$ depends on the length d of the dislocation segment. Let us denote by n the ratio d to b, where b is the length of the Burgers vector. Our considerations will be restricted to $n \geq 10$. If $n < 10$, we should speak rather of a dislocation kink. For $n = 10$ the function $l(k)$ is displayed in Fig. 3. It is easily seen that the relative maxima decrease rapidly as the absolute value of k_2 increases, which is the more pronounced the larger n is. This permits us to employ in the sequel an approximate form of $l(k)$ defined as

$$l(k_2) = \begin{cases} 1 - ak_2^2 & 0 \leq |k_2| \leq \dfrac{K}{n} \\ R_n & \dfrac{K}{n} \leq |k_2| \leq K \end{cases} \tag{4.5}$$

$$a = \frac{\pi^2 - 4}{\pi^2}\frac{n^2}{K^2}.$$

R_n is the average value of $l(k)$ on the segment $(K/n, K)$. Prior to selecting a specific method of estimation, we study the asymptotic behavior of R_n defined as

$$R_n \stackrel{\mathrm{df}}{=} \frac{1}{K - \frac{k}{n}}\int_{K/n}^{K}\frac{\sin^2\frac{k_2 d}{2}}{\left(\frac{k_2 d}{2}\right)^2}\mathrm{d}k_2 = \frac{n}{(n-1)K}I. \tag{4.6}$$

We are interested in R_n and nR_n as $n \to \infty$. Let us notice that these quantities are always positive. Since $\sin^2 x \leq 1$,

$$\int_{K/n}^{K}\frac{\sin^2\frac{k_2 d}{2}}{\left(\frac{k_2 d}{2}\right)^2}\mathrm{d}k_2 \leq \left(\frac{2}{d}\right)^2\int_{K/n}^{K}\frac{1}{k_2^2}\mathrm{d}k_2 = \frac{(n-1)4K}{\pi^2 n^2}$$

and thus

$$R_n \leq \frac{4}{\pi^2}\cdot\frac{1}{n}, \qquad R_n \cdot n \leq \frac{4}{\pi^2}. \tag{4.7}$$

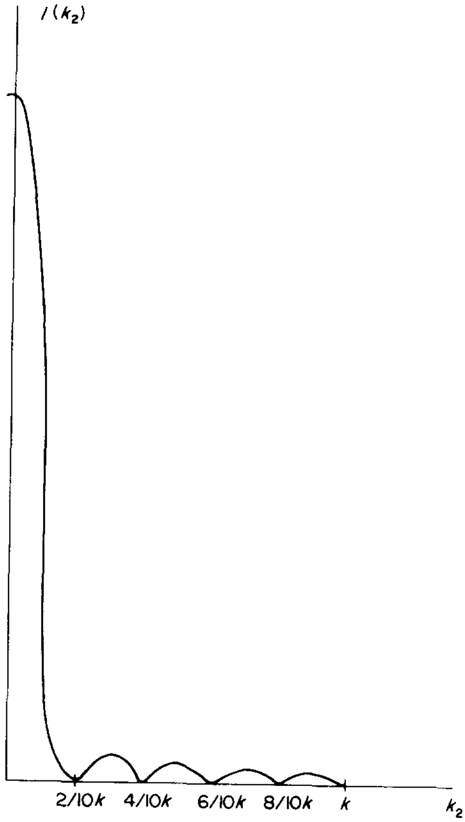

Fig. 3.

The idea to introduce R_n results from the behavior of the function $\sin^2 x/x^2$. We are more interested in estimating R_n, rather than presenting exact values. From different approximations such as (1) replacing $l(k)$ by straight-line segments; (2) replacing $\sin^2 x$ by its average value; or (3) replacing $1/k^2$ by its average value, we obtain the following estimates for R_n and nR_n

(1) $$R_n = \frac{2}{\pi^2}\frac{1}{n-1}\left[1 + 2\sum_{l=1}^{(n-2)/2}(2l+1)^{-2}\right]; \qquad \lim_{n\to\infty} R_n n = \frac{2}{\pi^2}\left(\frac{\pi^2}{4} - 1\right) \tag{4.8}$$

(2) $$R_n = \frac{2}{\pi^2}\cdot\frac{(n-1)^2}{n^3}; \qquad \lim_{n\to\infty} R_n \cdot n = \frac{2}{\pi^2} \tag{4.9}$$

(3) $$R_n = \frac{2}{\pi^2}\cdot\frac{(n-k)^4}{n^5}; \qquad \lim_{n\to\infty} R_n \cdot n = \frac{2}{\pi^2}. \tag{4.10}$$

In all cases

$$\lim_{n\to\infty} R_n \cdot n = \text{const}, \qquad \lim_{n\to\infty} R_n = 0. \tag{4.11}$$

5. ENERGY OF A SEGMENT OF AN EDGE DISLOCATION

From general formulas (3.13), taking advantage of the approximations (4.2) and (4.5), we obtain the following expression for the energy of the segment of an edge dislocation which is pinned to two semi-infinite screw dislocation lines,

$$W = \frac{b^2 d^2 c_2^2(0)\rho}{8\pi^2}\left\{\int_0^{K/n} dk_2 \iint A_1^0(\bar{k})[1 - R_n - ak_2^2 - hk^2]\, dk_1\, dk_3 \right.$$
$$\left. + R_n \int_0^K dk_2 \iint A_1^0(\bar{k})[1 - hk^2]\, dk_1\, dk_3\right\}. \tag{5.1}$$

The difference in the factor of two between (5.1) and (3.13) is due to the change in the limits of integration over k_2 from $-K$ to K, to 0 to K. Besides, the integration over the volume of the sphere is replaced in the present case by the integration over the volume of a cylinder of the same volume as the sphere. This replacement makes the expressions more easily interpretable in later discussions. It appears to be justified because the values near the boundary contribute but little to the total expression, since by far the major part comes from the contributions at and near the center of the volume. A rigorous estimate of the error introduced by such a replacement is, however, still lacking.

If we neglect dispersion by setting $h = 0$ in (5.1), we obtain the following expression for the energy of edge dislocations per unit of length

$$\omega = \frac{b^2\mu}{8\pi}\left\{\frac{1}{1-\nu}\left[(1-R_n)\left(n \operatorname{arctg}\frac{1}{n} + \ln(1+n^2)\right) - \frac{A}{3}\left(\ln(1+n^2) - n^2 + n^3 \operatorname{arctg}\frac{1}{n}\right)\right.\right.$$
$$\left. + R_n \cdot n\left(\frac{\pi}{4} + \ln 2\right)\right] - \left[(1-R_n)2\left(1 + n - n\sqrt{\left(1+\frac{1}{n^2}\right)}\right)\right.$$
$$\left. -\frac{2}{3}A\left(-2n^3 + 1 - n^3\sqrt{\left(1+\frac{1}{n^2}\right)} + 3n^3\sqrt{\left(1+\frac{1}{n^2}\right)}\right) - 2R_n \cdot n(2-\sqrt{2})\right] \tag{5.2}$$

where $A = (\pi^2 - 4)/\pi^2$ and, further, $c_2^2(0)$ and $\alpha(0)$ have been replaced by expressions in terms of the elastic constants μ and ν, as

$$c_2^2(0) = \frac{\mu}{\rho}, \qquad \alpha(0) = \frac{\mu}{2(1-\nu)}\frac{1}{\rho}.$$

The additional dispersion term is

$$\Delta\omega_d = -\frac{b^2\mu H}{12\pi}\left\{\frac{1}{1-\nu}\left[\left(n \operatorname{arctg}\frac{1}{n} + \frac{1}{2} - \frac{\ln n}{n^2}\right) + R_n \cdot n\left(\frac{\pi}{4} + \frac{1}{2} + \frac{1}{2}\ln 2\right)\right]\right.$$
$$\left. - \left[n\left(\sqrt{\left(1+\frac{1}{n^2}\right)}\right)^3 - n - \frac{1}{n^2} + R_n \cdot n2(\sqrt{2}-1)\right]\right\} \tag{5.3}$$

where $H = \pi^2/24$.

In expressions (5.2) and (5.3) the parameters A and H have on purpose, not been absorbed into the other numerical factors, such that the dependence of the energy expressions on assumed simplifications would remain in clear evidence.

6. THE ENERGY OF THE SEGMENT OF A SCREW DISLOCATION

From general formulas (3.13) we can obtain the expression analogous to (5.1) which would be applicable for a screw dislocation. Omitting calculational details, we obtain the following expression for the energy per unit of length of a screw dislocation segment pinned to two semi-infinite edge dislocation lines.

$$\omega = \frac{b^2\mu}{4\pi}\left\{\left[(1-R_n)\left(n \operatorname{arctg}\frac{1}{n} + \frac{1}{2}\ln(1+n^2)\right) - \frac{A}{3}\left(n^2 - n^3 \operatorname{arctg}\frac{1}{n} + \frac{1}{2}\ln(1+n^2)\right)\right.\right.$$
$$\left. + R_n \cdot n\left(\frac{\pi}{4} + \frac{1}{2}\ln 2\right)\right] - \frac{1}{1-\nu}\left[\left(n \operatorname{arctg}\frac{1}{n} - n\right) + \frac{n}{\sqrt{\left(1+\frac{1}{n^2}\right)}}(1-R_n)\right.$$
$$\left.\left. - A\left(2n^3 + n^2 - n^3\sqrt{\left(1+\frac{1}{n^2}\right)} - \frac{n^3}{\sqrt{\left(1+\frac{1}{n^2}\right)}} - n^3 \operatorname{arctg}\frac{1}{n}\right) + R_n \cdot n\left(\frac{\pi}{4} + \frac{\sqrt{2}}{2} - 1\right)\right]\right\}. \tag{6.1}$$

The additional dispersion terms are

$$\Delta\omega_w = -\frac{b^2\mu H}{12\pi}\left\{\frac{3}{2}+\frac{3}{2}R_n\cdot n-\frac{1}{1-\nu}\left[\left(5n-\frac{2}{n^2}+2+4n\left(\sqrt{\left(1+\frac{1}{n^2}\right)^3}\right)-9n\sqrt{\left(1+\frac{1}{n^2}\right)}\right.\right.\right.$$
$$\left.\left.\left.-2n\,\mathrm{arctg}\frac{1}{n}+\frac{\ln(n^2+1)}{n^2}\right)+R_n\cdot n\left(5-\sqrt{2}-\frac{\pi}{2}+\ln 2\right)\right]\right\}. \qquad (6.2)$$

7. ASYMPTOTIC EXPRESSIONS

The expressions (5.2), and (5.3), as well as (6.1) and (6.2) are the more accurate the larger n. Due to their complicated structure, however, their dependence on n is not readily recognizable. For this reason it is desirable to establish asymptotic relation for large n. As $n\to\infty$, (5.2) and (5.3) become

$$\omega_0{}^k = \frac{b^2\mu}{4\pi}\left(1-\frac{A}{3}\right)\left[\frac{\ln n+G_1}{1-\nu}-(1+G_2)\right] \qquad (7.1)$$

where

$$G_1 = \frac{1}{1-\frac{A}{3}}\left[\frac{1}{2}\left(1+\frac{A}{9}\right)+\frac{1}{2}(R_n\cdot n)_\infty\left(\frac{\pi}{4}+\ln 2\right)\right];$$
$$G_2 = \frac{(R_n\cdot n)_\infty(2-\sqrt{2})}{1-\frac{A}{3}} \qquad (7.2)$$

and

$$\Delta\omega_d{}^k = -\frac{b^2\mu}{8\pi}H\left[\frac{1}{1-\nu}+\frac{1}{3}(R_n\cdot n)_\infty\left(\frac{1+\pi/2+\ln 2}{1-\nu}-4(\sqrt{2}-1)\right)\right]\Big\}. \qquad (7.3)$$

The subscript ∞ indicates that the value at ∞ has to be taken. We recall that $(nR_n)_\infty = \text{const}$.

As $n\to\infty$, (6.1) and (6.2) become

$$\omega_0{}^s = \frac{b^2\mu}{4\pi}\left(1-\frac{A}{3}\right)\left[\ln n+L_1-\frac{1+L_2}{1-\nu}\right] \qquad (7.4)$$

where

$$L_1 = \frac{1}{1-\frac{A}{3}}\left[1-\frac{A}{9}+(R_n\cdot n)_\infty\left(\frac{\pi}{4}+\frac{1}{2}\ln 2\right)\right]; \qquad L_2 = \frac{(R_n\cdot n)_\infty\left(\frac{\pi}{4}+\frac{\sqrt{2}}{2}-1\right)}{1-\frac{A}{3}} \qquad (7.5)$$

and

$$\Delta\omega_d{}^s = -\frac{b^2\mu}{8\pi}H\left[1+(R_n\cdot n)_\infty\left(1-\frac{2/3(5-\sqrt{2}-\pi/2+\ln 2)}{1-\nu}\right)\right]. \qquad (7.6)$$

Expressions (7.1) and (7.4) can be rewritten as

$$\omega_0{}^k = \frac{b^2\mu}{4\pi}\left(1-\frac{A}{3}\right)\left[\frac{\ln(n/r_1)}{1-\nu}-(1+G_2)\right] \qquad (7.7)$$

$$\omega_0{}^s = \frac{b^2\mu}{4\pi}\left(1-\frac{A}{3}\right)\left[\ln(n/r_2)-\frac{1+L_2}{1-\nu}\right] \qquad (7.8)$$

where

$$\ln r_1 = -G_1, \qquad \ln r_2 = -L_1.$$

For $A = (\pi^2-4)/\pi^2$ and $(nR_n)_\infty = 2/\pi^2$, the following values for the constants r_1, r_2 are obtained

$$r_1 = 0.427, \qquad r_2 = 0.234. \qquad (7.9)$$

For the same A and $(nR_n)_\infty = 4/\pi^2$ the constants are

$$r_1 = 0.353, \qquad r_2 = 0.176. \tag{7.10}$$

We would like to establish the range of validity of (7.7) and (7.8) so as not to deal with the much more complicated expressions (5.2) and (6.1). Numerical calculations have been performed and are summarized in Table 1. It is seen that in the range of n which is of interest, good accuracy of simplified expressions is obtained. For edge dislocations for $n = 10$ (for $(nR_n)_\infty \equiv R = 2/\pi^2$). The difference is approximately 1.3% and for $n = 100$ it is only 0.5%. Thus expressions (7.7) and (7.8) are applicable in the whole range of n. It should be emphasized that besides their simple form, expressions (7.7) and (7.8) do not depend on R_n, but only on the limiting value $(nR_n)_\infty$. The comparison of the two second and third column, for edge and screw dislocations, respectively, indicates that the estimation of the limit $(nR_n)_\infty$ has no strong influence on the numerical values. For example, for edge dislocations the difference is decreasing from 4% for $n = 10$ to 2% for $n = 100$. Thus, expressions (7.7) and (7.8) will be used as energy expressions, whereby

$$2/\pi^2 \leq (nR_n)_\infty \leq 4/\pi^2.$$

It is noted that the dispersion contributions (7.3) and (7.6) do not depend on n, are negative for both types of dislocations and vary in the following ranges as a function of $(nR_n)_\infty$

$$0.35 \leq \Delta\omega_d^k \Big/ -\frac{b^2\mu}{8\pi} H \leq 0.40, \qquad \nu = \frac{1}{3} \tag{7.11}$$

$$0.22 \leq \Delta\omega_d^s \Big/ -\frac{b^2\mu}{8\pi} H \leq 0.23, \qquad \nu = \frac{1}{3}. \tag{7.12}$$

For $H = \pi^2/24$, $R = 2/\pi^2$ and $\nu = 1/3$ we obtain

$$\Delta\omega_d^k = -\frac{b^2\mu}{4\pi} 0.35, \qquad \left(0.40 \text{ for } R = \frac{4}{\pi^2}\right) \tag{7.13}$$

$$\Delta\omega_d^s = -\frac{b^2\mu}{4\pi} 0.22, \qquad \left(0.23 \text{ for } R = \frac{4}{\pi^2}\right). \tag{7.14}$$

For small values of n, the dispersion decreases in a significant manner the value of the energy. Of course, with increase of n this influence is decreasing because the dispersion contributions remain constant and the principal part of the energy, given by (7.7) and (7.8) are increasing as n increases. We have to keep in mind, however, that the model assumed here deals only with a medium with weak dispersion. It is possible that taking into account long

Table 1. Values of dislocation energies per unit of length in units $\omega/(b^2\mu/4\pi)$ for $\nu = 1/3$

n	Edge Dislocation			Screw Dislocation		
	From (5.2)	From (7.1)		From (6.1)	From (7.4)	
		$R=2/\pi^2$	$R=4/\pi^2$		$R=2/\pi^2$	$R=4/\pi^2$
10	2.84	2.89	3.01	1.64	1.66	1.74
20	3.68	3.72	3.84	2.20	2.22	2.30
30	4.17	4.21	4.33	2.52	2.54	2.62
40	4.51	4.55	4.67	2.76	2.77	2.85
50	4.78	4.82	4.94	2.94	2.95	3.03
60	5.00	5.04	5.16	3.08	3.09	3.17
70	5.19	5.23	5.35	3.21	3.22	3.30
80	5.36	5.39	5.51	3.32	3.32	3.40
90	5.50	5.53	5.65	3.41	3.42	3.50
100	5.63	5.66	5.78	3.50	3.50	3.58

range interactions (strong dispersion) could have a much more pronounced influence on the values of the energy and for a large range of n.

The dependence of energies in the range $n \in [10, 100]$ on Poisson's ratio ν is given in Table 2. The values are calculated from (7.7) and (7.8) for $R = 2/\pi^2$ and $A = (\pi^2 - 4)/\pi^2$. The last row in Table 2 contains the values for the dispersion $\Delta\omega$.

8. COMPARISON WITH CLASSICAL THEORY OF ELASTICITY

The self-energies per unit length of dislocations are given in classical elasticity by[5]

$$\omega_1 = \frac{b^2\mu}{4\pi} \ln \frac{n}{\zeta} \tag{8.1}$$

for a screw dislocation and

$$\omega_2 = \frac{b^2\mu}{4\pi(1-\nu)} \ln \frac{n}{\zeta} \tag{8.2}$$

for an edge dislocation, where ζ is the dimensionless core parameter, in general taken equal to 5. The comparison of (8.1) and (7.8) shows the essential difference of properties of the energy of a screw dislocation in the two models: in a pseudo-continuum it depends on ν. Of course this is connected with the fact that we considered a segment of a screw dislocation pinned to two semi-infinite screw dislocation lines. Because of the slow rate of increase of the logarithmic term, however, the influence of the second term, even for large n, remains significant. The logarithm term itself is multiplied by a factor $(1 - A/3) < 1$. Such, even for large values of n when the constant terms are negligible, the values of the energy are smaller than it would follow from expression (8.1).

In addition to the logarithmic term, the energy expression contains also the constant term L_1, which can be represented as $-\ln r_2$ (formula (7.8)). For edge dislocation the analogous constant is represented as $-\ln r_1$, (formula (7.7)). The interpretation of expressions (7.7) and (7.8) could be as follows. The pseudo-continuum, looked upon as a continuum, introduces a uniquely defined core parameter, always smaller than unity, for both kinds of dislocations and regardless of the value of A. Since, however, it is always smaller than unity, the pseudo-continuum is a continuum description of a discrete system. It should be yet emphasized that the energies are given by expression (7.1) and (7.4), supplemented by dispersion effects given by (7.3) and (7.6). The forms (7.7) and (7.8) are identical to (7.1) and (7.4), respectively, written, however, in a different way such as to facilitate interpretation and comparison. In an elastic continuum the necessity of introducing the notion of a core follows from the singularity of the corresponding integral when approaching the dislocation line; in a pseudo-continuum this problem does not exist at all: all functions are finite, $\delta(x)$ is replaced by $\delta_B(x)$ and the region of integration in k-space is also finite.

Table 2. Energy of dislocations for different values of ν, in units $\omega/(b^2\mu/4\pi)$

n	Edge Dislocation			Screw Dislocation		
	ν=0	ν=1/3	ν=1/2	ν=0	ν=1/3	ν=1/2
10	1.62	2.89	4.16	2.11	1.66	1.21
20	2.17	3.72	5.24	2.66	2.22	1.76
30	2.50	4.21	5.92	2.99	2.54	2.09
40	2.73	4.55	6.38	3.22	2.77	2.32
50	2.91	4.82	6.74	3.40	2.95	2.50
60	3.06	5.04	7.03	3.54	3.09	2.64
70	3.18	5.23	7.28	3.67	3.22	2.77
80	3.29	5.39	7.48	3.78	3.32	2.87
90	3.38	5.53	7.68	3.87	3.42	2.97
100	3.47	5.66	7.85	3.95	3.50	3.05
$\Delta\omega$	-0.23	-0.35	-0.49	-0.23	-0.22	-0.21

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